The 21st International Conference on Solid Compounds of Transition Elements

Programme and Abstracts
<table>
<thead>
<tr>
<th>Time</th>
<th>Sunday</th>
<th>Monday</th>
<th>Tuesday</th>
<th>Wednesday</th>
<th>Thursday</th>
<th>Symposium</th>
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<tr>
<td>08:50</td>
<td>Opening</td>
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<tr>
<td>09:00</td>
<td>Claudia Felser</td>
<td>Stuart Parkin</td>
<td>Bob Cava</td>
<td>Bobet</td>
<td>Staunton</td>
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<td>09:30</td>
<td>Sven Lidin</td>
<td>Vitalij Pecharski</td>
<td>Andrei Shevelkov</td>
<td>Grbovic</td>
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<td>Skryabina</td>
<td>Ebert</td>
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<td>11:00</td>
<td>Kamenev deVisser</td>
<td>Kaczorowski Romaka</td>
<td>Yoshimura Held</td>
<td>Antipov Belashchenko</td>
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<td>11:30</td>
<td>Wilhelm Mironova-Ulmane</td>
<td>Balakrishnan Klimeczuk</td>
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<td>Furukawa Park</td>
<td>Kawamura Gamza Khmelevskiy</td>
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<td>Pospisil Olu</td>
<td>Isobe Svanidze Haniki Chang</td>
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<td>Toshiro Takabatake</td>
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<td>14:00</td>
<td>Gladyshevskii Abd-Elmeguid Aoki Grin Fruchart Spalek</td>
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<td>Daniel Khomskii</td>
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<td>Saccone Wsiewski Ikeda Dronskowski Kuznetsov Kądzielawa-Major Zegrodnik</td>
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<td>15:00</td>
<td>Registration</td>
<td>Paul-Boncour Kolincio Dzabek Olynyk Kurbakov Verchiknuk Grebenyuk Verchenko Bartolome Strelovsko Tomczak Kubo</td>
<td>Announcement SCTE 2020, Closing</td>
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<td>Andreev Baran Yoshikawa Yokota Amon Korshunov Šlebarski Didelot Levytskyi Babic Opletal</td>
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plenary: 45 min; invited: 30 min, oral: 15 min
Conference Chair
Ernst Bauer
Technische Universität Wien

Conference Secretary
Herbert Müller
Technische Universität Wien

Conference Website
https://scte18.conf.tuwien.ac.at/

Conference email
secretary@scte18.conf.tuwien.ac.at

International Advisory Committee
F. Bartolomé (Zaragoza) O. Karis (Uppsala)
J. Bartolomé (Zaragoza) A. Mar (Edmonton)
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D. Fruchart (Grenoble) H. Noël (Rennes)
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Yu. Grin (Dresden) A.V. Shevelkov (Moscow)
H. Hillebrecht (Freiburg) A. Szytula (Krakow)
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D. Kaczorowski (Wroclaw)

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M. Reissner TU Wien, Abstracts
P. Rogl Uni. Wien, Programme
G. Rogl Uni. Wien, Programme
H. Sassik TU Wien, Programme

Plenary Speakers
Robert Cava, Princeton University, USA
Claudia Felser, MPI Dresden, Germany
Daniel Khomskii, Cologne University, Germany
Sven Lidin, Lund University, Sweden
Stuart Parkin, MPI Halle, Germany
Vitalij Pecharski, Iowa State University, USA
Andrei Shevelkov, Moscow State University, Russia
Toshiro Takabatake, Hiroshima University, Japan
Invited Speakers

M. Abd-Elmeguid  Y. Grin  V. Romaka
E. Antipov        K. Held   A. Saccone
Y. Aoki           M. Ikeda  E. V. Sampathkumaran
G. Balakrishnan   D. Kaczorowski C. Sekine
K. Belashchenko   K. Kamenev A. Shick
J.-L. Bobet       M. Klicpera T. Shiroka
A. Bombardi       T. Klimczuk J. Spałek
L. Degiorgi       J. Kudrnovsky J. Staunton
A. de Visser      A. Kuznetsov A. Strydom
R. Dronskowski    V. Levitskyi L. Szunyogh
H. Ebert          T. Mori   S. Tence
O. Eriksson       J.-G. Park E. C. Tereshina
D. Fruchart       J. Pospisil J. Tobola
Y. Furukawa       A. Provino P. Wiśniewski
R. Gladyshevskii  X. Qiu    K. Yoshimura
J. Grbović Novaković

General

The SCTE 2018 will follow a series of conferences, dating back more than 50 years, with recent meetings in Annecy, France, (2010), Lisboa, Portugal (2012), Genova, Italy, (2014) and Zaragossa, Spain (2016). The SCTE has always been a forum, where new ideas and discoveries – related to the solid state chemistry and solid state physics of d- and f-element compounds – are presented and discussed.

The conference will deal with the structure, crystal chemistry, chemical bonding, and magnetic and electronic transport properties of different classes of intermetallic compounds. The field of hydrides, borides, carbides, silicides and homologues, pnictides, as well as chalcogenides, oxides and halides (especially those of low oxidation state exhibiting metal or semimetal properties) will also be covered.

Fundamental and applied research in the areas of solid state chemistry, physics and materials science of compounds containing d- and f- elements will be included.

Conference Site

The conference will be held in the Institute building “Freihaus” of the Technische Universität Wien, using the lecture rooms V and VI. The poster session will also be held in the “Freihaus”, Wiedner Hauptstrasse 8-10, 1040 Wien (see the campus map).

Technische Universität Wien is located in the city center of Vienna, thus conveniently accessible by the Vienna public transport system. The nearest station to the conference site is “Karlsplatz”, to where the underground-lines U1, U2 and U4 are bound. Additionally, the tramway lines 62, 65 as well as 1, 2, D, J, Bus 4 and “Badner Bahn” are nearby. Parking slots for private cars are available in a public park house within the conference building (about € 90.-/week and € 4.-/hour).

Currency

The official currency in Austria is the EURO (€). Foreign currencies can be exchanged in Euro in all banks. The airport and most railway stations have exchange desks and money is available in numerous cash dispensers, prepared for major international cards. Hotels, restaurants, and many shops and travel agencies accept credit cards.
Language
The conference language is English. The language of Austria is German.

Conference Fees
Early bird rate: € 390.- until January 31, 2018
Regular fee: € 450.- until March 19, 2018
Students & retirees: € 290.- until March 19, 2018
Accompanying persons: € 140.- until March 19, 2018
Onsite: cash

Your SCTE 2018 conference fees include:

- Admission to all technical sessions
- Conference material, including the book of abstracts
- One printed version of the conference proceedings (students and retirees will not receive the printed versions of the conference proceedings)
- Daily coffee breaks
- Welcome reception on Sunday, March 25, 2018
- Conference dinner on Wednesday, March 28, 2018

Accompanying person’s conference fees include:
- Welcome reception on Sunday, March 25, 2018
- Conference dinner on Wednesday, March 28, 2018
- Daily coffee breaks
- Two guided tours in Vienna

Note:
- All participants must register with full remittance
- Payment after March 15, 2018 is only possible at the conference site (in cash, Euros).

Registration
On-site registration at the conference will open on Sunday, March 25, 2018 at 15:00. All conference participants, including speakers, must register at the conference and will receive an official conference package that includes Abstract Booklet, badge, etc. Every participant must wear her/his official conference badge to enter the conference building and technical sessions.

Technical Programme
The conference will start at Monday, March 26, 2018 at 8:50 and end on Thursday, March 29, 2018 around 15:30. For details of the programme, sessions and a list of oral contributions see also: https://scte18.conf.tuwien.ac.at/
Scientific Programme

The scientific programme consists of 8 plenary lectures (45 min, including discussion) scheduled at each conference day. There are 13 scientific sessions consisting of invited (30 min, including discussion) and contributed talks (15 min, including discussion). On Thursday, March 29, 2018 (morning session), a symposium on “Finite temperature simulation of magnetism” is arranged.

Both overhead projection and computer-based presentations will be available for speakers. If you wish to present your talk using this capability, please bring your presentation on a memory stick and hand over to the technical assisent of the session at least 30 minutes before the session starts, preferably the day before your talk. Otherwise bring your own laptop computer, and have it powered on and ready to be connected.

Please note:
The electric supply network provides 230V AC; plugs are type C and F.
The connection to the beamer is either HDMI type A (standard size) or VGA.
You will be responsible for promptly connecting to the projector. The presentation will begin immediately after introduction by the session chair.

Poster sessions with approx. 80 presentations are scheduled on Monday, March 26 and Tuesday, 27 March, 2018, each from 17:30 to 19:00. Posters will be on display at all day. The poster panels have a width of 100 cm and are reaching from the floor to a height of 180 cm. Adhesive tapes will be provided to fix the poster on the boards.

Proceedings

Attendees of the SCTE 2018 are invited to submit their conference contributions (plenary talks, invited talks, contributed talk and posters) as manuscripts to the proceedings of the SCTE’2018. As in previous years, the conference proceedings will be published by Trans Tech Publications Ltd after a standard reviewing process.


Internet Access

WLAN is available at most sites of the Conference building. For details contact the Conference Registration Desk.

Lunch and Coffee Breaks

Coffee, tea and mineral water as well as cakes will be served during the coffee breaks. Lunch can be taken in the student canteen (Mensa) situated in conference site (Institute building “Freihaus”, 1st floor, yellow tower). Alternatively, a large number of restaurants and pubs can be found nearby the conference site within walking distance (2-10 min). A list of nearby restaurants will be given in the Conference Package.

Social Events

The Welcome Reception will be held on Sunday, March 25 in the student canteen (Mensa, Institute building “Freihaus”). A buffet and beverages will be served.

On Wednesday, March 28 the conference dinner is held in the “Kuppelsaal” of the Technische Universität Wien at 19:00. This location is very close to the conference site.

Two guided tours to major Vienna attractions are included in the accompanying persons programme without additional costs.
Insurance

The organisers cannot accept any liability or responsibility for death, illness, or injury to the person or for loss of or damage to property of participants and accompanying persons which may occur either during or arising from the conference. Participants are advised to make their own arrangements in respect of health and travel insurance.

Conference Office

SCTE 2018
Institute of Solid State Physics
Technische Universität Wien
Wiedner Hauptstrasse 8-10
A-1040 Wien
Austria

During the conference

Tel: ++43 1 58 801 13801  Tel: ++43 1 58 801 13020

Email: secretary@scte18.conf.tuwien.ac.at

For latest information on the conference please visit our website at:

https://scte18.conf.tuwien.ac.at
The 21st International Conference on Solid Compounds of Transition Elements

Conference Programme

Sunday, March 25, 2018: Afternoon

15:00 Registration
18:00 Welcome Reception
Monday, March 26, 2018: Morning

08:50 Opening

Plenary Session: (FH HS 1)

09:00 C. Felser Topological Materials with liquid electrons (Mo-P1)
09:45 S. Lidin Complex materials studied by temperature dependent synchrotron x-ray diffraction (Mo-P2)
10:30 Coffee

Parallel sessions:

11:30 Session A (FH HS 6) Session B (FH HS 5)
13:00 Lunch
14:00 Session A (FH HS 6) Session B (FH HS 5)
15:30 Coffee
16:00 Session A (FH HS 6) Session B (FH HS 5)
17:30 Poster Session
Session A (FH HS 6): Monday, March 26, 2018

11:00 Kamenev
State-of-the-art instrumentation for studies of structural, magnetic and electronic properties of materials at the extremes of pressures, temperatures and magnetic fields (Mo-A1i)

11:30 F. Wilhelm
Chiral magnets probed with X-rays (Mo-A2)

11:45 N. Mironova-Ulmane
Temperature dependent Raman spectroscopy studies of SrTiO$_3$ and SrTi$_{18}$O$_3$ (Mo-A3)

12:00 Y. Furukawa
Hedgehog Spin-vortex Crystal Magnetic Order in the New Magnetic Superconductors CaK(Fe$_{1-x}$Ni$_x$)$_4$As$_4$ revealed by $^{75}$As Nuclear Magnetic Resonance (Mo-A4i)

12:30 J. Pospisil
Two different paramagnetic regimes in the U(Co,Rh)Ge compounds above TC (Mo-A5i)

13:00 Lunch

14:00 R. Gladyshevskii
Understanding Phase Diagrams of Intermetallic Systems using Crystal Chemistry (Mo-A6i)

14:30 A. Saccone
Synthesis, Structural Relationships, Chemical Bonding in Selected Ternary Germanides Containing Rare Earth Metals (Mo-A7i)

15:00 V. Paul-Boncour
Field induced ferromagnetic state in Y$_{1-x}$Er$_x$Fe$_2$Dy deuterides ($0 < x \leq 0.5$, $y \approx 4.2$) (Mo-A8)

15:15 K. Kolincio
Interaction between charge density wave and magnetism in RniC$_2$ family (Mo-A9)

15:30 Coffee

16:00 E. V. Sampathkumaran
Magnetic frustration anomalies in kagome lattices of the type R$_3$Ru$_4$Al$_{12}$ ($R$ = Rare-earths) (Mo-A10i)

16:30 A. Provino
New R$_3$TaM$_3$Ge$_2$ quaternary compounds ($R$ = rare earth; $T$ = transition metal) (Mo-A11i)

17:00 A. Andreev
Influence of substitution in the Fe sublattice on the magnetism of HoFe$_5$Al$_7$ (Mo-A12)

17:15 S. Baran
Magnetic and thermal properties of R$_3$Ni$_2$In$_4$ ($R$ = Gd–Tm) (Mo-A13)

17:30 Poster Session
<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Topic</th>
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<tbody>
<tr>
<td>11:00</td>
<td>A. de Visser</td>
<td>Nematic superconductivity in topological materials (Mo-B1i)</td>
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<td>11:30</td>
<td>G. Balakrishnan</td>
<td>Structural and magnetic investigations of skyrmion phases (Mo-B2i)</td>
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<td>12:00</td>
<td>J. Park</td>
<td>2D magnetism in magnetic van der Waals materials (Mo-B3i)</td>
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<td>12:30</td>
<td>X. Qiu</td>
<td>Optical properties of Weyl semimetal TaAs (Mo-B4i)</td>
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<tr>
<td>14:00</td>
<td>M. Abd-Elmeguid</td>
<td>Emergence of Novel Ground States in Mott-Insulators at High Pressure (Mo-B5i)</td>
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<td>14:30</td>
<td>P. Wiśniewski</td>
<td>Magnetor transport in rare-earth-based half-Heusler phases and monopnictides - non-trivial topology, superconductivity, antiferromagnetism and extreme magnetoresistance (Mo-B6i)</td>
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<td>15:00</td>
<td>S. Dzsaber</td>
<td>Kondo insulator to semimetal transformation tuned by spin-orbit coupling (Mo-B7)</td>
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<td>15:15</td>
<td>A. Oliynyk</td>
<td>Prediction of Novel Compounds and Rapid Property Screening through a Machine Learning Approach (Mo-B8)</td>
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<td>16:00</td>
<td>L. Degiorgi</td>
<td>Optical properties of the electronic nematic phase in FeSe (Mo-B9i)</td>
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<td>E. Constable</td>
<td>Spectroscopic study of quantum spin liquid candidate Tb₂Ti₂O₇ reveals vibronic coupling (Mo-B10)</td>
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<td>16:45</td>
<td>D. Szaller</td>
<td>Exotic magnetoelectric excitations of the multiferroic SmFe₃(BO₃)₄ (Mo-B11)</td>
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<td>17:00</td>
<td>A. Yoshikawa</td>
<td>Melt growth of Ir/Ir-Rh alloy &quot;FLEXIBLE&quot;wires using micro-pulling down method (Mo-B12)</td>
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<td>17:15</td>
<td>Y. Yokota</td>
<td>Growth of Co-Cr-Mo Alloy Fiber Crystal by Alloy-Micro-Pulling-Down Method, and the Microstructure and Mechanical Property (Mo-B13)</td>
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<td>Poster Session</td>
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Tuesday, March 27, 2018: Morning

**Plenary Session:** (FH HS 1)

09:00  S. Parkin  Spin Orbitronics: chiral domain walls and magnetic anti-skyrmions (Tu-P1)

09:45  V. Pecharsky  High-throughput search for caloric materials: The CaloriCool approach (Tu-P2)

10:30  Coffee

**Parallel sessions:**

11:30  Session A (FH HS 6)  Session B (FH HS 5)

13:00  Lunch

14:00  Session A (FH HS 6)  Session B (FH HS 5)

15:30  Coffee

16:00  Session A (FH HS 6)  Session B (FH HS 5)

17:30  Poster Session
Session A (FH HS 6): Tuesday, March 27, 2018

11:00  D. Kaczorowski  Magnetic ordering and superconductivity in Ce-Pd-In Kondo lattices (Tu-A1i)
11:30  T. Klimczuk  Crystal structure and physical properties of the cage compounds RV$_2$Al$_{20}$ and AV$_2$Al$_{20}$ (Tu-A2i)
12:00  Y. Kawamura  Superconductivity of Alkalline-Earth-Filled Skutterudites (Tu-A3)
12:15  M. Gamza  Large positive magnetoresistance in a novel superconductor Ca$_{3+x}$Co$_4$Sn$_{13-y}$ (Tu-A4)
12:30  M. Isobe  Charge Order and Spin-1/2 Dimer Formation Induced by Ag$^+$ Order in δ-Ag$_{2/3}$V$_2$O$_5$ (Tu-A5)
12:45  E. Svanidze  Novel Canonical Heavy Fermion Compound (Tu-A6)
13:00  Lunch
14:00  Y. Aoki  Unconventional 4f-Electron Magnetism in Ln(O,F)BiS$_2$ Layered Superconductors (Tu-A7i)
14:30  M. Ikeda  Strain as tuning parameter for the coupled nematic/structural phase transition in Co doped BaFe$_2$As$_2$ (Tu-A8i)
15:00  A. Kurbakov  Diffraction Studies of New Quasi-two-dimensional Frustrated Magnetics with Honeycomb Sublattices of Transition Ions (Tu-A9)
15:15  A. Szytula  Influence of doped 3d atom on the magnetic order in fourfold NiMnGe:T compounds (Tu-A10)
15:30  Coffee
16:00  T. Shiroka  Nodeless superconductivity and time-reversal symmetry breaking in the noncentrosymmetric superconductor Re$_{24}$Ti$_5$ (Tu-A11i)
16:30  S. Tence  Hydrogenation of intermetallics: A new synthetic route for iron-based superconductors (Tu-A12i)
17:00  A. Amon  Cluster formation in the superconducting complex intermetallic compound Be$_{21}$Pt$_5$ (Tu-A14)
17:15  M. Korshunov  Spin resonance peak in the superconducting state of iron pnictides and chalcogenides (Tu-A15)
17:30  Poster Session
Session B (FH HS 5): Tuesday, March 27, 2018

11:00  V. Romaka  DFT calculations in Half-Heusler systems (Tu-B1i)
11:30  J. Tobola  Electronic structure, magnetic and electrochemical properties of Li- and Na-ion battery systems in view of KKR-CPA calculations (Tu-B2i)
12:00  S. Khmelevskyi  Longitudinal integration measure in classical spin space: application to first-principle based simulations of the magnetism of ferromagnetic metals. (Tu-B3)
12:15  O. Janson  Spin model of the Heisenberg antiferromagnet \( \text{Li}_3\text{Ni}_2\text{SbO}_6 \): the relevance of third-neighbor exchanges (Tu-B4)
12:30  A. Hariki  LDA+ DMFT approach to core-level spectroscopy; application to 3d transition-metal compounds (Tu-B5)
12:45  H. Chang  Speed up method for solid solution problem by DFT calculations (Tu-B6)
13:00  Lunch
14:00  Y. Grin  Multi-center bonding in \( \gamma \)-brass phases (Tu-B7i)
14:30  R. Dronskowski  Carbodiimides of the Transition Metals: From Basic Research to First Applications (Tu-B8i)
15:00  D. Grebenyuk  Mixed Ligand Complexes of Rare Earth Carboxylates with Aminoligands as Precursors for MOCSD of Thin Films (Tu-B9)
15:15  V. Verchenko  Joint melt of two p-metals: New approach to synthesis of intermetallic compounds with functional properties (Tu-B10)
15:30  Coffee
16:00  C. Sekine  High Temperature and High Pressure Synthesis and Magnetic Properties of Arsenic-Based Filled Skutterudite compounds (Tu-B11i)
16:30  E. C. Tereshina  Multifunctional phenomena in rare-earth intermetallic compounds with a Laves phase structure (Tu-B12i)
17:00  A. Ślebarski  Electronic structure, magnetic, electric transport, and thermal properties of \( \text{Ce}_3\text{PdGe}_2 \) (Tu-B13)
17:15  E. Didelot  Closo-boranes of 3d transition metals, synthesis and characterization (Tu-B14)
17:30  Poster Session
Wednesday, March 28, 2018: Morning

**Plenary Session: (FH HS 1)**

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<th>Time</th>
<th>Speaker</th>
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<tr>
<td>09:00</td>
<td>R. Cava</td>
<td>Physical and Chemical Properties of Several New Intermetallic Superconductors (We-P1)</td>
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<td>09:45</td>
<td>A. Shevelkov</td>
<td>Iron Compounds with Strong Electron Correlations, Beyond Ferroarsenide Superconductors (We-P2)</td>
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**Parallel sessions:**

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### Session A (FH HS 6): Wednesday, March 28, 2018

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<tr>
<td>11:00</td>
<td>K. Yoshimura</td>
<td>Recent Progress in Itinerant Magnetism and Spin Fluctuations in Intermetallics and Compounds (We-A1i)</td>
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<tr>
<td>11:30</td>
<td>A. Bombardi</td>
<td>The puzzling Ru: A synchrotron journey in the electronic properties of some ruthenium oxides (We-A2i)</td>
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<tr>
<td>12:00</td>
<td>M. Klicpera</td>
<td>Vibron quasi-bound states in Ce intermetallics (We-A3i)</td>
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<tr>
<td>12:30</td>
<td>K. Nadeem</td>
<td>Disordered and Frustrated Magnetization in Coated MnFe₂O₄ Nanoparticles Prepared by Microwave Plasma Synthesis (We-A4)</td>
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<td>12:45</td>
<td>J. Cieslak</td>
<td>Magnetic properties of multicomponent AlₓFeNiCrCo High Entropy Alloys (We-A5)</td>
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<tr>
<td>14:00</td>
<td>D. Fruchart</td>
<td>Local peculiarity of the crystal structure of hexagonal pnicotides of Fe₂P type impacting the stability of the magnetic structure and the MC effect apart the ordering temperature (We-A6i)</td>
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<td>14:30</td>
<td>A. Kuznetsov</td>
<td>Many Faces of a Single Cuboctahedron: Structure and Bonding of Group 10 - Main Group Metal Cu₃Au-type Intermetallics and Derivatives (We-A7i)</td>
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<tr>
<td>15:00</td>
<td>F. Bartolomé</td>
<td>Modification of magnetism of Cr₁₀ wheel molecules on metallic (111) surfaces and bulk (We-A8)</td>
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<tr>
<td>15:15</td>
<td>S. Streltsov</td>
<td>Magnetic properties of FeO₂ and FeO₂H possible constituents of Earth’s lower mantle (We-A9)</td>
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<td>16:00</td>
<td>T. Mori</td>
<td>Magnetic Properties and Thermal Conductivity of Layered Borides (We-A10i)</td>
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<td>16:30</td>
<td>A. Strydom</td>
<td>Unusual order in the new compound Ce₂Rh₂Ga (We-A11i)</td>
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<tr>
<td>17:00</td>
<td>V. Levytskyi</td>
<td>Crystal Chemistry of Ternary Rare Earth Transition Metal Carbides : Recent Studies (We-A12i)</td>
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Session B (FH HS 5): Wednesday, March 28, 2018

11:00 K. Held  Probing the topological nature of SmB$_6$ by dynamical mean field theory (We-B1i)
11:30 L. Szunyogh  Multiscale study of itinerant magnetism based on first principles (We-B2i)
12:00 A. Akbari  Mixed-pairing superconductivity in 5d Mott insulators with antisymmetric exchange: Application to Sr$_2$IrO$_4$ (We-B3)
12:15 L. Pourovskii  DFT+Dynamical Mean-Field Theory Approach to Crystal-Field Splitting in Hard-Magnetic Rare-Earth Intermetallics (We-B4)
13:00 Lunch
14:00 J. Spalek  Spin-triplet superconducting phase of ferromagnetic UGe$_2$: An example of Hund metal (We-B5i)
14:30 E. Kądzielawa-Major  Coexistent ferromagnetic-superconducting phases in the renormalized mean-field theory: Application to UGe$_2$ (We-B6)
14:45 M. Zegrodnik  Coexisting charge- and pair-density-wave states in the single-band models of copper-based high-temperature superconductors (We-B7)
15:00 J. M. Tomczak  Kondo Insulators vs. Transition Metal-based narrow-gap Intermetallics (We-B8)
15:15 K. Kubo  Superconductivity in an $f^2$ System with the $\Gamma_3$ crystalline electric field ground state (We-B9)
15:30 Coffee
16:00 C. Chung  Mechanism of strange metal state near a heavy fermion quantum critical point (We-B10)
16:15 O. Pavlosiuk  Planar Hall Effect and Chiral Anomaly in Half-Heusler Antiferromagnet DyPdBi (We-B11)
16:30 M. Fidrysiak  Finite-temperature dynamics of d=3 antiferromagnets near quantum criticality: The case of TlCuCl$_3$ (We-B12)
16:45 S. Mankovsky  Electronic structure, magnetic and response properties of B20 A$_{1-x}$B$_x$Ge alloys (A, B = Mn, Fe, Co, Rh) (We-B13)
17:00 E. Babic  Electronic structure mediated vitrification of transition metal alloys (We-B14)
17:15 P. Opletal  Single crystal of URhGa in ambient and hydrostatic pressure (We-B15)
19:00 Conference Dinner
Thursday, March 29, 2018: Morning

Parallel sessions:

11:30  Session A  Symposium:
(FH HS 6)  Finite temperature simulation of magnetism (FH HS 5)

12:45  Lunch

13:30  Plenary Session

15:00  Announcement SCTE 2020, Closing

Plenary Session: (FH HS 6)

13:30  T. Takabatake  Magnetic Ordering in Cerium-based Kondo Semiconductors
(Th-P1)

14:15  D. Khomskii  Orbital-selective effects in transition metal compounds
(Th-P2)

15:00  Announcement SCTE 2020, Closing
Session A (FH HS 6): Thursday, March 29, 2018

09:00  J. Bobet  New ternary RE-TM-Mg alloys for Hydrogen Energy Applications: Clean Production and Storage (Th-A5i)
09:30  J. G. Novakovic  Hydrogen desorption for Mg/MgH₂ modified thin films (Th-A2i)
10:00  N. Skryabina  Oscillating behavior of physical and mechanical properties of alloys at hydrogenation (Th-A3)
10:15  M. Shelyapina  Transition metal induced bcc phase magnesium as issue for fast hydrogen sorption kinetics and low stability of MgH₂ (Th-A4)
10:30  Coffee
11:00  E. Antipov  Alkali and transition metal fluoride-phosphates as perspective cathode materials for metal-ion batteries (Th-A1i)
11:30  G. Buzanov  Overstoichiometric Lithium and Lithium-magnesium Manganese Oxide Spinels Synthesis Using Hydride Intercalation Method (Th-A6)
11:45  G. Rogl  How nano-composites influence physical, mechanical and thermal properties of high ZT-skutterudites (Th-A7)
12:00  S. Vitta  Effect of substitutions on the thermoelectric and magnetic properties of half-Heusler alloys - HfNiGe and ZrNiSn variants (Th-A8)
12:15  G. Eguchi  Anisotropic heat and charge transport in the cubic clathrate Ba₈Au₆₋ₓGe₄₀₊ₓ (Th-A9)
12:30  M. Pasturel  Low temperature synthesis of intermetallics for energy (Th-A10)
12:45  Lunch
**Symposium "Finite temperature simulation of magnetism"
(FH HS 5): Thursday, March 29, 2018**

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<tr>
<td>09:00</td>
<td>J. Staunton</td>
<td>Extending Density Functional Theory (DFT) to finite temperatures to describe spintronics, refrigeration and permanent magnetic effects. (Th-S1i)</td>
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<tr>
<td>09:30</td>
<td>A. Shick</td>
<td>LDA+Hubbard-I approximation for modelling of f-electrons systems (Th-S2i)</td>
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<tr>
<td>10:00</td>
<td>H. Ebert</td>
<td>Impact of finite temperatures on the response functions of magnetic solids (Th-S3i)</td>
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<tr>
<td>11:00</td>
<td>K. Belashchenko</td>
<td>Temperature-Dependent Magnetic Anisotropy from First Principles (Th-S4i)</td>
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<td>11:30</td>
<td>J. Kudrnovsky</td>
<td>The spin-disorder resistivity: the disordered local moment approach (Th-S5i)</td>
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Abstracts
Topological Materials with liquid electrons

Claudia Felser
Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Topology a mathematical concept became recently a hot topic in condensed matter physics and materials science. One important criteria for the identification of topological material is the band inversion and the crystal symmetry. In my talk I focus on new topological semimetals: Weyl semimetals. Binary phosphides are the ideal material class for a systematic study of Weyl physics. Weyl points, a new class of topological phases was also predicted in NbP, NbAs, TaP, MoP and WP₂. In NbP micro-wires we have observed the chiral anomaly but NbP has served also as a model system for astrophysics: realizing the gravitational anomaly in NbP and the hydrodynamic flow of electrons in WP₂. MoP and WP₂ show exceptional properties such as high conductivity higher than copper, high mobilities and a high magneto-resistance effect. In magnetic materials, the Berry curvature measured via the classical anomalous Hall effect helps to identify interesting candidates for magnetic topological materials and devices.

Complex materials studied by temperature dependent synchrotron x-ray diffraction

S. Lidin, L. Folkers
Lund University, CAS, Lund, Sweden

Synchrotron radiation has a number of advantages compared to in-house sources that allows qualitatively different studies. The superior flux is certainly important as it turns weak features into hard facts and makes studies at multiple pressures or temperatures feasible without compromising data quality. Further, choosing an appropriate wave-length, the contrast between elements may be enhanced. This contribution will focus on these features for the study of a number of complex systems.

Sn₃Sb₂ was synthesized in-situ at the beam-line Cristal at the Soleil light source by heating a single crystal of stistaite together with a piece of tin. The elemental contrast was enhanced by using radiation with a wave-length close to the absorption edge of tin. For this study all the above mentioned features of synchrotron radiation are essential: The satellite reflections are weak, but enhanced by the choice of wave-length and the high flux and the measurement of an entire sequence of temperature dependent data ensures that the relevant phase is measured.

The TII type structures of AuIn and BiPd were studied at the Soleil and Diamond light sources. Both compounds undergo a sequence of phase transformations where the structure first discommensurates and the super structure reflections give way to incommensurate satellite reflections and then the satellite reflections are smeared out into diffuse scattering.
Mo-A1i, 11:00

State-of-the-art instrumentation for studies of structural, magnetic and electronic properties of materials at the extremes of pressures, temperatures and magnetic fields

Konstantin V. Kamenev

† Centre for Science at Extreme Conditions, The School of Engineering, The University of Edinburgh, Peter Guthrie Tait Road, Edinburgh EH9 3FD, UK

Historically high-pressure (HP) research has been an area that is heavily dependent on the availability of the experimental equipment. Many of the discoveries in HP science followed promptly from breakthroughs in instrumentation development, which provided researchers with higher pressure limits or larger sample volumes. A limited availability of commercial pressure cells and the need to remain at the cutting edge of the research make it likely that anyone working in this field will at some point engage in designing new or in modifying existing HP equipment. This presentation aims to introduce an engineering approach to developing pressure cells and to present such generic tools as computer aided design (CAD) and finite element analysis (FEA).

The use of engineering methods in the design of HP equipment will be illustrated using recently developed pressure cells. This includes a range of piston-cylinder and opposed-anvil cells for measuring magnetic susceptibility at high pressure. The examples of using Finite Element Analysis for miniaturization of the pressure cells and their components will include miniature pressure cells for X-ray diffraction and magnetic property measurements. Some new devices for neutron scattering at high pressure will also be presented such as a large volume pressure cell with optimized transmission for inelastic neutron scattering. The first 3D-printed diamond anvil cell will be presented to illustrate the advantages of using this fast developing manufacturing technique.

Mo-A2, 11:30

Chiral magnets probed with X-rays

F. Wilhelm and A. Rogalev

ESRF-The European Synchrotron, 71 avenue des Martyrs, 38000 Grenoble, France

Magnetic order breaks time reversal symmetry and in chiral magnetic systems, additionaly, space inversion symmetry is broken. Chiral magnets are abundant, existing as metals and molecules, semiconductors and insulators. These symmetry conditions are satisfied in magneto-electric media and multiferroics and also in chiral crystals subjected to a magnetic field. Interstingly, in such systems, in addition to natural and magnetic circular dichroisms, a magneto-chiral dichroism can be observed. It is a non-reciprocal effect featuring an unbalanced absorption of unpolarized light and its sign depends on both the relative orientation of the light propagation direction, the applied magnetic field and the sample chirality. Despite the fundamental interest in a phenomenon breaking both parity and time-reversal symmetries, magneto-chiral dichroism is one of the least investigated aspects of light–matter interaction most likely because of the weakness of the effect. It has been experimentally evidence only in 1997 [1] in the visible range and a few years later in the X-ray range [2]. A major strength of X-ray magneto-chiral dichroism (XMCD) is its element specificity and edge selectivity inherent to any X-ray absorption spectroscopy. It is interesting to note that, while X-ray magnetic circular dichroism (XMCD) provides information on the orbital and spin magnetic moment of the absorbing atom, XMCD gives access to a more elusive quantity: the anapole orbital current or orbital toroidal moment carried by the absorbing atom. Orbital toroidal currents seem to be involved in different phenomena ranging from multiferroicity to superconductivity, and XMCD offers a unique possibility to its accurate determination. Applications of this new technique to a number of non-centrosymmetric magnetic systems ranging from ferromagnetic chiral crystals Mn$_{1-x}$Fe$_x$Ge, multiferroic Ga$_2$Fe$_3$O$_7$ crystal and chiral single molecule magnets [3] will be presented here.

Mo-A3, 11:45

**Temperature dependent Raman spectroscopy studies of SrTiO$_3$ and SrTi$^{18}$O$_3$**

N. Mironova-Ulmane$^1$, A. Anspoks$^1$, L. Puust$^2$, I. Sildos$^2$, M. Itoh$^3$, J. Purans$^1$

1 Institute of Solid State Physics, University of Latvia, Kengaraga street 8, LV-1063 Riga, Latvia
2 Institute of Physics, University of Tartu, W.Ostwaldi tn 1, 50411, Tartu, Estonia
3 Tokyo Institute of Technology, Laboratory for Materials & Structures, Midori Ku, 4259-J2-19 Nagatsuta, Yokohama, Kanagawa 2268503, Japan

Strontium titanate is a model quantum paraelectric in which, in the region of dominating quantum statistics, the ferroelectric (FE) instability is inhibited due to nearly complete compensation of the harmonic contribution into ferroelectric soft mode frequency by the zero-point motion contribution. The enhancement of atomic masses by the substitution of $^{18}$O with $^{16}$O decreases the zero-point atomic motion, and low-T ferroelectricity in SrTi$^{18}$O$_3$ is realized 1.

In this study, we report on temperature dependent (T=10-300K) Raman spectra measurements in SrTiO$_3$ and SrTi$^{18}$O$_3$. Raman spectra were measured at room temperature through 50x microscope objective using Renishaw inVia micro-Raman spectrometer equipped with argon laser (514.5 nm, max cw power $P_{cw}=10$ mW) with the cryostat. The spectral signal was dispersed by the 2400 grooves/mm grating onto Peltier-cooled (-60°C) CCD detector. We have identified modes (e.g. 171 and 519 cm$^{-1}$) correlated with FE phase, as well as modes (e.g. 145 and 422 cm$^{-1}$) associated with tetragonal phase. As x-ray diffraction studies does not detect any structural changes in FE phase1, and x-ray absorption studies2,3 reveal that the local structure of the Ti is the same in whole temperature range (10 - 300K), we suggest that SrTi$^{18}$O$_3$ as an example of dynamic FE phase transition, where average structure does not change, but the relative movement of the ions is strongly correlated, and this correlation (e.g. of Ti-Ti chains) is responsible for macroscopic FE phase. This suggestion is supported by the theory of formation of lower symmetry dynamical clusters in ferroelectrics4.


Mo-A4i, 12:00

**Hedgehog Spin-vortex Crystal Magnetic Order in the New Magnetic Superconductors CaK(Fe$_{1-x}$Ni$_x$)$_4$As$_4$ revealed by $^{75}$As Nuclear Magnetic Resonance**

Yuji Furukawa,

Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50014, USA

Following the discovery of unconventional superconductivity (SC) in Fe-based superconductors, many pnictides have been investigated in the search for unconventional SC and other novel properties. Quite recently, a new Fe-based SC, CaKFe$_2$As$_2$, with a transition temperature of $T_c=52$ K has been discovered [1]. Here we have carried out nuclear magnetic resonance (NMR) measurements to investigate the electronic and magnetic properties of single crystalline CaKFe$_2$As$_2$. In this talk, based on the NMR data, we will discuss the details of superconducting properties and magnetic fluctuations of CaKFe$_2$As$_2$[2], which will be compared with those in other Fe-based SCs such as 122 systems. In addition, we will report the observation of the hedgehog spin-vortex order in the antiferromagnetic state in Ni-doped CaK(Fe$_{1-x}$Ni$_x$)$_2$As$_2$ ($T_n=52$ K and $T_c=9$ K for $x=0.05$) [3,4]. Furthermore, the Ni doping $x$ dependence of magnetic fluctuations will be presented and discuss a possible quantum critical behavior in Ni-doped CaK(Fe$_{1-x}$Ni$_x$)$_2$As$_2$.

This work was performed in collaboration with Q.-P. Ding, J. Cui, P. Wiecki, K. Rana, P. C. Canfield, S. L. Bud’ko, A. E. Böhmer, W. R. Meier, Y. Lee, V. Borisov, R. Valentí, P. Orth, and R. Fernandes.


*This work was supported by the US Department of Energy, Division of Material Science. Ames Laboratory is operated for the US Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.

Oral
The ferromagnetic superconductors UCoGe and URhGe have the easy magnetization axis in the ferromagnetic state along the orthorhombic c-axis. Magnetization behavior in fields along b, however, plays important role in physics of these materials. URhGe at 2 K undergoes a first-order metamagnetic transition at $H_R = 12.5$ T whereas the $M(H)$ curve of UCoGe exhibits a broad S-shape around $H_m \approx 50$ T. The $\chi_b(T)$ curve of URhGe shows a sharp peak at $T_{\chi_b} = 9.5$ K ($= T_C$) but a broad maximum around $T_{\chi_b} = 37$ K ($>> T_C = 3$ K) for UCoGe\textsuperscript{1}. Our detailed study of UCo$_{1-x}$Rh$_x$Ge single-crystals has revealed the evolution of the characteristic temperature ($T_{\chi_b}$) and magnetic fields ($H_R$, $H_m$) with Co/Rh concentration. For $x \leq 0.3$ we observed $T_{\chi_b} > T_C$ and for $x \geq 0.4$ $T_{\chi_b} = T_C$. The characteristic field of the $M(H)$ anomaly develops in each of the two regions with very different trend. Two different paramagnetic regimes can be distinguished in the $H$-$T$ phase diagrams: a) low-temperature field-polarized paramagnet for $H < H_R$ for high $x$, b) correlated paramagnetic regime with ferromagnetic fluctuations for $T < T_{\chi_b}$ and $H < H_m$ for low $x$. We will discuss relations of these paramagnetic regimes in normal state to the role of spin fluctuations in pairing mechanism and the character of the field-induced re-entrant superconductivity domes of parent compounds\textsuperscript{2,3}.

\textsuperscript{1} W. Knafo et al., Phys. Rev. B \textbf{86}, 184416 (2012)
\textsuperscript{2} F. Levy et al., Science \textbf{309}, 1343 (2005)
\textsuperscript{3} B. L. Wu et al., Nat. Commun. \textbf{8}, 14480 (2017)

Mo-A6i, 14:00

**Understanding Phase Diagrams of Intermetallic Systems using Crystal Chemistry**

Roman Gladyshevskii\textsuperscript{1}

\textsuperscript{1}Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya St. 6, 79005 Lviv, Ukraine

Ternary intermetallic systems with rare-earth elements, d-elements, and p-elements of group IIIA (Al, Ga, In), IVA (C, Si, Ge, Sn, Pb), and/or VA (Sb, Bi) will be discussed. The phase diagrams of many of these systems are complex and contain a large number of compounds of similar composition; temperature- and composition-induced structural changes are often observed. For deformation, substitution, ordering, vacancy and filled-up derivatives the structural transformations can be described in terms of group-subgroup relationships. Homologous series of structures will be discussed. The knowledge of the relations between the compositions and crystal structures of the compounds provides important information on the interaction of the elements and the phase diagrams.
Mo-A7i, 14:30

**Synthesis, Structural Relationships, Chemical Bonding in Selected Ternary Germanides Containing Rare Earth Metals**

Adriana Saccone, Riccardo Freccero, Serena De Negri, Pavlo Solokha

*Dept. of Chemistry and Industrial Chemistry, University of Genova, via Dodecaneso 31, 16146, Genova, Italy*

Rare-earth binary and ternary germanides form a group of polar intermetallics extensively studied with respect to crystal structure, chemical bonding, and physical properties. These compounds show intriguing crystallographic properties (defective structures, superstructures, modulated structures), characteristic Ge-based covalent fragments (dumbbells, 2D motifs, more complex 3D fragments), and interesting physical properties (giant magnetocaloric effect, superconductivity, anomalous thermal expansion).

In our laboratory several ternary systems R-M-Ge (R=rare earth metal, M=another metal) have been explored with respect to phase equilibria and crystal chemistry of intermediate compounds. Existence and crystal structures of these germanides are strongly influenced by the nature of R and M: consequently they became good candidates for studies of structure/bonding/properties relationships.

In the framework of these studies, different synthetic routes were followed, such as induction/arc melting, thermal treatments, synthesis in flux medium.

Among the numerous Ge-rich intermetallics discovered in these systems, the $R_xMGe_{10-x}$, $R_xM_2Ge_5$, $R_xM_5Ge_8$, and $R_xMGe_6$ series will be presented and discussed. Emphasis will be given on peculiarities like vacancies ordering phenomenon ($R_xZn_{1-x}Ge_2$), different polymorphs or twin formation ($R_xMGe_{10-x}$, $R_xPdGe_6$), “coloring” accompanied by symmetry reduction ($R_xM_2Ge_5$, $R_xMGe_6$). Common structural features will be also highlighted in view of a deeper investigation of the chemical bonding of these germanides.


Mo-A8, 15:00

**Field induced ferromagnetic state in Y_{1-x}Er_xFe_2D_y deuterides (0 < x ≤ 0.5, y≈4.2)**

V. Paul-Boncour 1, O. Isnard 2, M. Guillot 3

1 ICMPE, UPEC - CNRS, 94320 Thiais, France
2 Institut Néel, University of Grenoble Alpes - CNRS, BP 166X, 38042 Grenoble, France
3 LNCMI, CNRS, BP166, 38042 Grenoble Cedex 9, France

Y_{1-x}Er_xFe_2 compounds crystallize in the cubic MgCu_2 type structure and are ferrimagnetic. Hydrogen (deuterium) insertion strongly modifies their crystallographic and magnetic properties and particularly original results were observed for an H (D) content close to y=4.2. Deuterium insertion into tetrahedral sites induces a lowering of the crystal symmetry into a monoclinic structure (Pc space group). At low temperature the ground state is ferromagnetic with an antiparallel orientation of the Fe and Er moments in the (a, c) plane. Below 30 K, a field induced forced ferri-ferromagnetic (Ferri-F) transition is observed for a transition field $B_{trans}$ of only 8 T, whereas such transitions have been observed for $B_{trans} ≥ 40$ T in $R_xM_{17}$ ($R$= Er, Tm, $M$= Fe, Co)5 and 60 T in ErFe_{11}TiH$_3$ compounds. Such low value of $B_{trans}$ can be attributed to the strong reduction of the Er-Fe exchange interaction by (H) insertion. Beside, $B_{trans}$ is not sensitive to the Er content and remains almost constant up to 30 K. Upon heating and at low field a transition towards an antiferromagnetic (AF) state is observed at $T_{F\text{-}AF}$ which decreases linearly from 84 K (x=0) to 39 K (x=0.5). This first order transition is attributed to an itinerant electron metamagnetic behavior of the Fe sublattice and is accompanied by a cell volume contraction. Above $T_{F\text{-}AF}$ a metamagnetic transition from AF towards F state is observed. $B_{trans}$ increases linearly versus temperature and the d$B$/d$T$ slope increases with the Er content. If this transition is mainly related to the itinerant character of the Fe moments, Er moments parallel to the Fe moments are also induced above $B_{trans}$. This study reveals the strong influence of D (H) insertion on both crystal and magnetic structures as well as on the Er-Fe and Fe-Fe interactions.

Interaction between charge density wave and magnetism in $R\text{NiC}_2$ family

K. K. Kolincio, M. Roman, J. Strychalska-Nowak, M. J. Winarski, T. Klimczuk

Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland

The interaction between charge density wave (CDW) and various types of ordering as magnetism and superconductivity is a long-standing area of interest. The family of ternary compounds described by formula $R\text{NiC}_2$ (where $R$ is a rare-earth metal) has been found to exhibit both Peierls instability, superconductivity and a large variety of magnetic ground states, which yields an unique opportunity to explore the mechanisms of the interplay between these states.

From detailed analysis of transport, galvanomagnetic, thermal and magnetic properties we conclude that the coupling between magnetism and CDW strongly depends on the magnetic state. The interaction varies from constructive as for PrNiC$_2$, where the magnetic anomaly enhances the Fermi surface nesting, through weakly destructive in GdNiC$_2$ with the CDW state partially suppressed by Zeeman splitting of conduction bands in the paramagnetic state, to a further (yet still partial) suppression by antiferromagnetic groundstate and a complete destruction of the Peierls instability due to field induced ferromagnetic transition.

$^*$Authors gratefully acknowledge the financial support from National Science Centre (Poland), grant number: UMO-2015/19/B/ST3/03127.
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Magnetic Frustration Anomalies in Kagome Lattices of the type, $R_3\text{Ru}_4\text{Al}_{12}$ (Rare-earths)

E.V. Sampathkumaran

Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumba – 400005, India

Non-metallic materials containing magnetic ions arranged in kagome lattice structure have been attracting a lot of attention in the field of geometrically frustrated magnetism. However, geometrically frustrated magnetism of intermetallic compounds possessing kagome lattice features has been scarcely explored in the literature. Here, we present an overview of our results of bulk magnetic measurements [1-3] on the intermetallics, $R_3\text{Ru}_4\text{Al}_{12}$ ($R$ = Gd, Tb, Dy, and Er) containing (distorted) kagome nets, exhibiting long range magnetic order at ($T_N$) 18.5, 22, 7 K, and <2K respectively. The point of emphasis is that there is an evidence for anisotropic re-entrant spin-glass-like behavior (below 12 K) for the Tb case. Such glassy characteristics presumably arise from geometrical frustration and it is interesting that such features are observed without chemical doping. However, no magnetic frustration effects could be observed for the Gd case. We therefore speculate that orbital anisotropy may play a crucial role for magnetic frustration features in the Tb case.

References
New R₃TAl₃Ge₂ quaternary compounds (R = rare earth; T = transition metal)

Alessia Provino 1,2, A. K. Pathak 3, M. K. Kashyap 4, T. A. Hackett 3, V. K. Pecharsky 3,5, P. Manfrinetti 1,2

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The formation of new quaternary compounds with formula R₃TAl₃Ge₂, where R is a rare earth element and T is a transition metal of the first and second period, has been studied by means of XRD, DTA and SEM-EDX analyses. We have found the compound R₃TAl₃Ge₂ for R = Gd and Tb and T = Cr, Mn, Fe, Co, Ni and Cu to form; they crystallize in the hexagonal Y₃NiAl₃Ge₂-type (hP9, P-62m, Z = 1). Figure 1 shows the trend of the lattice parameters for the Gd compounds. Investigation of their physical properties is now underway. Theoretical calculations to explain their formation, relative stability as a function of the rare earth size and transition metal, and their magnetism have been performed. Preliminary results will be presented.

Part of work, performed at the Ames Laboratory, was supported by the Office of the Basic Energy Sciences, Materials Sciences and Engineering Division of the U.S. Department of Energy. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract DE-AC02-07CH11358.

Mo-A12, 17:00

Influence of substitution in the Fe sublattice on the magnetism of HoFe₅Al₇

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Effects of the Co and Cr substitution for Fe on the strongly anisotropic ferrimagnet HoFe₅Al₇ (tetragonal crystal structure of the ThMn₁₂₋₁ type) are studied on single-crystalline samples grown in a triarc furnace by Czochralski method. For HoFe₅₋ₓCoₓAl₇, we found the homogeneity range up to x = 2.5. The Co substitution results in a shrinkage of the tetragonal lattice within the basal plane, whereas the c parameter does not change. The exchange interactions and magnetic anisotropy are strongly affected by the Co substitution. The strong decrease of the Curie temperature Tc in HoFe₅₋ₓCoₓAl₇ compounds with increasing Co content is very unusual. Tc linearly falls from 216 K for x = 0 to 67 K for x = 2.5, which is unexpected because the Co substitution for Fe in 3d-4f intermetallic compounds usually increases the magnetic ordering temperatures due to the strengthening of exchange interactions. At the same time, the compensation temperature changes very little between 65 K and 72 K. At 2 K, spontaneous magnetic moment increases from 2 μB at x = 0 to 4.2 μB at x = 2.5. In contrast to Co substitution where the number of 3d electrons increases, a substitution of Fe by Cr leads to a smaller number of 3d electrons. Nevertheless, Tc also decreases, moreover, very drastically. In HoFe₅Cr₇ it is only 22 K. Magnetization measurements have been performed in pulsed magnetic fields up to 58 T. The compounds exhibit a high magnetic anisotropy of the easy-plane type with the [110] axis as the easy-magnetization direction. Along the easy axis, two first-order field-induced magnetic transitions (at 17 T and 37 T) are observed for HoFe₅Al₇ and one transition at 27 T for HoFe₅CoAl₇. The magnetization curve has an S-shape for HoFe₅₋ₓCoₓAl₇. With Cr substitution, the second transition observed in HoFe₅Al₇ shifts to 34 T. The magnetization curve below 8 T could be interpreted as showing a modified first transition of HoFe₅Al₇ - it becomes the second order and starts at very low field.

Oral
Magnetic and thermal properties of R₃Ni₂In₄ (R = Gd–Tm) *

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The R₃Ni₂In₄ (R = Gd–Tm) compounds are a new interesting series of intermetallics whose crystal structure was for the first time reported in 2016 by B. Heying et al.¹ The compounds crystallize with the hexagonal Lu₃Co₂In₄-type structure (space group P6) which is a reduced symmetry derivative of the ZrNiAl-type structure.

In this presentation we report magnetic and thermal properties of R₃Ni₂In₄ (R = Gd–Tm) investigated by magnetometric and heat capacity measurements. The polycrystalline samples were obtained by arc melting under argon atmosphere followed by annealing in vacuum at 1070 K for one week. All measurements were performed with the use of a Physical Properties Measurement System (PPMS) equipped with the VSM, ACMS and HC options. Magnetic susceptibilities of all investigated compounds, taken at 50 Oe, shows at low temperatures maxima typical of transition from paramagnetic to antiferromagnetic state. In case of some compounds (R = Gd, Ho) the maxima are very broad suggesting a spin-glass character of the magnetic ground state. The transition temperatures, as determined from magnetic susceptibility and heat capacity measurements, vary from about 3 K (R = Ho, Tm) to about 23 K (R = Tb). Reciprocal magnetic susceptibilities, collected at 1 kOe, show the Curie-Weiss behavior in a wide temperature range. The values of effective magnetic moments are very close to those predicted theoretically for the R⁺³ ions. Such a result clearly indicates that rare earth ions are the source of magnetism in the investigated intermetallics.

The results are compared with those obtained for the isostructural R₃Co₁.₇₅In₄ (R = Ho, Er, Tm) compounds².³

*The research was carried out with the equipment purchased thanks to the financial support of the European Regional Development Fund in the framework of the Polish Innovation Economy Operational Program (contract no. POIG.02.01.00-12-023/08).
² S. Baran, Yu. Tyvanchuk, Ya. Kalychak and A. Szytuła, accepted for publication in Phas. Trans.

Nematic superconductivity in topological materials

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Topological insulators have generated a wide research interest, because they offer access to novel quantum states with unprecedented properties. Most interestingly, the concept of topological insulators can be transferred to superconductors, where the superconducting gap plays the role of the band gap of the insulator. Here we focus on recent developments in the family of intercalated Bi₂Se₃-based crystals, such as Cu₃Bi₂Se₃ and Sr₃Bi₂Se₃, where field-angle dependent measurements of the transport, thermal and magnetic properties reveal spontaneously broken rotational symmetry in the macroscopic superconducting properties, for instance in the upper critical field [1,2]. This unusual property can be explained by recent theoretical models for topological superconductors in terms of nematic superconductivity associated with a two-component superconducting order parameter (E₉ representation) [3]. The experimental results provide evidence for unconventional superconductivity with an odd-parity spin-polarized triplet Cooper-pair state (Δ₅-pairing).

Structural and magnetic investigations of skyrmion phases

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Recent studies report the existence of skyrmions in materials with a different chiral space group from that of the B20 compounds, such as GaV$_4$S$_8$ [1] and Co$_{10-x}$Zn$_{10-y}$Mn$_x$S$_8$ [2]. This has motivated us to embark upon a study of several classes of skyrmion materials and explore a wide composition range of each of the above family of compounds: i.e., GaV$_4$X$_8$ ($X$=S, Se, Te), Co$_{10-x}$Zn$_{10-y}$Mn$_x$S$_8$ and the Cu$_{2-x}$A$_x$OSeO$_3$ ($A$=Zn, Ni). Investigations of the effects of substitution and the resulting structural order/disorder on the existence of the skyrmion phase in these materials sheds light on the origin, the formation, and tuning of the skyrmion lattices.

A number of the above materials have been synthesized and structural investigations have been carried out using both powder and single crystal X-ray diffraction. A study of the magnetic properties of these materials has also been carried out by ac and dc magnetic susceptibility measurements. We present a detailed structural and magnetic study of these interesting classes of materials demonstrating the structural similarities of these materials and the correlation with their magnetic properties.


2D magnetism in magnetic van der Waals materials*

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There has been a huge increase of interests in two-dimensional van der Waals materials over past ten years or so. Despite the impressive list of new materials and the novel physics it has come to offer, there is the conspicuous absence of one particular class of materials: magnetic van der Waals systems. In this talk, I will identify and illustrate how we might be able to benefit from exploring these so-far neglected materials.

*This work was supported by the Institute for Basic Science in Korea (IBS-R009-G1).
The temperature and frequency dependence of the optical response in Weyl semimetal TaAs has been studied systematically. It is found that the optical conductivity of TaAs features a narrow Drude response alongside a linear dependence on frequency. The weight of the Drude peak decreases upon cooling, following a $T^2$ temperature dependence, in good agreement with theoretical predictions. Two linear components with distinct slopes dominate the low-temperature optical conductivity. A comparison between our experimental results and theoretical calculations suggests that the linear conductivity below $\sim 230$ cm$^{-1}$ arises purely from interband transitions near the Weyl points. Strong coupling between an infrared-active phonon and electronic transitions near the Weyl points has also been observed, which demonstrates itself as a Fano resonance in the lineshape. The resulting asymmetry in the phonon line shape, conspicuous at low temperatures, diminishes continuously with increasing temperature. This behavior originates from the suppression of electronic transitions near the Weyl points due to the decreasing occupation of electronic states below the Fermi level ($E_F$) with increasing temperature, as well as Pauli blocking caused by thermally excited electrons above $E_F$. Our findings open a route for exploring exotic physical phenomena through phonon properties in Weyl semimetals.

References


Mo-B5i, 14:00

Emergence of Novel Ground States in Mott-Insulators at High Pressure

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In Mott-insulators, the metal insulator (MI) transition is driven by strong correlation effects associated with electron-electron interactions and the interplay between the charge, spin and orbital degrees of freedom. These are strongly coupled to the lattice and thus can be tuned by external pressure. In this contribution, I will discuss recent results on the change of transport, magnetic and structural properties of some selected Mott-insulators (EuNiO$_3$, GaNb$_4$S$_8$) by tuning these systems across the MI transition with external pressure. A special emphasis will be given to the appearance of unusual metallic state in EuNiO$_3$ and superconductivity in GaNb$_4$S$_8$ at/near the pressure-induced MI transition. The experimental results provide new insight in understanding the interplay between these degrees of freedom and their impact on the formation of anomalous ground states at high pressure.

Mo-B6i, 14:30

**Magnetoresistance in rare-earth-based half-Heusler phases and monopnictides – non-trivial topology, superconductivity, antiferromagnetism and extreme magnetoresistance**

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We review our studies of $R_eT_eX$ half-Heusler phases and $R_eX$ monopnictides ($R_e$ = Y, Lu, Gd–Er; $T_e$ = Pd, Pt; X = Bi, Sb). Several of these compounds exhibit band inversion essential for topological non-triviality of electronic states. Superconductivity of half-Heusler phases, often coexisting with antiferromagnetic order, seems highly unconventional (due to their non-centrosymmetric crystal structure and very low carrier densities) and possibly realized via exotic pairing of $j = 3/2$ fermions. Magnetoresistance of these phases is huge, with sign depending on magnetic character of $R_e$. Shubnikov–de Haas effect is universally observed, revealing small Fermi surfaces and very light charge carriers. New data on several $R_eT_eSb$ are also presented. Some of $R_eX$ monopnictides also possess topologically non-trivial electronic states. The question how Dirac-like structures present in their electronic structure contribute to extremely large magnetoresistance in these compounds remains open.

In several monoantimonides their extraordinary magnetotransport properties (extreme magnetoresistance and low-temperature resistivity plateau) could be ascribed in full to nearly perfect charge compensation of bulk 3D Fermi surfaces. Our comprehensive analysis of Fermi surface reveals the same for YBi and LuBi.

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Mo-B7, 15:00

**Kondo insulator to semimetal transformation tuned by spin-orbit coupling**

Sami Dzsaber¹, Lukas Prochaska¹, Andrei Sidorenko¹, Gaku Eguchi¹, Robert Svagera¹, Monika Waas¹, Andrey Prokofiev¹, Claudia Hradil², Qimiao Si³, Silke Paschen¹,³

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The recent discovery of topologically non trivial bandstructures in non-interacting electron systems triggered an enormous effort to look for their strongly interacting counterparts. Until recently, focus was on the topological Kondo insulator SmB₆ (ref. 1). Very recently, a gapless version - dubbed Weyl-Kondo semimetal - has attracted much attention. Herein we present the growth of a series of $\text{Ce}_2\text{Bi}_3(\text{Pt}, \text{Pd})_3$ single crystals starting form the archetypal Kondo insulator $\text{Ce}_2\text{Bi}_3\text{Pt}_3$ (ref. 4). Upon gradually replacing the 5d element Pt by the much lighter 4d element Pd, we observe an insulator-to-semimetal transition, that we attribute to the decreasing of spin-orbit coupling. Most interestingly, the low-temperature electronic specific heat coefficient $C/\text{T}$ of $\text{Ce}_2\text{Bi}_3\text{Pd}_3$ is linear in $\text{T}$. This is the hallmark of a strongly correlated system with linear electronic dispersion, just as recently predicted for a Weyl-Kondo semimetal.

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Oral
Optical properties of the electronic nematic phase in FeSe

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FeSe undergoes a structural tetragonal-to-orthorhombic transition below 90 K, which breaks the four-fold rotational symmetry of the tetragonal phase, without any subsequent onset of magnetic ordering. The substantial anisotropy of the transport properties in the broken symmetry state is ascribed to an electronic nematic phase. FeSe thus provides an opportunity to address the impact of nematicity on its intrinsic physical reflectivity measurements over a broad spectral range that probe the optical response to variable uniaxial stress, detwining the specimen and acting as an external symmetry breaking field, and as a function of temperature across the structural transition [1]. We extract the optical conductivity through Kramers-Kronig transformation. Our data reveal an astonishing anisotropy of the optical response in the mid-infrared-to-visible spectral range, which bears testimony of an important polarization of the underlying electronic structure in agreement with ARPES results. Our findings at high energy scales support models for the nematic phase based on an orbital-ordering mechanism, supplemented by orbital selective hand renormalization. The far-infrared response of the charge dynamics moreover allows establishing the link to the dc resistivity. The dc limit of the optical conductivity indeed agrees with the measured transport properties, deploying an anisotropy typical of hole-doped iron-based materials. Our optical results at energies close to the Fermi level furthermore emphasize scenarios based on scattering by anisotropic spin-fluctuation, shedding new light on the origin of nematicity in FeSe.


Oral
Spectroscopic study of quantum spin liquid candidate Tb₂Ti₂O₇ reveals vibronic coupling

Evan Constable¹, L. Bergen¹, R. Ballou¹, J. Robert¹, C. Decorse¹, J.-B. Brubach¹, P. Roy¹, E. Lhotel¹, V. Simonet¹, S. Petit¹ and S. deBrion¹

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Within a solid crystal vibronic coupling describes the interaction between the electronic energy levels and the phonon modes of the structure, often leading to a ground state that is considerably perturbed in comparison to an uncoupled system. In the context of magnetic rare-earth pyrochlores (RE₂Ti₂O₇, RE = Dy, Ho), large crystal field splitting of the electronic energy levels and geometric frustration leads to exotic magnetic behavior in the form of a highly degenerate spin ice ground state. The possibility that quantum fluctuations due to vibronic coupling could melt the spin ice state forming a quantum spin liquid is an interesting prospect. It is thought that this process could be present in Tb₂Ti₂O₇ as it does not appear to feature long-range order or a spin ice phase. Indeed, our investigations reveal favorable symmetry and energy conditions for vibronic coupling. Using optical spectroscopic techniques we find evidence of a hybridization of crystal-field-phonon modes present across a broad temperature range. This vibronic process supports a collective state between the ground and excited levels that provides a crucial path for quantum spin-flip fluctuations that inhibit the stabilization of conventional magnetism.

Exotic magnetoelectric excitations of the multiferroic SmFe₃(BO₃)₄

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Magnetoelectric (ME) multiferroics (MFs), i.e. materials simultaneously hosting ferroelectric and magnetic order, have been attracting enormous interest due to their potential in information-technology applications.¹² Rare-earth ferroborates are a particularly interesting family of MF crystals, where the strong spin-orbit interaction at the rare-earth sites results in the coupling of the magnetic and electric degrees of freedom. The ME response of the material is enhanced by the antiferromagnetic ordering of the iron spins.¹³ The same ME coupling appears in the optical regime as different absorption of counter-propagating light beams, where transparent and dark directions can be swapped by reversing the magnetic field.¹⁴ Furthermore, due to the ME coupling the strength of absorption at spin-wave resonance frequencies can also be tuned by electric field, opening the path for practical applications.¹⁵

Melt growth of Ir/Ir-Rh alloy “FLEXIBLE” wires using micro-pulling down method

Akira Yoshikawa1,2,3, Rikito Murakami1,3, Yuui Yokota2, Kei Kamada2,3, Yasuhiro Shoji1,3, Shunsuke Kurosawa2,4, Yuji Ohashi2, Akihiro Yamaji1, Masao Yoshino1,3

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We have developed alloy wire elaboration process using micro-pulling down method (Alloy-micro-pulling down method, A-μ-PD method). It is melt growth process. For example, with alumina crucible, we have succeeded in growing Pd-In-Fe and NiFeCoGa wires. Recently, we also succeeded in growing Ir were (Tm=−2447°C) with diameter of 1 mm and with length of more than 10 m by zirconia crucible which can be used at over 2500°C. The grown wires have shown excellent flexibility due the elongated coarse grains along growth direction, therefore, it is highly expected to apply A-μ-PD method to produce thermocouples. For practical application, there are some problems to be solved in: (i) to make wires with diameter as thin as 0.5 mm, which is equivalent to existing commercial thermocouples, (ii) to evaluate thermo-electromotive force (EMF) at high temperature. In this research, we aimed to fabricate deformable Ir/Ir-Rh thermocouple by A-μ-PD method and measure the EMF. Ir and Rh powders (99.9% purity) were used as raw materials. Pure Ir and Ir-40 wt.% Rh were pelletized by arc melting, and then wires with diameter of 0.5 mm were produced in an A-μ-PD furnace (Micropuller A-01, C&A corp.) using zirconia crucibles. In order to observe the structure by scanning electron microscope (SEM, J-7800F, JEOL), after mechanical polishing, cross section polishing (CP) treatments with argon ion beam were performed to remove surface strain. The crystal grain size and crystal orientation were evaluated by the electron back scatter diffraction (EBSD) technique. From the BSE images, the grown wire consists of several large and oriented crystal grains. In addition, the EMF was evaluated using a tubular furnace and a commercially available thermocouple. At this time, the reference junction was kept at 0 °C. The EMF curve showed good correspondence with that of existing thermocouple.

Growth of Co-Cr-Mo Alloy Fiber Crystal by Alloy-Micro-Pulling-Down Method, and the Microstructure and Mechanical Property

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Co-Cr-Mo (CCM) alloys have been used as biomedical applications for human body such as a stent. However, it is difficult to process them into complicated shapes due to the poor workability. In our previous studies, the alloy-micro-pulling-down (A-μ-PD) method has been developed to grow alloys with specific shapes from the melt directly, and platinum-group metal fiber crystals could be grown1. In this study, we tried to grow the CCM alloy fiber crystal by the A-μ-PD method, and the microstructures and mechanical property were investigated. Co, Cr and Mo powders (3N) were mixed as a nominal composition of Co-28Cr-6Mo (mass%) and pre-melted CCM alloy ingots were set in a Al2O3 crucible with a φ2 mm hole at the bottom. The ingots were heated up to the melting point by the high frequency induction heating. After it was completely melted, the melt was pulled down through the hole using an Ir wire in Ar+3%H2. Obtained alloy fibers were polished and treated by the cross-sectional polisher. Microstructures on the treated surfaces were observed the Electron Back-Scattered Diffraction (EBSD). Tensile tests of the grown fibers were performed by a universal testing machine. CCM fiber crystals could be grown at 0.1, 0.3 and 0.5 mm/min growth rates. Large hcp ε phase was observed in the CCM fiber grown at 0.1 mm/min. On the other hand, fcc γ phases were partially formed in the hcp ε phase of the CCM fiber grown at 0.5 mm/min. The results suggest that the growth rates affected the phase formation of the CCM fiber. We will report details of crystal growths, microstructures and tensile tests of the CCM fibers.

Mo-PO1

Synthesis and magnetic susceptibility of YCrB₄-type compounds by arc-melting method

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The rare earth aluminum tetraborides α-RAlB₄ having YCrB₄-type (orthorhombic Pham) have attracted increasing attention with recent reports of interesting electronic and physical properties [1-3]. α-RAlB₄ (R = Er, Ho) compounds from a solution with Al-rich self-flux have been synthesized by arc-melting method [4,5]. However the question of crystal growth and the properties of the solid solution R[AlₓFeₓCrᵧ]B₄ are still not elucidated completely. In this work we report the crystal synthesis of R[AlₓFeₓCrᵧ]B₄ compounds from the high temperature Al, Fe and Cr mixed flux-mediated arc-melting method. The starting atomic of R : Al : B was fixed as 1 : 10 : 3. In the cases of R = Er and Ho, when we substituted Al flux with Fe in 10 at% and Cr in 5 at%, YCrB₄-type compounds were synthesized, when the amount of Fe and Cr decreased, R tetraboride kR₄ or Ho dodecaboride HoB₁₂ crystals were mainly coexisting. The lattice parameters and chemical analysis of R[AlₓFeₓCrᵧ]B₄ compounds with YCrB₄-type structure obtained by a single phase, were for Er[AlₓFeₓCrᵧ]B₄ ; a = 0.5917(1), b = 1.1442(2), c = 0.3433(1) nm, Er[Al₀.₀₁Fe₀.₁₅Cr₀.₆₂]B₃₈, for Ho[AlₓFeₓCrᵧ]B₄ ; a = 0.5933(3), b = 1.1451(5), c = 0.3506(4) nm, Ho[Al₀.₂₀Fe₀.₁₅Cr₀.₆₁]B₄₆, respectively. The magnetic susceptibility of powder samples of Er[AlₓFeₓCrᵧ]B₄ were measured by using a SQUID magnetometer in the temperature range of 300 K to 1.8 K. Superconductivity was not observed in any of the Er[AlₓFeₓCrᵧ]B₄ down to a temperature of 1.8 K. The antiferromagnetic transition of Er[AlₓFeₓCrᵧ]B₄ with Neel transition temperature were each observed at 7N = 6.5 K (magnetic field ; 5 kOe) and 7N = 5.8 K (magnetic field ; 10 kOe).


Mo-PO2

Crystal growth and physical properties of Lu(Al₁ₓT₄)B₄ (T = Cr, Fe) by Al-self flux

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In the known ternary R-Al-B systems (R = rare earth), four types of ternary structures have been reported, namely the YCrB₄-type (α-type, Pham) [1, 2], ThMoB₄-type (β-type, Cmmm) [3], the Y₂ReB₄-type (R₂AlB₄, Phm) [1, 4, 5] and the MgAlB₄-type (RAIB₁₄, Imma) [6]. The rare earth aluminum tetraborides α-RAlB₄ have attracted increasing attention with recent reports of interesting electronic and physical properties [7]. However the question of crystal growth and the properties of the solid solution Lu(Al₁ₓT₄)B₄ (T = Cr, Fe) are still not elucidated completely. In this work we report the experimental conditions for growing crystals of Lu(Al₁ₓT₄)B₄ (T = Fe, x = 0 ~ 0.100; T = Cr, x = 0 ~ 0.015) from the high temperature Al and T mixed flux. In addition, the size and morphology of crystal, measurements of micro-Vickers hardness and electrical resistivity were studied. The starting materials used were Lu₂O₃, Fe, Cr, crystalline B, and button-like Al. Mixtures of the materials in atomic ratio (B/Lu₂O₃ = 9.0) were placed in an Al₂O₃ crucible and heated in an Ar atmosphere at soaking temperature 1773 K for 5 h. As-grown the crystals were measured using a Vickers diamond indenter at room temperature. The maximum dimensions and morphology of obtained crystals were the size of about 0.7 × 0.5 mm for cubic crystal of Lu(Al₁ₓCr₄)B₄ and 5.2 × 0.2 mm for prismatic crystal of Lu(Al₁ₓFe₄)B₄. The values of micro-Vickers hardness of Lu(Al₁ₓFe₄)B₄ (x = 0.005 ~ 0.030) and Lu(Al₁ₓCr₄)B₄ (x = 0.005, 0.010) are in the ranges of 16(2.1) ~ 20(2.8) and 13(2.0) ~ 16(2.9) GPa, respectively. The electrical resistivity of the Lu(Al₁ₓFe₄)B₄ crystals will be debated in detail by poster presentation.

Crystalline growth and some property of Tm(Al1−xMo)xB4 compound by Al-flux

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The rare earth aluminum tetraborides α-RAIB4 (R = rare earth) have attracted increasing attention with recent reports of interesting electronic and physical properties [1,2]. TmAlB4 has especially been a compound of interest, and to try to further modify it, in this work we investigate the solid solution Tm(Al1−xMo)xB4. We report the experimental conditions for growing crystals of a new compound Tm(Al1−xMo)xB4 (x = 0 − 0.05) from the high temperature Al and Mo mixed flux. When authors substituted Al-flux with Mo in 0.2 or 0.5 at% Tm(Al1−xMo)xB4 crystals with YCrB4-type structure was synthesized, and also included MoAlB4 crystals. The starting materials used had purity 99.5 ~ 99.9 % for Tm2O3, Mo, crystalline B4, and button-like Al. Mixtures of the materials in atomic ratio (B/TmO3 = 9.0) were placed in an Al2O3 crucible and heated in an Ar atmosphere at soaking temperature 1773 K for 5 h, and then slowly cooled down at a rate of 50 K/h to room temperature. The maximum dimensions and morphology of obtained Tm(Al0.995Mo0.005)B4 crystal was silver-metallic unsettled plate-like crystal 2.2 mm square, and 7.0 × 0.1 mm for needle crystal of MoAlB4. The lattice parameters of Tm(Al0.995Mo0.005)B4 crystal with YCrB4-type obtained from Al0.995Mo0.005 mixed flux were a = 0.5988(7), b = 1.1582(2), c = 0.3544(6) nm, V = 0.2458(2) nm3 (larger values as the lattice parameters of TmAlB4 (a = 0.597157(6), b = 1.1472(1), c = 0.34773(3) nm [3])). In addition, the measurements of micro-Vickers hardness and electrical resistivity of Tm(Al1−xMo)xB4 were studied. The micro-hardness of Tm(Al1−xMo)xB4 was compared with Tm(Al1−xTc)B4 (T = Cr, Fe) crystals obtained by a recent report [4], and will be discussed by poster presentation.

References:

Crystal Growth Optimization of Ni2Mn1+xGa1-x Magnetic Shape Memory Alloys

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The Heusler alloy Ni2MnGa exhibits magnetic shape memory effects (MSM) where a large magneto-crystalline anisotropy in the low-symmetry martensite structure allows for re-orientation of twinved structural domains by application of a magnetic field due to high twin-domain boundary mobility. This structural reorientation provides strains of up to 6%. The high speed of twin boundary motion makes this a good system for use in actuators. The transition to the distorted martensite structure can be easily tuned to room temperature by altering the Ga:Mn ratio, with the general formula Ni2Mn1+xGa1-x, and this has allowed the possibility of device manufacture, such as μpumps for lab-on-a-chip applications. Additionally, room temperature ferromagnetism has allowed the first observation of skyrmions at room temperature with no applied field, highlighting the potential for skyrmionics applications. To allow scaling up for use in applications, the synthesis of high quality single crystals must be well controlled and reproducible. The influence of impurity inclusions on both macroscopic and microscopic properties has previously been highlighted as well as the stoichiometry sensitivity of observed superstructure. We will present our efforts to optimize the reproducible growth of high quality single crystals of Ni2Mn1+xGa1-x with 0 < x < 0.2. Characterization through microscopy, magnetometry, composition analysis (EDX), thermal gravimetric analysis and diffraction methods will be presented.*

* This work was supported by the OP VVV project MATFUN under Grant CZ.02.1.01/0.0/0.0/15_003/0000487 (www.matfun.eu)
2 Phatak, C. et al., Nano Lett. 2016, 16, 4141;
Mo-PO5

The Influence of the Mn Content on the Structural and Magnetic Properties of Bulk CuMnAs Compound

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CuMnAs is a room temperature antiferromagnetic semi-metal, which has recently attracted experimental and theoretical interest in the research fields of antiferromagnetic spintronics1,2, and physics of Dirac fermions3. In the bulk form, the compound is known to have an orthorhombic (Pnma) crystal structure with lattice parameters $a = 0.6859$ nm, $b = 0.3867$ nm and $c = 0.7320$ nm1, while tetragonal structure (P4/nma) with lattice parameters $a = b = 0.3820$ nm and $c = 0.6318$ nm is formed when the materials is grown on GaAs (001) or GaP (001) substrates2,4. The composition analysis suggests Mn deficiency in the studied tetragonal films4.

Our current studies on bulk CuMnAs shows that the crystal structure and magnetic properties are very sensitive to the exact composition. While stoichiometric CuMnAs has orthorhombic structure and it orders antiferromagnetically below 350–400 K, already less than 10% of the Mn deficiency turns the material to tetragonal phase with similar lattice parameters to thin films and higher Neél temperature than in the orthorhombic case. On the other hand, Mn excess leads to orthorhombic structures with the unit cell doubled along the $a$-direction (compared to the stoichiometric CuMnAs); this structure was previously reported for CuMnAs2 and Cu2Mn2As3 compounds5. We will present studies of the central part of the Cu-Mn-As ternary system.

2 K. Olejník et al, Nature Communications 8 15434 (2017)
4 P. Wadley et al., Nature Communications 4 2322 (2013)

Mo-PO6

Functionalization of siloxane derivatives by attaching polar groups

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Methyl-substituted disiloxanes as well as oligomeric siloxanes with their intrinsic characteristics (high flexibility and hydrophobicity conferred by Si-O bond particularity and presence of methyl groups attached to silicon atoms, respectively) are effective platforms for modification of the active sites to obtain compounds with unusual properties. Both linear and cyclic siloxane derivatives were used as substrates for attaching polar moieties (i.e., triazole or carboxylic groups) on the silicon atom resulting a series of original compounds with added value, two examples being showed in Figure 1.

Figure 1. Tetramethyldisiloxane end-functionalized with triazole cycles (a) and hexamethycyclotrisiloxane functionalized with carboxyl groups (b), both functions being attached to the siloxane substrate by thioether bridge

In all cases, proper mercapto-derivatives were used as polar group providers and either alkylation or thiol-ene addition as chemical routes. The reaction conditions are established for each pair of reactants. The obtained products were structurally characterized by spectral (IR and NMR) an elemental analysis and X-ray single crystal diffraction, where appropriate. Properties of the compounds were investigated, some of them showing good biological activity, metal complexing ability and ionic conductivity, in the last cases the compounds being of interest as liquid electrolyte for Li batteries.

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Mo-PO7

Cs-corrected STEM Observation for Al-Rh-Cu Decagonal Quasicrystal

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On the basis of Cs-corrected high-angle annular detector dark-field (HAADF)- and annular bright-field (ABF)-scanning transmission electron microscopy (STEM) observation, the structure of an Al-Rh-Cu decagonal quasicrystal (DQC) formed with two quasiperiodic planes along the periodic axis in an annealed Al$_x$Rh$_{14.5}$Cu$_{18.5}$ alloy has been investigated. Heavy atoms of Rh, and mixed sites (MSs) of Al and Cu atoms projected along the periodic axis can be clearly recognized as separate bright dots in HAADF-STEM images, and consequently arrangements of Rh atoms and MSs on the two quasiperiodic planes can be directly determined from those of bright dots in HAADF-STEM images. The Rh atoms are arranged in pentagonal tiling formed with pentagonal and star-shaped pentagonal tiles with an edge-length of 0.76 nm, and also MSs with a pentagonal arrangement are located in the pentagonal tiles with definite orientations. The star-shaped pentagonal tiles in the pentagonal tiling are arranged in $\tau^3$ (golden ratio)-inflated pentagonal tiling with a bond-length of 2 nm. From arrangements of Rh atoms located in pentagonal tilings with a bond-length of 2 nm, which are generated by the projection of a hyper-cubic lattice in a five-dimensional superspace, occupation domains in the perpendicular space are derived. Al atoms as well as Rh atoms and MSs are represented as dark dots in ABF-STEM images. The present model of the Al–Rh–Cu DQC is basically different from the structure proposed by single crystal X-ray diffraction in respect of the presence of the 0.76 nm pentagonal tiling of Rh atoms and MSs of Al and Cu atoms.

Mo-PO8

The crystal structure of two novel cage-like aluminides *

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Two novel intermetallic compounds from Al-rich region of the Ce-Rh-Al phase diagram were synthesized using arc-melting technique. The crystal structure of Ce$_2$Rh$_3$Al$_{20}$ was analyzed by means of powder X-ray diffraction and Rietveld analysis. In the case of Ce$_2$Rh$_7$Al$_{28}$, structure determination was performed using single-crystal X-ray diffraction data. Single crystals were selected from crashed polycrystalline ingots. The compound Ce$_2$Rh$_7$Al$_{28}$ of the new structure type crystallizes in orthorhombic space group (SG) Cmcm, Pearson symbol cC156 with a=9.1570(4), b=31.3790(14), c=8.9414 (17) Å, V=2569.2(17) Å$^3$. Intermetallics Ce$_2$Rh$_7$Al$_{14}$ has a tetragonal structure closely related to Ce$_2$Ru$_3$Al$_{15}$, SG I4$_1$/amd, Pearson symbol hH36, a=9.0000(15), c=31.7640(11) Å, V=2572.9(6) Å$^3$. Three cerium atoms (4c site) in Ce$_2$Rh$_7$Al$_{20}$ and two cerium atom (8e site) in Ce$_2$Rh$_7$Al$_{14}$ are coordinated by 18 and 20 Rh and Al atoms, forming the 3D- frameworks of large icosahedral voids. This feature resembles the high coordinated Ce environment seen in CeRh$_2$Al$_{15.7}$ and CeRh$_2$Al$_{10}$. With the exception of the disordered Ce1 in Ce$_2$Rh$_7$Al$_{28}$, the closest Ce-Ce contacts in both compounds are about 4.5 Å.

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Mo-PO9

Novel ternary gallides of the structural family Ce\(_{2+n}\)Rh\(_{3+3n}\)Ga\(_{1+2n}\)(n=0\(\div\)6)*

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The direct alloying of cerium, rhodium, and gallium results in the formation of intermetallic compounds with sequence of related structures, forming a new homologous series. Structures of 9 ternary intermetallic compounds of Ce-Rh-Ga system containing 50 at.% of rhodium were determined from single-crystal X-ray diffraction data. The compounds are built up of columns of alternating combination of the fragments of CeRh\(_5\)Ga with Mg\(_2\)Cu\(_3\)Si structure (MgZn\(_2\)-type) or Mg\(_2\)Ni\(_3\)Si (MgCu\(_2\)-type) and fragments of CeRh\(_5\)Ga with CeCo\(_5\)B\(_2\) structure (CaCu\(_5\)-type), forming the homologous series R\(_{2+2n}\)T\(_{3+3n}\)M\(_{1+2n}\) (n=0\(\div\)6). They can be grouped in two different structural series: trigonal (R-3m) and hexagonal (P6\(/mmc\)) group, depending on Laves-type fragment.

<table>
<thead>
<tr>
<th>n</th>
<th>Ce(<em>{2+n})Rh(</em>{3+3n})Ga(_{1+2n})</th>
<th>R-3m</th>
<th>Z=3</th>
<th>a=5.614(2)</th>
<th>c=11.932(5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n=0</td>
<td>Ce(_2)Rh(_5)Ga</td>
<td>P6(/mnc)</td>
<td>6</td>
<td>a=5.556(3)</td>
<td>c=15.680(8)</td>
</tr>
<tr>
<td>n=2</td>
<td>Ce(_2)Rh(_5)Ga(_3)</td>
<td>R-3m</td>
<td>3</td>
<td>a=5.554(3)</td>
<td>c=34.98(2)</td>
</tr>
<tr>
<td>n=3</td>
<td>trig-Ce(_2)Rh(_5)Ga(_3)</td>
<td>R-3m</td>
<td>3</td>
<td>a=5.563(4)</td>
<td>c=46.36(6)</td>
</tr>
<tr>
<td>n=4</td>
<td>hex-Ce(_2)Rh(_5)Ga(_3)</td>
<td>P6(/mcc)</td>
<td>2</td>
<td>a=5.597(3)</td>
<td>c=31.40(3)</td>
</tr>
<tr>
<td>n=5</td>
<td>trig-Ce(_2)Rh(_5)Ga(_3)</td>
<td>R-3m</td>
<td>3</td>
<td>a=5.574(8)</td>
<td>c=57.82(2)</td>
</tr>
<tr>
<td>n=6</td>
<td>hex-Ce(_2)Rh(_5)Ga(_3)</td>
<td>P6(/mcc)</td>
<td>6</td>
<td>a=5.592(12)</td>
<td>c=38.116(10)</td>
</tr>
</tbody>
</table>

* The work was performed under support of Ministry of Education and Science of Russia, Contract N16.552.11.7081 and RFBR (research Grant No. 15-03-04434).

Mo-PO10

Novel ternary aluminide Ce\(_4\)Ru\(_3\)Al\(_2\) *

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The crystal structure of a novel ternary intermetallic aluminide Ce\(_4\)Ru\(_3\)Al\(_2\) was determined from the synchrotron X-ray powder diffraction data collected on an almost single-phase alloy. The compound crystallizes with an orthorhombic crystalline structure of new type: space group Pnma, lattice parameters \(a=22.0592(5)\) Å, \(b=4.62213(6)\) Å, \(c=7.54309(8)\) Å, \(Z=4\). It can be presented as packing of coupled trigonal prisms with Ru-atoms located inside the prisms and quadrilaterals Ru\(_2\)Al\(_2\) residing in between them. The new structure is closely related to those of the equiatomic germanides YbAl\(_4\)Ge and CaCu\(_5\) [1-2], which have similar atomic order with a total of nine crystallographic sites of the same multiplicity. However, while in the germanides, each type of atoms occupies three sites, in Ce\(_4\)Ru\(_3\)Al\(_2\), Ce atoms are distributed over four sites, Ru atoms occupy three sites, and Al atoms are located at two sites. A remarkable feature of Ce\(_4\)Ru\(_3\)Al\(_2\) is extremely small values of some Ce-Ru distances, ranging from 2.300(1) to 2.572(1) Å. Only one of the four inequivalent Ce atom exhibits a regular distance from its nearest neighbors, exceeding 3.235(1) Å. In concert with the structural characteristics, Ce\(_4\)Ru\(_3\)Al\(_2\) was established by means of low-temperature magnetic and electrical transport measurements to exhibit a coexistence of valence fluctuations and local moment magnetism, attributable to the Ce atom sublattices with anomalously short and normal Ce-Ru interatomic distances, respectively. Due to the ¼ fraction of Ce\(^{3+}\) ions with fairly stable 4f\(^{1}\) electronic configuration, Ce\(_4\)Ru\(_3\)Al\(_2\) orders antiferromagnetically at \(T_N=2\) K and shows Kondo behavior in its electrical resistivity. In this respect, the novel aluminide resembles the gallide Ce\(_2\)Rh\(_5\)Ga\(_3\) that also bears in its crystalgraphic unit cell Ce ions with diverse valence states [3].

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Poster
Mo-PO11

New ternary indides with 2D intergrowth CsCl- and AlB2-related slabs*

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New ternary indides of approximate RE,RuIn3 composition were obtained by arc-melting during investigation of interaction of rare earths with ruthenium and indium. Compounds were studied by powder and single crystal XRD, and EMPA. Earlier, Ce11RuIn9 of Nd11PdIn9-type was structurally characterized. Tm, Yb, and Lu do not form ternaries of such stoichiometry. La, Pr, Nd, Sm, Gd, Tb, Dy, Ho, and Er indides were found to crystallize with four new structure types. Crystallographic data of the first representatives are listed in the Table:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Sp. Gr.</th>
<th>Cell dimensions, Å</th>
<th>Prototype</th>
<th>R1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gd3Ru3In7</td>
<td>Pmma</td>
<td>28.869(12), 3.7660(12), 8.030(3)</td>
<td>Y5Cu3Mg8</td>
<td>5.38</td>
</tr>
<tr>
<td>Tb3RuIn3</td>
<td>PbAm</td>
<td>11.338(7), 16.262(9), 3.645(2)</td>
<td>-</td>
<td>3.46</td>
</tr>
<tr>
<td>Ho3Ru3In4</td>
<td>P2/nm</td>
<td>12.926(7), 3.5688(2), 18.9908(9), β=105.58(3)</td>
<td>-</td>
<td>5.52</td>
</tr>
<tr>
<td>Sm3Ru3In3</td>
<td>Pbam</td>
<td>31.451(3), 37.221(2), 3.7268(3)</td>
<td>Nd8Ir0.98In16.02</td>
<td>4.94</td>
</tr>
</tbody>
</table>

The structures are built of two types of layers stacking along the shortest axis and represent new members of intergrowth structures of CsCl- and AlB2-related slabs.

* This work was supported by RFBR (project 18-03-00477).

Mo-PO12

Novel cerium germanide Ce2RuGe: synthesis, crystal structure, physical properties *

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Novel ternary intermetallic phase Ce2RuGe was synthesized via arc-melting of the constituents and subsequent annealing at 700 °C. Its crystal structure was determined from the powder X-ray diffraction data collected at room temperature. The compound crystallizes in the orthorhombic structure of a new type: space group P2221, lattice parameters: a = 4.38231(5) Å, b = 4.31823(5) Å, c = 9.91491(15) Å, Z = 2. In the fully ordered unit cell of Ce2RuGe, there are two crystallographic positions for Ce atoms, single site with Ru atoms, and single site with Ge atoms, each with the multiplicity of two. The crystal structure is built of infinite zigzag-like chains of the Ru and Ge atoms, propagating along the [010] direction. The essential feature is a very short interatomic distance between the Ce1 atoms and the Ru atoms being equal to 2.225(2) Å, while the Ce2-Ru distance is of regular length. This structural property gives rise to distinctive physical behavior of the compound that exhibits the coexistence of valence fluctuations associated with unstable 4f shell of the Ce1 ions and a long-range ferromagnetic order that emerges in the Ce2 ions sublattice below Tc = 8.5(3) K, as revealed by means of magnetization, heat capacity and electrical resistivity measurements, performed on a polycrystalline sample of Ce2RuGe in wide temperature and magnetic field strength ranges.

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Mo-PO13

**CaCu$_5$-type related structures in the Pr-Ni-Al system**

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During the investigation of the interaction of the components in the Pr-Ni-Al ternary system at 970K, the existence of two new ternary compounds PrNi$_{5.8}$Al$_x$ ($x=2.69$, 2.91) has been established. The crystal structure of both compounds has been investigated by single crystal method. Good quality single crystals of the PrNi$_{2.31}$Al$_{2.69}$ and PrNi$_{2.09}$Al$_{2.91}$ ternary compounds were isolated from the same alloy of total composition Pr : 2.22Ni : 2.78Al. Intensity data of PrNi$_{2.31}$Al$_{2.69}$ and PrNi$_{2.09}$Al$_{2.91}$ were collected at room temperature on a STOE StadiVari diffractometer equipped with a Mo-Kα micro focus source and a Pilatus 300K detector. The PrNi$_{2.31}$Al$_{2.69}$ compound crystallises in space group $P6/m$ (a = 14.045(2) Å, c = 4.0792 (8) Å; $R_1 = 0.0243$, $wR_2 = 0.0421$, 668 independent reflections), whereas the crystal structure of PrNi$_{2.09}$Al$_{2.91}$ compound was refined in space group $P6/mmm$ (a = 15.882(2) Å, c = 4.0933(8) Å, $R_1 = 0.0214$, $wR_2 = 0.0372$, 836 independent reflections). Both structures PrNi$_{5.8}$Al$_x$ ($x=2.69$, 2.91) are derived from the hexagonal CaCu$_5$-type, in which the binary PrNi$_5$ compound ($x=0$) crystallizes*. Interestingly, the known ternary PrNi$_2$Al$_3$ compound ($x=3$) is an ordered superstructure of CaCu$_5$-type*. Therefore, the partial substitution of nickel by aluminum atoms in PrNi$_{5.8}$Al$_x$ up to $x=2.69$ leads at first to the much disordered structure of PrNi$_{2.31}$Al$_{2.69}$ (Z=7), whereas further increasing of Al-content in PrNi$_{5.8}$Al$_x$ results in a gradual atomic ordering in the structures of PrNi$_{2.09}$Al$_{2.91}$ ($x=2.91$, Z=9) and PrNi$_2$Al$_3$ ($x=3$, Z=1).


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Mo-PO14

**The Family of the Pd$_5$TlAs Structure Type Compound: Synthesis, Crystal Structure, and DFT Calculations**

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The Pd$_5$TlAs structure type was first reported by El-Boragy et al. Pd$_5$TlAs is built from alternating layers of face-sharing thallium-centered palladium cuboctahedra and flat arsenic atom layers along the c axis. The paper by El-Boragy et al lists many palladium- and platinum-based compounds as crystallizing within this type. However, no information about these compounds, apart from the unit cell metrics often deduced from the multi-phase samples, has been given. Here we present the synthesis and investigations of a series of the palladium- and platinum-rich mixed phosphides and selenides belonging to the Pd$_5$TlAs structure type, including Pd$_3$InP, Pd$_3$InS, Pd$_3$ZnP, Pd$_3$ZnP, and Pd$_3$ZnSe. We have succeeded in obtaining either phase-pure samples, or samples with minimal amount of binary impurities, and for some of the compounds we even obtained single crystals. The structures were refined based on either powder or single-crystal data. The noticeable trend is that the compounds of the Pd$_5$TlAs type are more abundant for phosphorus and arsenic, while the chalcogen-containing ones are relatively rare and, in fact, are limited to a few selenium-containing ones. We also present a detailed crystallographic analysis of the structures in the series, most importantly, the distortions of cuboctahedra upon the formation of the compounds, as well as details of the electronic structure and bonding analysis based on the DFT calculations. The possibilities of the formation of the homologous series are also discussed, based on our search for the compounds of the Pd$_3$M$_3$Q- and Pd$_3$M$_3$Q-type (M=In, Zn; Q=P, As, Se) which can be considered a second homologue in the series after the Pd$_5$TlAs-type compounds.

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$^*$ This work was supported by RSF (Russian Science Foundation), grant No. 17-73-10492
Mo-PO15

Substitution effects on structure and magnetic properties of $\text{Cr}_3(\text{Ni}_{1-x}\text{Co}_x)\text{Si}_2$

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The intermetallic compounds with $\beta$-Mn structure type (or its derivatives) in systems $\text{Cr}-\text{Me}-\text{Si}$ was reported previously [1]. We continued this research because the symmetry of these structures makes it possible to search for magnetic skyrmions. The samples $\text{Cr}_3(\text{Ni}_{1-x}\text{Co}_x)\text{Si}_2$ was synthesized from a mixture of the elements by arc melting and subsequent annealing at 1100°C. The crystal structure was determined using powder X-ray diffraction technique ($\text{CuK}_\alpha$, radiation, Huber Image Plate Camera G670). The compound $\text{Cr}_3\text{NiSi}_2$ (space group $P2_13$, Pearson symbol $cP20$, $a = 6.1195\,\text{Å}$, $Z = 2$) crystallize with structure type $\text{AuAl}_2$ [2], that is an ordered substitution derivative of the $\beta$-Mn structure type. The crystal structure of $\text{Cr}_3\text{NiSi}_2$ can be understood as packing of icosahedrons formed by Ni or Cr and centered by Si atoms (Figure). In the samples with $x \neq 0$, the Ni/Co positions are partially occupied also by cobalt atoms. In the region of homogeneity, when nickel is replaced by cobalt, the unit cell parameter varies from 6.1195 to 6.1232 Å. Magnetic properties of these samples were studied at the temperature range 1.8–400 K and showed that all investigated compounds are paramagnetic. The observed change in the magnetic characteristics of a substance is a function of the isomorphous substitution of atoms.


Mo-PO16

Synthesis, structure and magnetic properties of $\text{DyCu}_5\text{Sn}$ and $\text{TmCu}_5\text{Sn}$

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The intermetallic compounds $\text{DyCu}_5\text{Sn}$ and $\text{TmCu}_5\text{Sn}$ were prepared by arc melting, annealed at 870 K and characterized by XRPD analysis and magnetic property measurements. The crystal structure $\text{DyCu}_5\text{Sn}$ was determined by using single-crystal X-ray diffraction technique (space group $Pnma$, Pearson symbol $cP28$, $a = 8.20527(8)\,\text{Å}$, $b = 4.96931(5)\,\text{Å}$, $c = 10.5722(1)\,\text{Å}$, $V = 431.08(2)\,\text{Å}^3$, $Z = 4$) and refined to $R_F = 0.032$ for 41 refined parameters and 1540 unique reflections. The compound crystallizes with $\text{CeCu}_5\text{Au}$ structure type [1] (ordered variant of $\text{CeCu}_6$-type [2]). The crystal structure $\text{TmCu}_5\text{Sn}$ is isotypic and was refined using the full-profile powder X-ray diffraction data ($a = 8.19834(8)\,\text{Å}$, $b = 4.96607(5)\,\text{Å}$, $c = 10.5607(1)\,\text{Å}$, $V = 429.96(2)\,\text{Å}^3$). Coordination numbers of atoms are 19 for Dy(Tm), 12-16 for Cu and 14 for Sn. The magnetic properties were studied in the temperature range 1.8–400 K and showed that in the paramagnetic state both studied compounds are Curie-Weiss paramagnets. $\text{DyCu}_5\text{Sn}$ orders antiferromagnetically at low temperatures and exhibit a metamagnetic transition. The stannide $\text{TmCu}_5\text{Sn}$ does not exhibit any magnetic ordering down to 1.8 K.

Mo-PO17

Crystal Structure of the Compound Sc$_{1.33}$Pd$_3$Al$_8$
with Layers of R Atoms and Al$_3$ Triangles

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The crystal structure of the new ternary aluminide Sc$_{1.33}$Pd$_3$Al$_8$ was refined by the Rietveld method from X-ray powder diffraction data (STOE Stadi P diffractometer, Cu $K\alpha_1$ radiation). It crystallizes with a Gd$_{1.33}$Pt$_3$Al$_8$-type structure: $hR51-14.00$, $R=3m$, $a = 4.29094(3)$, $c = 38.1599(4)$ Å, $R_p = 0.0465$, $R_B = 0.0411$. The main feature of the structure of Gd$_{1.33}$Pt$_3$Al$_8$ is a statistical distribution of Gd atoms and Al$_3$ triangles within atomic layers of composition Gd$_2$Al$_3$ (Gd$_{0.67}$Al within the unit cell). During the final cycles of the refinement, the occupancies of the corresponding sites were fixed at occ. = 0.67 for Sc in Wyckoff position 6c and occ. = 0.33 for Al in 18h. The unit cell of the compound of Sc$_{1.33}$Pd$_3$Al$_8$ contains six Sc$_{0.67}$Al layers, nine Pd and eighteen Al layers along the crystallographic direction [001]. The Sc atoms center 20-vertex polyhedra (hexagonal prisms of composition Al$_3$Pd$_6$ with three Sc and five additional Al atoms capping the eight faces). The coordination polyhedra around the Pd and Al atoms are icosahedra, or derivatives of these with one or two missing vertices. Together with the structures of Y$_2$Co$_5$Ga$_9$, Sc$_{0.67}$Fe$_2$Si$_5$, Er$_2$Pt$_6$Al$_{14}$, and ErNi$_3$Al$_9$, the structure of Gd$_{1.33}$Pt$_3$Al$_8$ forms a family of intergrowth structures built up of three kinds of monoatomic layer.

Mo-PO18

Crystal Structure of the DyNi$_4$Si Compound

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Some time ago$^\dag$ we reported the existence of the ~Dy$_{16}$Ni$_6$Si$_{22}$ compound with unknown structure. We present here the results of a single-crystal X-ray diffraction study performed on this compound. The alloy was prepared by arc-melting the components under argon in an arc furnace, and was annealed at 1070 K under vacuum for 1 month. Integrated intensities were measured with graphite-monochromatized Mo $K\alpha$ radiation on an Xcalibur Atlas CCD diffractometer. The crystal structure was refined by the full-matrix least-squares method on $F^2$ using SHELXL$^\ddag$. The present investigation led to the following data for the crystal structure and the refined composition DyNi$_{10.86(4)}$Si: Pearson symbol $hP40$, space group $P6_3/mmc$, $a = 8.1990$, $c = 8.6840(7)$ Å, $R = 0.0173$, $R_w = 0.0275$. The refined atomic coordinates and displacement parameters are the following: Dy 6$h$ 0.18975(2) 0.37950(4) 1/4 $U_{eq} = 0.01085(10)$ Å$^2$, Ni1 12$k$ 0.16285(4) 0.32570(8) 0.58575(6) $U_{eq} = 0.00958(13)$ Å$^2$, Ni2 6$h$ 0.56382(6) 0.12764(11) 1/4 $U_{eq} = 0.00834(17)$ Å$^2$, Ni3 4$f$ 1/3 2/3 0.99607(10) $U_{eq} = 0.0087(2)$ Å$^2$, Ni4 2$b$ 0 0 1/4 $U_{eq} = 0.0197(6)$ Å$^2$ occ. = 0.829(6), Ni5 2$a$ 0 0 0 $U_{eq} = 0.0152(11)$ Å$^2$ occ. = 0.428(6), Si 6$g$ 1/2 0 0 $U_{eq} = 0.0083(3)$ Å$^2$. The structure belongs to a large family of structures related to EuMg$_{5.2}$ with representatives among ternary aluminides, silicides, germanides, etc.


Mo-PO19

Crystal Structures and Electrical Properties of the Ternary Compounds DyGa₃₋ₓGeₓ (x = 0.08-0.48 and x = 0.68-0.80)

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The ternary compounds DyGa₂₋₂.₅₂Ge₀.₈₈₋₀.₄₈ and DyGa₃₋₂.₅₂Ge₀.₆₈₋₀.₈₀ with homogeneity ranges along the isoconcentrate 25 at.% Dy were found in the system Dy–Ga–Ge at 600°C. Their crystal structures were refined by the Rietveld method, on X-ray powder diffraction patterns collected at room temperature on a diffractometer STOE Stadi P (Cu Ka₁-radiation), using the program package FullProf Suite. The crystal structure of the compound DyGa₂₋₂.₅₂Ge₀.₈₈₋₀.₄₈ belongs to the structure type Mg₃In (Pearson symbol hR48, space group R-3m, a = 6.1707(3)-6.22374(10), c = 27.7297(15)-28.1185(5) Å), the structure of the compound DyGa₃₋₂.₅₂Ge₀.₆₈₋₀.₈₀ to the type PuAl₃ (hP24, P6₃/mmc, a = 6.0970(3)-6.1091(6), c = 14.3153(8)-14.3528(14) Å). Gradual substitution of Ge atoms for Ga atoms in DyGa₃₋ₓGeₓ at 600°C leads to the formation of three structure types: Ta(Rh₃₃Pd₀.₆₇)₃ (binary compound DyGa₃), Mg₃In (ternary compound DyGa₂₋₂.₅₂Ge₀.₈₈₋₀.₄₈), and PuAl₃ (ternary compound DyGa₃₋₂.₅₂Ge₀.₆₈₋₀.₈₀), which all three belong to the family of close-packed structures. The increase of the Ge content in the phases of the system DyGa₃₋ₓGeₓ leads to a decrease of the hexagonality of the structure.

The temperature dependences of the electrical resistivity and the differential thermoelectric power were studied by the potentiometric method in the temperature range 80-380 K on single-phase alloys of composition Dy₂₋₂.₅₆Geₓ (DyGa₂₋₀.₈₈Ge₀.₃₂, a = 6.19987(3), c = 27.9435(7) Å) and Dy₃₋₂.₅₆Ge₁₋ₓ (DyGa₃₋₀.₆₈Ge₀.₃₂, a = 6.0970(3), c = 14.3153(8) Å). The gradual increase of the electrical resistivity with increasing temperature, and the small negative values of the differential thermoelectric power (S = -2 - -4.2 µV/K) indicate metallic type of conductivity.

Mo-PO20

Structural Evolution in the Systems TAl₃₋ₓGeₓ (T = Zr, Hf)

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The interaction of the components in the ternary systems [Zr, Hf]–Al–Ge has not been investigated previously and information on phase equilibria or crystal structures of ternary phases is absent in the literature. The aim of the present work was to study the structural evolution in the alloys ZrAlₓ₁Geₓ, and HfAlₓ₁Geₓ (x = 0-0.8) at 600°C when the Al atoms are progressively replaced by Ge atoms. The alloys were synthesized from the pure metals by arc melting under argon atmosphere, and annealed under vacuum at 600°C for 720 h. Phase analyses and refinements of the crystallographic parameters were performed using X-ray powder diffraction patterns collected on a diffractometer DRON-2.0M (Fe Kα-radiation). The crystal structures were refined by the Rietveld method using the program package FullProf Suite.

The crystal structures of the binary compounds ZrAl₃ and HfAl₃ at 600°C belong to the structure type ZrAl₃ (tI₆, I₄/mmm: a = 4.00930(11), c = 17.2718(7) Å for ZrAl₃; a = 3.9849(3), c = 17.1443(15) Å for HfAl₃). Substitution of Ge atoms for Al atoms in ZrAl₃ and HfAl₃ leads to the formation of the ternary compounds ZrAlₓ₂Ge₀.₅ and HfAlₓ₂Ge₀.₆, respectively, with limited homogeneity ranges. Their crystal structures belong to the tetragonal structure type TiAl₃ (tI₈, I₄/mmm: a = 3.92395(11), c = 9.0476(4) Å for ZrAlₓ₂Ge₀.₅; a = 3.9021(2), c = 8.9549(8) Å for HfAlₓ₂Ge₀.₆).

Similar TiAl₃-type ternary phases have been reported in the related systems [Ti, Zr, Hf]–Al–Si. The structure types ZrAl₃ and TiAl₃ are both built up from close-packed layers in c stacking. The coordination polyhedra of all the atoms in both structures are cuboctahedra.

Mo-PO21

New Quaternary Compounds \(R_3\text{MnAl}_3\text{Ge}_2\) (\(R = \text{Rare Earths}\))

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Nine new compounds \(R_3\text{MnAl}_3\text{Ge}_2\) (\(R = \text{Sm-Lu}\)) were synthesized by arc melting under an Ar atmosphere and annealed at 600°C for 1800 h. Their crystal structures were studied by X-ray powder diffraction (dифрактометр DRON-2.0M, Fe Kα radiation). All of the compounds crystallize in the hexagonal structure type \(Y_3\text{NiAl}_3\text{Ge}_2\): Pearson symbol \(hP9\), space group \(P-62m\). The cell parameters of the isotypic compounds \(R_3\text{MnAl}_3\text{Ge}_2\) decrease with decreasing radius of the rare-earth metal from Sm to Lu.

| Crystallographic parameters of \(R_3\text{MnAl}_3\text{Ge}_2\) compounds |
|-----------------|--------|----------|
| Compound        | \(a, \text{ Å}\) | \(c, \text{ Å}\) | \(V, \text{ Å}^3\) |
| \(Y_3\text{MnAl}_3\text{Ge}_2\) \(\dagger\) | 6.9780 | 4.2108 | 177.57 |
| \(\text{Sm-MnAl}_3\text{Ge}_2\) | 7.0501(6) | 4.2893(5) | 184.63(3) |
| \(\text{Gd-MnAl}_3\text{Ge}_2\) | 7.0162(6) | 4.2554(4) | 181.41(3) |
| \(\text{Tb-MnAl}_3\text{Ge}_2\) | 6.9749(7) | 4.2104(5) | 177.39(5) |
| \(\text{Dy-MnAl}_3\text{Ge}_2\) | 6.9514(6) | 4.2102(5) | 176.19(3) |
| \(\text{Ho-MnAl}_3\text{Ge}_2\) | 6.9347(9) | 4.1908(7) | 174.54(4) |
| \(\text{Er-MnAl}_3\text{Ge}_2\) | 6.9099(9) | 4.1739(7) | 172.59(4) |
| \(\text{Tm-MnAl}_3\text{Ge}_2\) | 6.8923(8) | 4.1587(6) | 171.09(4) |
| \(\text{Yb-MnAl}_3\text{Ge}_2\) | 6.8986(9) | 4.2228(8) | 174.04(6) |
| \(\text{Lu-MnAl}_3\text{Ge}_2\) | 6.8645(9) | 4.1309(8) | 168.57(7) |


Mo-PO22

Two novel polar intermetallics \(\text{Lu}_5\text{Pd}_4\text{Ge}_8\) and \(\text{Lu}_3\text{Pd}_4\text{Ge}_4\):
crystal structure and chemical bonding analysis

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The two novel \(\text{Lu}_5\text{Pd}_4\text{Ge}_8\) and \(\text{Lu}_3\text{Pd}_4\text{Ge}_4\) polar intermetallics were prepared by direct synthesis of pure constituents. Their crystal structure was determined by single crystal X-ray diffraction analysis: \(\text{Lu}_5\text{Pd}_4\text{Ge}_8\) is monoclinic, \(P2_1/m\), \(\text{mp}34\), \(a = 5.7406(3)\), \(b = 13.7087(7)\), \(c = 8.3423(4) \text{ Å}\), \(\beta = 107.8(1)\), \(Z = 2\); \(\text{Lu}_3\text{Pd}_4\text{Ge}_4\) is orthorhombic, \(\text{Immm}\), \(a22\), \(a = 4.1368(3)\), \(b = 6.9192(5)\), \(c = 13.8229(9) \text{ Å}\), \(Z = 2\). The \(\text{Lu}_5\text{Pd}_4\text{Ge}_8\) analyzed crystal is one more example of non-merohedral twinning among the rare earth containing germanides.

Focusing on all known Ge-rich compounds in the Lu–Pd–Ge system a regular trend of the complexity of the Ge covalent fragments, connected through Pd contacts, can be highlighted as a function of composition. An increase of the Ge content causes a reduction of its valence electron concentration which reflects in a higher number of Ge–Ge covalent interactions: isolated Ge atoms and dumbbells in \(\text{Lu}_5\text{Pd}_4\text{Ge}_8\) evolving to dumbbells and four membered \(cis\) Ge chains for \(\text{Lu}_3\text{Pd}_4\text{Ge}_4\) and to infinite zigzag chains and corrugated 3-bonded layers for the Ge-richest \(\text{Lu}_5\text{Pd}_4\text{Ge}_8\) phase. As derives from the electronegativity values difference of constituents and the absence of a gap at \(E\), is more appropriate to assign these compounds to the class of polar intermetallics rather than classical Zintl phases.

In this contribution, a deeper description of chemical bonding is discussed on the basis of DOS, pDOS and COHP curves analysis. The integrated COHP values permits to discern the strongest covalent interaction to be among Ge–Ge within the \(cis\) Ge4 chains and dumbbells followed by Ge–Pd, Ge–Lu and Lu–Pd contacts.
**Mo-PO48**

**Pd(Pt)-Cu-B systems: formation and crystal structure of new Th\(_7\)Fe\(_3\)-type related compounds.**

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A novel series of ternary metal borides of the Th\(_7\)Fe\(_3\) structural family was observed in the Pd(Pt)-Cu-B systems from as cast and annealed at 600 °C - 650 °C alloys. The \(h\)-(Pd\(_{0.73}\)Cu\(_{0.27}\))B\(_3\) (≡Pd\(_{0.02}\)Cu\(_{0.98}\)B\(_3\), space group \(P6_3cm\), \(a=12.9426(9)\)Å, \(c=4.8971(4)\)Å, single crystal XRD data) forms a unique structure type. Further substitution of Cu by Pd led to formation of a Mn\(_7\)C\(_3\)-type structure, \(o\)-(Pd\(_{0.93}\)Cu\(_{0.07}\))B\(_3\) (≡Pd\(_{0.46}\)Cu\(_{0.54}\)B\(_3\), space group \(Pnma\), \(a=4.8971(2)\)Å, \(b=7.5353(3)\)Å, \(c=12.9743(6)\)Å, single crystal XRD). Isotypic LT \(h\)-(Pd\(_{0.70}\)Cu\(_{0.30}\))B\(_3\) (≡Pt\(_{1.00}\)Cu\(_{2.00}\)B\(_3\)) was observed in the Pt-Cu-B system as a low temperature phase (\(T\leq600\) °C) (powder XRD), whereas the ThFe\(_3\)-type (HT \(h\)-(Pd\(_{0.73}\)Cu\(_{0.27}\))B\(_3\) ≡ Pt\(_{1.10}\)Cu\(_{1.90}\)B\(_3\), space group \(P6_3mc\), \(a=7.4671(1)\)Å, \(c=4.9039(1)\)Å, powder XRD) proved to be stable at high temperature. The three structures are built of columns of face connected metal octahedra and columns of metal tetrahedra alternatingly fused by common faces and vertices. Boron atoms are found in trigonal prisms formed by metal atoms. Phase relations in the Pd(Pt)-Cu-B systems at 650 °C (600 °C) within the relevant concentration fields will be discussed. Superconductivity was discovered for Pt\(_{1.9}\)Cu\(_{2.1}\)B\(_3\) (Pd\(_4\)Cu\(_5\)B\(_7\)-type) and Pt\(_{3.1}\)Cu\(_{1.9}\)B\(_3\) (Th\(_7\)Fe\(_3\)-type) below 0.67 and 0.66 K, respectively. Despite the close value of the transition temperature the values of the upper critical field at 0 K differ as 0.37 T and 0.27 T for the two compounds.

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**Mo-PO23**

**Sn-containing Tetrahedrites as Prospective Thermoelectric Materials**

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Currently, natural and synthetic tetrahedrites are widely investigated as compounds possessing effective thermoelectric properties. Among them are the most studied and prospective Cu\(_{12.5}\)T\(_3\)Sb\(_5\)S\(_3\) solid solutions, in which two Cu\(^{2+}\) ions partly or fully substituted of the other two-valence cations T = Mn\(^{2+}\), Co\(^{2+}\), Ni\(^{2+}\), Zn\(^{2+}\) or mixed-valence Fe\(^{2+}/3+\) cation. Recently Cu\(_{12.5}\)Sn\(_x\)Sb\(_5\)S\(_3\) and Cu\(_{12.5}\)Ge\(_x\)Sb\(_5\)S\(_3\) with apparently Sn\(^{4+}\) and Ge\(^{4+}\) cations were synthesized. In this paper, we have for the first time found the limit of substitution of Sn for Cu in Cu\(_{12.5}\)Sn\(_x\)Sb\(_5\)S\(_3\), determined Sn site in the tetrahedrite structure and its oxidation state using the combination of synchrotron x-ray powder diffraction and \(^{119}\)Sn Mössbauer spectroscopy. We have found that: (i) Cu\(_{12.5}\)Sn\(_x\)Sb\(_5\)S\(_3\) solid solution contains no more than 0.8 Sn atoms per formula unit, (ii) Sn occupies only tetrahedrally-coordinated Cu\((1)\) site and (iii) Sn is presented in the +4 oxidation state.

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Poster
Mo-PO24

Calorimetric investigation of hydrogen interaction with Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}

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We have investigated the hydrogen interaction with Ti\textsubscript{0.9}Zr\textsubscript{0.1}Mn\textsubscript{1.3}V\textsubscript{0.6} applying the calorimeter of Tean-Calvet type connected with a Sieverts-type apparatus. The sample Ti\textsubscript{0.9}Zr\textsubscript{0.1}Mn\textsubscript{1.3}V\textsubscript{0.6} and its hydride Ti\textsubscript{0.9}Zr\textsubscript{0.1}Mn\textsubscript{1.3}V\textsubscript{0.6}H\textsubscript{2} were checked by X-ray diffraction which indicated that the starting sample was single-phase material with the hexagonal Laves phase structure C14 (MgZn\textsubscript{2}) and hydride of Ti\textsubscript{0.9}Zr\textsubscript{0.1}Mn\textsubscript{1.3}V\textsubscript{0.6}H\textsubscript{2} was single phase material with the hexagonal Laves phase structure C14 (MgZn\textsubscript{2}) too. The calorimetric study was carried out in the temperature range 60 - 130°C and a hydrogen pressure up to 50 atm. Absorption (desorption) partial molar enthalpy $\Delta$H\textsubscript{abs.}(des.) was determined from the heat effect of the reaction:

$$P=f(C), \Delta H_{\text{abs.(des)}}=f(C) \text{ and } \Delta S_{\text{abs.(des)}}=f(C)$$

The calorimetric data obtained for the Ti\textsubscript{0.9}Zr\textsubscript{0.1}Mn\textsubscript{1.3}V\textsubscript{0.6} – H\textsubscript{2} system at 60°C are presented in the Table:

<table>
<thead>
<tr>
<th>H/IMC</th>
<th>$\Delta H_{\text{abs}}, \text{kJ/molH}_2$</th>
<th>H/IMC</th>
<th>$\Delta H_{\text{des}}, \text{kJ/molH}_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7-1.5</td>
<td>30.3±0.2</td>
<td>0.7-1.5</td>
<td>27.4±0.5</td>
</tr>
<tr>
<td>1.5-2.3</td>
<td>31.4±0.2</td>
<td>1.8-2.2</td>
<td>31.2±0.3</td>
</tr>
<tr>
<td>2.3-2.7</td>
<td>33.4±0.2</td>
<td>2.3-2.7</td>
<td>33.4±0.8</td>
</tr>
</tbody>
</table>

As one can see from presented results the values of enthalpy of hydrogen reaction of absorption and desorption from the hydride phase increased with the rise of C. We assume that hydrogenation of IMC at definite conditions (increased temperature and pressure) may cause rearrangement of crystal structure of initial IMC and formation of some new different interstitial sites which are more energetic efficient for hydrogen. It should be emphasized that Ti\textsubscript{0.9}Zr\textsubscript{0.1}Mn\textsubscript{1.3}V\textsubscript{0.6} has very good hydrogen capacity (C~3) and very small hysteresis of pressure these properties are very important for the use of this compound in the technology purposes.

Mo-PO25

Thermodynamic properties of the two-dimensional quantum magnet Cu(tn)Cl\textsubscript{2} $^*$

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Previous studies of polycrystalline Cu(m)Cl\textsubscript{2}, (m = C\textsubscript{3}H\textsubscript{10}N\textsubscript{2}) identified the compound as an excellent realization of a two-dimensional (2d) quantum magnet. While no phase transition to magnetic long-range order was observed down to 50 mK, the response of the material to the applied magnetic field mimics a field-induced Berezinskii-Kosterlitz-Thouless transition theoretically predicted for the Heisenberg antiferromagnet (HAF) on a square lattice\textsuperscript{1}. While such behavior indicates extreme weakness of interlayer magnetic correlations, the character of the 2d magnetic lattice is not known\textsuperscript{3}.

The present work is focused on the determination of intra-layer exchange interactions. For that purpose, specific heat, magnetic susceptibility and elastic properties of a single crystal were experimentally investigated nominally at temperatures from 0.3 to 300 K. Since the quantitative analysis of the magnetic specific heat is highly sensitive to the estimation of the phonon contribution, various approaches were applied for its determination as the use of the diamagnetic isomorph Zn(m)Cl\textsubscript{2} and elastic constants. The resulting magnetic contribution was analyzed within a model of the spin $\frac{1}{2}$ HAF on the spatially anisotropic square lattice with the nearest-neighbour coupling $J$ and $J^\prime$. The best agreement was obtained for $J^\prime/J = 0.3$ and $J/k_B = 4.4$ K. However, susceptibility data suggest the co-existence of ferro and antiferromagnetic interactions within the magnetic layer, namely $J^\prime/J = -0.5$ and $J/k_B = 4.4$ K. Additional steps including first-principles study are discussed.

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Mo-PO26

The isothermal section of the Co–Cu–Hf ternary system at 1073 K

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Isothermal section at 1073 K of the ternary of Co–Cu–Hf system was investigated in the whole concentration range by means of powder X-ray diffraction, scanning electron microscopy (energy dispersive X-ray spectroscopy) and differential thermal analysis. All measured compositions and crystal structure refinements were performed at room temperature for quenched samples annealed at 1073 K for four weeks. The solubility ranges of binary compounds into ternary system were determined. It was found that 10 three-phase equilibria regions form in Co–Cu–Hf ternary system. No ternary compound was found in this system. The solubility of Cu is significantly larger in B2 CoHf intermetallic compound (38.2 at.%) than in Co2Hf, CoHf2 or Co23Hf6 (15.4, 10.4 and 7 at.% respectively). The maximum Co solubility (about 30 at.%) is found in Cu51Hf4 compound, which is much higher than in CuHf2, Cu10Hf3 and Cu8Hf3 (6.5, 8.4 and 5 at.% respectively).

Mo-PO27

Structural Phase Stability in (Ce,La)Pd2Al2-xGax Compounds*

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At room temperature (Ce,La)Pd2Al2-xGax compounds crystallize in the CaBe2Ge2 type of structure (P4/nmm) which is one of the two most frequent structural types in the RT2X2 (R: rare earth, T: transition metal, X: p-block element) family of materials. Interest in these compounds is driven by their physical properties at low temperature. For example the Ce based compounds exhibit antiferromagnetic order (< 2.8 K). Also CePd2Al2 is one of the very few Ce compounds discussed in the relation of enhanced magnetoelastic interaction resulting in the formation of a bound state between 4f electrons and phonons. On the other hand nonconventional superconducting behavior is observed in La based compounds below 2.8 K. All (Ce,La)Pd2Al2-xGax compounds undergo structural phase transitions at low temperatures to the orthorhombic structure described within the space group Cmme.

We studied the concentration dependence of the transition temperature (Ttr) by using the low temperature X-ray powder diffraction. Although at low temperature all the parent compounds have the same structure from symmetry point of view, the characteristics of the phase transitions are considerably different. This is reflected by a suppression of the transition temperature which we find in both the Ce and La composition series. With respect to this suppression we find that Al-rich and Ga-rich compounds show distinct onsets of the orthorhombic distortions. The stability of Al and Ga based parent compounds will be compared with our results of density function theory calculations. We also studied this transition on single crystalline LaPd2Al2 which indicates the formation of orthorhombic domains below Ttr.

* The work was supported by The Czech Science Foundation under grant no 17-04925J

Poster
We calculated structural properties, enthalpies of formation of six Silver - rare earth binary compounds Ag$_x$-Re$_{1-x}$ (Re=Gd, Sm) at (x=0.21, 0.33 and 0.5) using first principles calculations based on density functional theory (DFT). A set of self-consistent thermodynamic parameters formulating the Gibbs energy of various phases in the Ag-Re binary system were then obtained. A much better agreement was achieved between the calculated results and the reported experimental data.

Imporatn remarques about commun behavor of two systems and dependance of melting temperature as composition are observed.
Mo-PO30

Interaction of the Components in the \{Ce, Gd\}-{Ti, Zr}-Sb Systems

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The phase equilibria in the \{Ce, Gd\}-{Ti, Zr}-Sb systems were investigated at 600°C. The results show that the interaction of the components is more complicated in the systems with Zr than with those with Ti. The formation of two compounds (Ce\(_2\)Ti\(_7\)Sb\(_{12}\) and Ce\(_5\)TiSb\(_3\)) in the Ce-Ti-Sb system, and of one compound (Gd\(_2\)Ti\(_{11}\)Sb\(_{14}\)) in the Gd-Ti-Sb system, was confirmed; no additional ternaries were found. The crystal structures of Ce\(_2\)Ti\(_7\)Sb\(_{12}\) and Gd\(_2\)Ti\(_{11}\)Sb\(_{14}\) were refined from X-ray powder diffraction data \(^1\). In the Ce-Zr-Sb system, the formation of the Ce\(_2\)ZrSb\(_3\) compound was confirmed, and three new compounds were found in the ternary region: Ce\(_{0.08}\)Zr\(_{1.92}\)Sb\(_5\), ~CeZrSb\(_4\), and ~Ce\(_2\)Zr\(_2\)Sb\(_3\). In the Gd-Zr-Sb system the existence of a large homogeneity range was established for the GdZrSb compound along the isoconcentrate 33.3 at.\% Sb: Gd\(_{0.8}\)Zr\(_{1.4}\)Sb, and a new compound of approximate composition ~Gd\(_{0.8}\)Zr\(_{1.4}\)Sb was discovered. The crystal structure of Ce\(_{0.08}\)Zr\(_{1.92}\)Sb and the boundary compositions of the Gd\(_{1-}\)Zr\(_{1+}\)Sb phase (\(x = 0-0.905(18)\)) were refined from X-ray powder diffraction data. The higher complexity of the systems with zirconium is related to the higher number of ternaries formed. In both the Ce-Zr-Sb and Gd-Zr-Sb systems the formation of ternary compounds with high antimony content was observed, unlike in the systems with titanium. From the results of EDX analyses it was found that the solid solubility of the third component in the binary compounds is higher in the systems with zirconium than in the corresponding systems with titanium. For example, the GdSb compound according to our data dissolves about 5 at.% Ti and about 25.7 at.% Zr. We believe that this is due to the fact that the atomic radius of Zr is larger than that of Ti, i.e. closer to the radius of the rare-earth metal, which makes the isomorphic replacement in the structure easier.

\(^1\) O. Senchuk, Ya. Tokaychuk, R. Serkiz, P. Demchenko , R. Gladyshevskii, Phase equilibria in the Ce-Ti-Sb and Gd-Ti-Sb ternary systems at 600°C and the crystal structures of the Ce\(_2\)Ti\(_7\)Sb\(_{12}\) and Gd\(_2\)Ti\(_{11}\)Sb\(_{14}\) compounds, Chem. Met. Alloys 10(2) (2017) 76-92.

Mo-PO31

Phenomenological Mean-Field Theory and Scaling Analysis for Metamagnetism in Ce-Based Heavy Fermion Compounds

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Although a characteristic feature of heavy fermion compounds is the large Sommerfeld parameter of the specific heat, the metamagnetism which is observed in some heavy fermion compounds is also the intriguing phenomena. When the external magnetic field is increased, the magnetization suddenly raises at a metamagnetic field \(H_m\). To understand this phenomena, we explore the phenomenological mean-field theory which is independent of any microscopic mechanism. We write free energy as:

\[
\mathcal{F}(\tau) = \frac{1}{2} \text{Tr} \left( m \mathbf{m} + \mu_0 (m_\downarrow^2 + m_\uparrow^2) - (\tau / T_m) S_{\text{BW}} - k (m_\downarrow^2 - m_\uparrow^2) \right) + c_1 m_\downarrow^2 + c_2 m_\uparrow m_\downarrow m_\uparrow \left( m_\downarrow - m_\uparrow \right),
\]

where \(m_\downarrow, m_\uparrow\) are the sub-lattice magnetizations, \(h\) is the normalized external field, \(a_1, \ldots, c_2\) are parameters, and \(S_{\text{BW}}\) is the Bragg-Williams entropy which is not like Landau. \(^1\) By minimizing this free energy, we can obtain the sub-lattice magnetizations and the sub-lattice susceptibilities in thermal equilibrium. To reduce these results to the experimental data under the constant pressure condition, we use the scaling hypothesis

\[
M(\tau, V) = \frac{\mathcal{M}(\mathcal{H}, V)}{\mathcal{B}(\mathcal{H}, V)},
\]

where \(M(H, V)\), \(h(V)\) are the magnetization and the scaling field with the sample volume \(V\), respectively. \(^2\) Finally, we can explain the experimental data qualitatively. We also obtain the magnetic phase diagram which resembles the observations. In these analyses of CeRu\(_2\)S\(_2\)\(_3\), we use the experimental data of the compressibility, the molar volume, the magnetic Grüneisen parameter, and the maximum susceptibility values \(\chi(T_m=100K;0T)\) and \(\chi(T_m=10K;7.7T)\).


Mo-PO32

Phase transitions in ferromagnetic superconductors for example UGe$_2$
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Ural Federal University, Ekaterinburg, Russia, 2017

Phase transitions in the ferromagnetic superconductor UGe$_2$ were investigated in the pressure range from 0.3 GPa to 1.7 GPa within the framework of the Anderson periodic model extended by taking into account the pf-hooping. The electronic structure was simulated as a function of pressure (P), magnetization (M) on the basis of data on the pressure dependence of the effective masses. The spin-fluctuation mechanism of the singlet and triplet pairing was considered. It was shown that the strong ferromagnetic state realized near the superconducting temperature loses thermodynamic stability under electron-pairing conditions for f-like electrons. As a result, the phase transitions observed at low temperatures are a crossover of a first-order magnetic transition and a superconducting transition of the second order. With increasing temperature, the effect of the double exchange interaction is changed, which, in the accordance with the exp, leads to the appearance of a weak ferromagnetic state. It is found that the transition from the ferromagnetic phase to the phase of the ferromagnetic superconductor is accompanied by a jump of the zero-point fluctuations. In the phase diagram, the disappearance of the ferromagnetic superconductivity corresponds to a first-order phase transition. The developed representations are applicable to a group of ferromagnetic superconductors, in which the superconducting temperature (Tsc) is much lower than the Curie temperature (Tc).

Mo-PO33

Magnetic phase transition in MnSi based on the first principle calculations of electronic structure and spin fluctuation theory*

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The chiral ferromagnetic helicoid MnSi is a prototype of skyrmion materials for spintronic. The causes of spin structure are antisymmetric relativistic Dzyaloshinskii – Moriya interaction effects of intra-atomic and interstitial Coulomb correlations. However, the first principle LDA+U+SO calculations of the electronic structure of MnSi’s ground ferromagnetic state give some equal, in terms of magnetic state stability, solutions with different values of Coulomb interaction. In this case, the values of the magnetic moments of the ground state differ markedly from experimental observations. In connection with this, we develop a phenomenological spin fluctuation theory, in which along with local magnetization (obtained from the LDA calculations), we introduce mean square spin correlators, which correspond to zero and thermal spin fluctuations.

The expressions obtained for the magnetic susceptibility, in accordance with the results of calculations of the electronic structure, show lambda-like anomalies near the Neel temperature. At the same time, numerical analysis of possible methods of electronic structure description results to a conclusion that the magnetic transition is a crossover of first-order thermodynamic phase transition and quantum transition, accompanied by an abrupt disappearance of zero-spin fluctuations. The best quantitative agreement with experimental results is realized with the parameter of the intra-atomic Coulomb interaction U=6.8eV.

It is shown that a skyrmion phase with huge ferromagnetic spin correlations and chiral fluctuations is realized in narrow temperature intervals. However, the experimental data do not provide quantitative information on the field of existence of the chiral fluctuations.

*The results were obtained within the framework of the assignment of the Ministry of Education and Science of the Russian Federation, the contract 3.9521.2017/8.9
Mo-PO34

The features of yttrium dodecaboride single crystal thermionic properties
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Rare earth (RE) hexaborides, first of all, lanthanum hexaboride and composite materials based on it, are widely used in vacuum electronics as high-efficient cathode materials. There are known individual publications on thermionic properties of RE borides of other structure types: di-, tetra-, dodecaborides. In the present work thermionic properties of yttrium dodecaboride (YB12) single crystals are studied.

The YB12 single crystals were grown by crucible free inductive zone melting.*

YB12 thermionic current density was measured on primary heating in the temperature range from 1218 to 1978 K at p < 10⁻⁴ Pa. Only an effective electron work function φ is presented because of anomalous Schottky effect. Up to 1687 K temperature dependence of the YB12 electron work function is described by a linear function of the temperature φ(T) = −0.04297 + 22.6×10⁻⁴ T. At T > 1687 K deviation of the φ(T) from linearity towards lower values took place. Subsequent annealing of the YB12 samples during 6 h at 1978 K resulted in the thermionic current density increase as compared with initial YB12 at all temperatures. At present it is known that for RE dodecaborides (except TmB12) undergo phase transformation MeB12 → MeB4 in surface layer on its annealing in a vacuum p < 10⁻⁴ Pa that is due to the boron evaporation from dislocation outcrops. At p ≥ 10⁻² Pa phase transformation is intensified due to the surface bombardment by ions of the residual gases and evaporated boron ions. In the YB12 case the similar processes also result in formation of new phase depleted by boron and more emissive as compared with YB12. The new phase is yttrium hexaboride (YB6) that is the nearest one to the YB12 from the side with less content of boron unlike from other RE dodecaborides which don’t form hexaboride phase.

Mo-PO35

Spatio-temporal investigations on the interface propagation in a spin-crossover crystal observed by Optical Microscopy
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We study the spatio-temporal formation and spreading of the low-spin state (LS) during the thermal spin transition and the cooperative relaxation of the photo-induced metastable high spin (HS) state at low temperature, in the presence of a structural defect. The model is made of a two dimension rectangular-shaped lattice with discrete spins coupled by springs. The investigations are performed for a perfect lattice and a lattice with a hole (simulating the defect) with a fixed size. We found that the presence of the defect affects the thermal equilibrium by reducing the size of the thermal hysteresis at the transition. However, the transition temperature remains unchanged. The study of the low-temperature relaxation of the lattice from HS to LS state indicated the existence of three different regimes of the growth process: (i) a first regime of growth from one corner of the rectangle along the width, then followed by (ii) a second regime of longitudinal propagation at almost constant velocity and (ii) a third rapid regime (iii) when the system feels the surface or the border of the crystal. When a hole is injected inside the lattice, it results (i) in a deformation of the HS/LS interface when it approaches the defect position, and (ii) the slowing down of the relaxation process which is hindered by the presence of the defect. These results are in good agreement with available experimental data.


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Poster
Frustrated magnetism in the Eu-based intermetallic system EuIr$_2$P$_2$

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The compounds of the A$_2$Cu$_{24}$O$_{41}$-CuO$_2$ homologous series (so-called spin-ladder compounds), where A are alkaline-earth metals, the most famous among which is the Sr$_8$Ca$_6$Cu$_{24}$O$_{41}$ phase, are attractive objects for investigation as their structures are related to those of the high-$T_c$ superconductors. The aim of this work was the phase and structural analysis of samples of nominal composition A$_{14}$M$_2$O$_{41}$ with partial substitution on the alkaline-earth metal sites and on the Cu sites. The synthesis was carried out by solid state reaction at 920°C.

The crystal structure of the Sr$_8$Ca$_6$Cu$_{24}$O$_{41}$ compound can be described as a stacking of CuO$_2$, Sr/Ca, and CuO$_2$ layers along the [010] direction of space group Cccm. We made an attempt to replace the Ca$^{2+}$ ions ($r = 1.03$ Å) in the structure of this compound by smaller Eu$^{3+}$ ions ($r = 1.14$ Å) with the aim to decrease the interlayer spacing, which may favor the charge transfer for superconductivity. The study of the Sr$_8$Ca$_{4-x}$Eu$_x$Cu$_{24}$O$_{41}$ ($x = 1$–4) samples showed the following results: all the samples contained as main phase the (Sr,Ca)$_{14}$Cu$_2$O$_{41}$ (Cccm) phase, and as additional phases Eu$_2$CuO$_4$ (I4/mmm) and CuO (C2/c), the quantities of which grew with increasing Eu-content. The value of the cell parameter $b$ of the spin-ladder phase, which is most sensitive to substitutions, increased in comparison with that of the initial phase, as a result of the inclusion of the Eu atoms in the Eu$_2$CuO$_4$ phase and the change of the Sr/Ca ratio in the sample. The investigation of Sr$_8$Ca$_{6-x}$Mn$_x$O$_{41}$ ($x = 1$–4) samples indicated the formation of (Sr,Ca)$_{14}$Cu$_2$O$_{41}$ as the main phase and of additional Sr$_8$Mn$_2$CuO$_9$ ($P321$) and CuO (C2/c). In the case of analogous substitution by Zn atoms, all the samples contained, besides the main spin-ladder phase with constant cell parameters, the secondary phase ZnO ($P6_3mc$).

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Frustrated magnetism in the Eu-based intermetallic system EuIr$_2$P$_2$

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Frustration in magnetic systems is a topic of strong current interest, since it can result in very unusual ground states with intriguing properties, as e.g. spin liquids, spin ice, or magnetic monopole-like excitations. The vast majority of studies on frustration in magnetic systems have been performed on insulating spin systems, while frustrated metallic systems remain largely unexplored. Interesting effects may be expected for the later case from the interplay between itinerant electrons and frustrated magnetic degrees of freedom. We have recently synthesized the small-gap semiconductor EuIr$_2$P$_2$ and studied its magnetic properties. EuIr$_2$P$_2$ crystallizes in a trigonal, chiral structure P3$_2$21 which might lead to unconventional magnetism. The results of our bulk measurements have indeed revealed unusual magnetic states and magnetic transitions, as well as evidence for important frustration effects.

EuIr$_2$P$_2$ was in an early work proposed to order ferromagnetically based on the positive Curie-Weiss temperature, $\Theta_{CW}$, estimated from the high-temperature susceptibility (C. Lux, et al., J. Alloys and Comp. 200 (1993) 135-139). However, our recent measurements conclusively show that it orders antiferromagnetically at $T_{N1} = 5$ K, in spite of the positive $\Theta_{CW}$. Besides there is a second magnetic transition at $T_{N2} = 3$ K. The size of the specific heat anomaly at $T_{N1}$ is small compared to other S=7/2 Eu$^{2+}$ or Gd$^{3+}$ systems. Furthermore we observe a large tail in the specific heat above $T_{N1}$ indicative of strong magnetic fluctuations. These effects point to a magnetic structure with a significant degree of frustration due to different competing magnetic interactions.
Mo-PO38

**Revisiting Fe₆Ge₅: Overlooked Bridge between Two Sides of the Fe-Ge System**

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The Fe-Ge system is one of the richest binary intermetallic system in terms of the number of intermediate compounds and variety of crystal structures. It is possible to identify similar structural motifs in them, and the compounds themselves exhibit a wide spectrum of physical properties. Despite the large number of works devoted to the study of compounds in this system, a little to nothing is known about Fe₆Ge₅. The literature presents only the determination of its crystal structure ¹ performed with low accuracy.

We have reexamined the crystal structure of Fe₆Ge₅ and studied its magnetic behavior in the temperature range 2–400K on single crystals obtained by gas-phase chemical transport. The investigation of the temperature dependence of magnetic susceptibility and heat capacity of a Fe₆Ge₅ single crystal showed the presence of two antiferromagnetic-type phase transitions at 110 K and 330 K. Synthesis of Fe₆Ge₅, comparison of its crystal structure and physical properties with other compounds in the Fe-Ge system as well as a discussion of the reasons underlying such magnetic behavior of the compound will be presented in the poster.

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Mo-PO39

**The Competing Hyperfine Interactions in (Tb₁₋ₓYₓ)₀.₈Sm₀.₂Fe₂ Intermetallic Compounds**

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Rare-earth magnetic magnetic materials now are in demand for applications including permanent magnets, magnetocaloric and magnetostrictive materials. It is known that the structure and important magnetic properties of TbFe₂ may be modulated as by type of substituting rare-earth, their combination and mutual influence, concentration and resulting hyperfine interactions that can get the opportunity to obtain compounds with desired enhanced possibilities. The main idea of the work was to study the competition of different types of exchange interactions in rare-earth sublattices.

In our work, polycrystalline samples of (Tb₁₋ₓYₓ)₀.₈Sm₀.₂Fe₂ (x(Y)=0, 0.2, 0.4, 0.6, 0.8, 1.0) system have been alloyed at normal pressure in argon atmosphere. To reveal peculiarities of the structural and magnetic state of the samples we performed X-ray diffraction and Mössbauer spectroscopy study. The dependencies of structure parameters on the concentration have been determined. The detailed analysis of hyperfine Mossbauer spectra parameters distributions and their mutual correlations have been performed. The isotropic and anisotropic parts of magnetic hyperfine interactions have been resolved. The composition dependence of the subspectra hyperfine parameters and its correlations with spin reorientation behavior is discussed considering the competing influences of the anisotropy of the rare-earth sublattice and that of the exchange interactions.
Mo-PO40

**Novel cerium germanides Ce$_2$IrGe$_3$ and CeIrGe$_2$**

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The novel cerium ternaries, Ce$_2$IrGe$_3$ and CeIrGe$_2$, were studied by means of x-ray diffraction, magnetization, specific heat and electrical resistivity measurements, performed in wide ranges of temperature and external magnetic fields. Ce$_2$IrGe$_3$ was found to crystallize with slightly disordered hexagonal structure of the Ce$_2$CoSi$_3$ type, which is a derivative of the AlB$_2$ prototype. In turn, CeIrGe$_2$ was established to adopt the orthorhombic CeNiSi$_2$ type unit cell, which can be described as packing of two kinds of slabs, corresponding to the AlB$_2$ type and one half of the BaAl$_2$ type blocks. While CeIrGe$_2$ was characterized as a Kondo lattice that orders antiferromagnetically at $T_N = 4$ K, Ce$_2$IrGe$_3$ was found to exhibit a ferromagnetic-like ordering below $T_C = 4$ K, accompanied with several features typical for metallic spin glasses. Based on the thermodynamic and electrical transport data, the latter germanide was also described as a strongly correlated electron system.

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Mo-PO41

**The Solid Solution Series LuCo$_{1-x}$Ni$_x$C$_2$: Crystal Structure and Electronic Properties**

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A series of polycrystalline solid solutions LuCo$_{1-x}$Ni$_x$C$_2$ ($x = 0.0, 0.33, 0.5, 0.67, 1.0$) were investigated by means of x-ray diffraction and specific heat measurements as well as ab-initio electronic structure studies. The crystal structures of all investigated samples refer to the CeNiC$_2$-type structure * (space group $Amm\bar{2}$ and Pearson symbol oS8). The non-isoelectronic substitution of Co by Ni causes a small increase of the unit cell volume and a non-monotinous variation of the $a$ and $c$ lattice parameters, as earlier reported for HoCo$_{1-x}$Ni$_x$C$_2$.†

In order to analyze the changes in the electronic structure of this solid solution series, we used the projector augmented plane-wave (PAW) method in combination with the virtual crystal approximation (VCA). All calculations were performed using the PBE GGA (Perdew Burke Ernzerhof generalized gradient approximation) functional. For LuCoC$_2$ the density of states at the Fermi energy is mainly dominated by the 3$d$-band of Co, whereas for LuNiC$_2$ the 3$d$-band is almost filled and the contributions come from Lu, Ni and C. The 3$d$−band filling is successfully depicted via the VCA scheme, we present the variation of the density of states and band structure for the whole solid solution. The densities of states at the Fermi level are compared to experimental data and Fermi surface features will be discussed.

RF-Sputtered Co-Cr films with different thickness (103, 161, 200 and 280 nm) were deposited on glass substrate and then annealed at 600°C in argon atmosphere. The EDS spectra inferred that the Cr-content of as-deposited films was lightly varied with increasing film thickness whereas a cross-section SEM confirmed that the interface area between the deposited film and substrate was very smooth and the surface morphology were significantly depended on the film thickness. The XRD result showed that the as-deposited film displayed the HCP-Co (220), Cr (110) and Co-Cr (311) phases and the annealed film exhibited the obvious modification of phase structure. The Co-Cr (311) phase of the 103 and 161-annealed films was clearly disappeared signifying the segregation of Co and Cr atoms after heat treatment. The electrical resistance of as-deposited film was decreased with increasing film thickness whereas that of the annealed film with 161 nm-thicknesses showed the minimum electrical resistance. The VSM measurements showed the paramagnetic phase in all as-deposited films and ferromagnetic phase in annealed film excluding the annealed film with the thickness of 103 nm. The highest perpendicular coercivity and magnetization were observed in a 280 nm-annealed film. All result confirmed that the heat treatment improved the magnetic properties of the sputtered Co-Cr film by virtue of the modification of the phase structure and surface morphology.

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Mo-PO43

**Drastic changes of physical properties through H and C insertion in the NdScSi and GdScGe phases**

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The intermetallic systems with the CeScSi structure type (I4/mmm) are interesting for their potential sites for light element insertion within the vacant rare earth tetrahedra and the Sc-RE octahedra (RE = rare earth). So far, very little work has been carried out on the insertion of light elements and the effect this can have on the physical properties of these materials. The pristine NdScSi presents ferromagnetic order below $T_C = 171$ K. The insertion of hydrogen induces a drastic reduction of the Curie temperature while carbon insertion causes a more moderate one. Hydrogenation of the new carbide NdScSiC$_{0.5}$ induces a change in the type of magnetic order (from ferromagnetic to antiferromagnetic). Neutron diffraction studies show that this changes the magnetic coupling between the Nd planes. In the case of GdScGe, which is ferromagnetic below 350 K, the insertion of hydrogen severely reduces the magnetic order temperature and, interestingly, changes the electrical transport properties from metallic to non-metallic type (see figure). Band structure calculations have shown the role played by H in the drastic changes of magnetic and transport properties.
Mo-PO44

Characteristics of Patterned-Co film on Glass Substrate Prepared by RF-Sputtering*

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The structural, morphological and magnetic of as-sputtered and annealed Co films with different patterns (A, B, C, D and E) on glass substrate were studied. A cross-section SEM showed the film thickness of about 160 nm and smooth interfacing area between as-deposited film and substrate. The sputtered Co film was made in 5 different patterns including an un-patterned film by laser. The XRD result confirmed that all as-deposited Co film showed Co-O phase in (111) (200) directions and/or Co-(HCP) in (104), (212) and (204) directions. All annealed Co films exhibited Co$_3$O$_4$ in (220), (311), (400), (511) and (440) directions and/or Co-(HCP) in (105), (212), (411) and (501) directions. The maximum and minimum electrical resistances measured from four-point probe technique were found in B and C-patterned Co films, respectively. VSM result indicated that all as deposited film showed ferromagnetic phase with different shape of hysteresis loop whereas all annealed Co films displayed ferromagnetic with the sharp and un-saturation magnetization curves. For as-deposited film, the maximum and minimum perpendicular coercive filed were observed in E and D-patterned films, respectively. For annealed film, the maximum and minimum perpendicular coercive filed were observed in B and E-patterned films, respectively. The results implied that the magnetic parameters and electrical resistance of sputtered Co film were strongly depended on the morphological pattern of the films and heat treatment powerfully affected on the phase structure of RF-sputtered Co film gave rise to the modification of magnetic properties of the film.

*This work was supported by The Graduate School, Kasetsart University. The matching fund by Department of Physics, Faculty of Science, Kasetsart University and Kasetsart University Research and Development Institute–KURDI are also acknowledged.

Mo-PO45

Magnetic Study on $Y_2M_3Co_9P_7$ ($M$: Transition Metals) with Cations Ordered Zr$_2$Fe$_{12}$P$_7$-type Structure *

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We successfully synthesized polycrystalline samples of $Y_2M_3Co_9P_7$ ($M$ = Co, Fe, Mn, Cr, Ru, Mo), which have Zr$_2$Fe$_{12}$P$_7$-type structure with $M$ and Co selectively occupy the pyramidal site and tetrahedral site one, whose ratio is 1:3, respectively. For the case of $M$ = Co, corresponding to $Y_2Co_2P_7$ with original Zr$_2$Fe$_{12}$P$_7$-type structure, itinerant ferromagnetism has been observed below the Curie temperature $T_c$ = 153 K$^2$. By substituting Fe, Mn, or Cr for Co in the pyramidal site, $T_c$ increases to 233 K, 229 K, or 167 K, respectively. Whereas when Co in the pyramidal site is substituted by Ru or Mo, $T_c$ decreases to 21 K for $M$ = Ru and the compound shows exchange-enhanced Pauli paramagnetism for $M$ = Mo. In a case that Fe is substituted for Co in both sites, i.e., $Y_2Fe_2P_7$, the compound does not show ferromagnetism but shows Pauli paramagnetism$^5$. These results indicate that in $Y_2M_3Co_9P_7$ Co in the tetrahedral site is necessary for the realization of ferromagnetic ordering while transition metals in the pyramidal site can both enhance and reduce ferromagnetism. For the cases of $M$ being 3d transition metals, $T_c$ shows maximum around $M$ = Fe and Mn. This tendency is also seen in the cases of $M$ being 4d transition metals, i.e., $T_c$ decreases with changing $M$ from Ru to Mo. This trend may relate to larger spin density on the pyramidal site in comparison with that on the tetrahedral site observed in a case of Nd$_3Co_2P_7$$^4$. This may indicate that magnetic moments on the pyramidal site have rather localized nature and enhance ferromagnetism according to their size.

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Mo-PO46

Physical properties of half-Heusler lanthanide antimonides*

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We investigated several half-Heusler compounds (cubic MgAgAs-type crystal structure; space group $F\bar{4}3m$) of general composition $LnTnSb$, where $Ln$ is heavy rare earth element and $Tn$ stands for $d$-electron transition metal. This group of materials has attracted much attention due to big variety in their physical properties, like topologically non-trivial electronic states in LuPtSb\(^1\) or heavy fermion behavior in YbPtSb\(^2\). Up to date, only few $LnTnSb$ phases have been obtained in single-crystalline form. Motivated by our results obtained recently for the half-Heusler $LnTnB$ binary systems\(^3\) we performed investigations on high quality single crystals of $LnTnSb$ ($Ln$ = Er, Tm, Yb, Lu; $X$=Ni, Pd, Pt), grown from Bi-flux. Their crystal structures were verified from the X-ray diffraction data, and the low-temperature properties were studied by means of magnetization, magnetic susceptibility, electrical resistivity, magnetoresistivity and heat capacity measurements, performed in wide range of temperature and magnetic field. We found that the $LnNiSb$ phases are metallic-like, whereas the $LnPdSb$ compounds exhibit semiconducting-like conductivity at high temperatures and metallic-like behavior at low temperatures. All the investigated $LnTnSb$ phases are Curie-Weiss paramagnets that order magnetically at low temperatures. The $LnPdSb$ compounds show at low temperatures non-linear non-saturating negative magnetoresistance (for ErPdSb, reaching $-40\%$ in a field of 14T).

* Work supported by the National Science Centre (Poland); grant no. 2015/18/A/ST3/00057.


Mo-PO49

2D infinite boron clustering in borides: ScRu\(_2\)B\(_3\) and Sc\(_2\)RuB\(_6\)

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New compounds, ScRu\(_2\)B\(_3\) and Sc\(_2\)RuB\(_6\) had been synthesized by arc-melting followed by annealing at 800 °C. ScRu\(_2\)B\(_3\) exhibits a new structure type with the space group $Cmcm$ (a=3.0195(2) Å, b=15.4056(8) Å, c=5.4492(3) Å). Sc\(_2\)RuB\(_6\) adopts the $Y\_2ReB_6$-type structure (space group $Pbam$; a=8.8545(2) Å, b=11.1620(3) Å, c=3.4760(1) Å ). ScRu\(_2\)B\(_3\) displays an unusual intergrowth of CeCo\(_2\)B\(_2\)- and AlB\(_2\)- related slabs; a striking feature is a boat configuration of puckered boron hexagons within infinite B\(_6\) nets. Sc\(_2\)RuB\(_6\) presents two-dimensional planar nets of condensed boron pentagons, hexagons and heptagons sandwiched between metal layers. In Sc/Y substituted $Y\_2ReB_6$-type, $Y$ atoms are distributed exclusively inside the boron heptagons. Exploration of the Sc-Ru-B system at 800 °C including binary boundaries employing EPMA and powder X-ray diffraction technique furthermore rules out the existence of previously reported "ScRuB\(_4\)" but confirms the formation and crystal structure of Sc\(_2RuB_4\). Sc\(_2RuB_4\) forms in cast alloys (LuRu\(_2\)B\(_4\)-type structure; space group $I4_{1}/acd$ (no. 142), $a=7.3543(2)$ Å, $c=14.92137(8)$ Å). Cell parameters and atomic coordinates have been refined for Sc\(_2RuB_4\), Sc\(_2RuB_6\) and ScRu\(_2\)B\(_3\) in the scope of generalized gradient approximation applying the Quantum Espresso package and the results achieved had demonstrated a good agreement with the experimental parameters. Ab initio electronic structure calculations indicate a moderate electronic density of states at the Fermi level for all the studied compounds. Electrical resistivity measurements characterize ScRu\(_2\)B\(_3\) and Sc\(_2\)RuB\(_6\) as metals in concert with electronic band structure calculations.

* The research work of O. Sologub. was supported by Austrian FWF project V279-N19.
Mo-PO47

**Synthesis and physical properties of TaIrGe and neighboring phases**

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Recently discovered half-Heusler TaIrGe was predicted and found to be a transparent hole-conductor with a large band gap¹. It was synthesized by the annealing of the mixed elements under vacuum. We attempted to obtain the same compound by the arc melting of the elements. However, this synthesis route did not easily produce a single-phase material. Also, the impurity phases had a profound effect on physical properties. Instead of the expected semiconducting behavior, the metallic electrical behavior and the onset of superconductivity at low temperatures were observed. Depending on the synthesis conditions, the superconducting impurities were found to be TaGe₂ and TaIr₂Ge₂ with the critical temperatures \(T_c\) of 1.8 K and 4.0 K, respectively. The compound TaIr₂Ge₂ with a novel structure and superconducting properties was only recently discovered². By adjustment of the amount of the input elements and of the synthesis conditions, we successfully reduced the amount of impurities to the point that the semiconducting behavior of the bulk TaIrGe phase could be measured.

High-throughput search for caloric materials: 
The CaloriCool approach*
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The high-throughput search paradigm adopted by the newly established caloric materials consortium – CaloriCool® – with the goal to substantially accelerate discovery and design of novel caloric materials will be discussed. We will begin with describing material selection criteria based on known properties, which are then followed by heuristic fast estimates and ab-initio calculations implemented in a set of automated computational tools, followed by measurements of thus identified compounds. We also demonstrate how theoretical and computational methods serve as a guide for experimental efforts by considering some representative examples from the field of magnetocaloric materials.

*This work is performed under auspices of the caloric materials consortium, CaloriCool®, which is a member of the Energy Materials Network and is supported by the Advanced Manufacturing Office of the Office of Energy Efficiency & Renewable Energy and managed jointly through the Advanced Manufacturing and Building Technologies Offices of the U.S. Department of Energy. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University of Science and Technology under Contract No. DE-AC02-07CH11358.

Plenary
Crystal structure and physical properties of the cage compounds RV$_2$Al$_{20}$ and AV$_2$Al$_{20}$

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Series of compounds with the stoichiometry RV$_2$Al$_{20}$ (R = rare earth metal) were synthesized by arc melting method in a high purity Ar atmosphere. The lattice constant, determined from the Rietveld refinement, increases with increasing radii of the rare earth metal, which is located inside a CN16 Frank-Kasper polyhedra formed by 16 Al atoms. The smallest a=1.44978 nm is observed for ScV$_2$Al$_{20}$, whereas the largest lattice parameter a= 1.4617 nm is observed for LaV$_2$Al$_{20}$. We used magnetic susceptibility, resistivity, and heat capacity measurements to characterize the superconducting state in MV$_2$Al$_{20}$, where M = Sc, Y and Lu. Superconducting critical temperature is 1.0 K, 0.57 K and 0.6 K for ScV$_2$Al$_{20}$, YV$_2$Al$_{20}$, LuV$_2$Al$_{20}$, respectively. Influence of the size of M atom (and possibly rattling effect) on superconductivity in this important class of materials will be discussed.

The second part of my presentation will focus on actinide based AV$_2$Al$_{20}$ (A = U, Np, Pu). Comparison of the crystallographic results with the reported data for RV$_2$Al$_{20}$ counterparts reveals distinctly different behavior of the lanthanide- and actinide-bearing compounds. This difference is likely caused by localized character of the 4f electrons, whereas itinerant character of the 5f electrons is suggested for U- and Np-containing phases.

TK and MW greatly acknowledge support from JRC, ITU “Actinide User Laboratory” program.
Superconductivity of Alkaline-Earth-Filled Skutterudites

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Filled skutterudites with a general chemical formula $\text{AX}_x\text{X}_2$ ($X = \text{Alkaline earth, Rare earth, } T = \text{Transition metal, } X = \text{Pnicogen}$) are one of the intensively studied compounds due to their unique physical properties. Some of the superconductor realized in the filled skutterudites have characteristic physical properties such as a unique heavy fermion superconductor in PrOs$_4$Sb$_{12}$ [1] and a positive pressure dependence of superconducting transition, $T_C$, in LaFe$_4$P$_{12}$ and YFe$_4$P$_{12}$[2]. We have recently succeeded in synthesizing new filled skutterudites, SrOs$_4$P$_{12}$ by high pressure and high temperature technique. As SrOs$_4$P$_{12}$ was found to be superconductor, we have investigated the physical properties of superconducting states of SrOs$_4$P$_{12}$ with magnetization, electrical resistivity, and specific heat measurements. The electrical properties were also investigated under pressure and in a magnetic field. We found SrOs$_4$P$_{12}$ is a bulk superconductor with two superconducting transition at $T_{C1} \sim 1.5$ K and at $T_{C2} \sim 1.0$ K. The specific heat at $T_{C1}$ and $T_{C2}$ increases by 15 mJ/molK and 5 mJ/molK, respectively. The entropy released by superconductivity is balanced out with that by the normal conductivity. $T_{C1}$ is rapidly suppressed by the magnetic field, while $T_{C2}$ is relatively difficult to be suppressed. $H_{C2}$ for $T_{C1}$ and for $T_{C2}$ can be estimated to be 6 kOe and 14 kOe, respectively. The $H_{C2}$-$T_C$ relationship from resistivity reflect both $T_{C1}$ and $T_{C2}$; $T_C$ decreases with field at a rate of 4.0 kOe/K at low field followed by a downward convex at 0.9 K and the $T_C$ decreases rapidly with field at a rate of 16.4 kOe/K at high field. This downward convex is suppressed by applying pressure. In other words, The $T_{C1}$ is sensitive to field but insensitive to pressure, while $T_{C2}$ is sensitive pressure but insensitive to field. $T_{C1}$ has positive pressure dependence at the field of 0 kOe, contrary to the negative dependence predicted by simple model based on BCS theory.

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Large positive magnetoresistance in a novel superconductor Ca$_{3+x}$Co$_4$Sn$_{13-y}$.*

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We report on a huge positive normal state magnetoresistance (MR) for a novel superconductor Ca$_{3+x}$Co$_4$Sn$_{13-y}$ (x $\approx$ 0.2; y $\approx$ 0.2) with $T_C \approx 5.5$ K. For crystals grown from Sn flux with the residual resistivity ratio (RRR) of 60, the MR is of 1000% at temperatures of 6 K in magnetic field of 9 T and does not show a tendency towards saturation. We demonstrate that for crystals with a wide range of RRR values from ~1 to 64, the magnitude of the MR scales with the RRR, MR $\approx 1.6(1) \cdot$ RRR$^{1.7(2)}$. We present results of structural, thermodynamic and transport measurements. With the help of the experimental data and electronic band structure results we address the origin of the extraordinarily large MR. Finally, we analyze the relationship between chemical composition and electronic properties for the ternary phase Ca$_{3+x}$Co$_4$Sn$_{13-y}$.

* This work was supported by the Royal Society, grant no. RG150773
Tu-A5, 12:30

Charge Order and Spin-1/2 Dimer Formation Induced by Ag⁺ Order in δ-Ag₂/₃V₂O₅

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Vanadium bronzes have attracted much interest as a playground of various quantum phenomena. They are essentially mixed valent oxides where metallic conductivity and novel phenomena with spin, charge and orbital degrees of freedom are exhibited. Recently we have investigated the δ-phase of vanadium bronze, focusing on the phase transition in δ-Ag₂/₃V₂O₅ which shows characteristic super-cooling effects. The structure consists of double trellis layer formed by edge/corner-shared VO₆ octahedra and Ag ions located between the layers in Fig. 1. We have observed the phase transition at around 230 K accompanied by jumps of magnetic susceptibility and resistivity¹. Structural analysis of the low-temperature triclinic phase reveals that Ag ion order and Vanadium dimer formation. Below the transition temperature the magnetic susceptibility shows a broad maximum around 110 K followed by spin gap behavior. We conclude that the phase transition in δ-Ag₂/₃V₂O₅ is a charge order into V⁴⁺ and V⁵⁺ induced by Ag ion order. The V⁴⁺ ions form dimers with the spin-gapped ground state. Also it can be super-cooled down to the lowest temperature by rapid cooling.


Tu-A6, 12:45

Novel Canonical Heavy Fermion Compound

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The field of heavy fermion physics emerged nearly four decades ago and has since become one of the central research directions of condensed matter physics. While significant progress has been made in understanding heavy fermion behavior and accompanying phenomena, the global trends still remain unclear. One of the avenues in the search for heavy fermions has focused on compounds with high coordination, and, therefore, low concentration of uranium atoms. This approach has proven fruitful in the case of antiferromagnetic U₂Zn₁₇ and UCd₁₁, as well as unconventional superconductor UBe₁₃. The two former compounds are also the only two canonical heavy fermions. In this work, we present the discovery of the third canonical heavy fermion U₁₁Hg₄₅. This compound exhibits an antiferromagnetic transition at T_N = 2 K, which can be suppressed by application of magnetic field. A high value of the Sommerfeld coefficient γ = 0.6 J/µmol K² is likely related to the high itineracy of the f-electrons, as evidenced by the high value of the Rhodes-Wohlfarth ratio along with the small entropy of the antiferromagnetic transition.

Oral
BiS₂-based layered superconductors Ln(O,F)BiS₂ (Ln: rare earth), which consist of alternating stacking of BiS₂ conductive layers and LnO block layers, have been attracting much attention. ARPES measurement has clarified that the conduction bands consist of Bi 6pₓ,6pᵧ electrons forming 2-dimensional Fermi surface. Because of strong spin-orbit coupling in Bi 6p orbital, the conduction electrons are expected to have spin polarized nature. Since 4f electrons of Ln ions in the block layers have magnetic degrees of freedom, it is an intriguing question whether the magnetism and superconductivity compete or coexist in this material. We have succeeded in growing high-quality single crystals of Ln(O₁₋ₓFₓ)BiS₂ series and have been investigating 4f-electron behaviors. Here we report findings of non-Fermi-liquid behaviors in Ln=Ce and heavy-fermion-like behaviors in Ln=Nd.

In CeOBiS₂, 4f-electrons have been found to be in a localized state with clear crystalline-electric-field (CEF) splitting. The CEF ground state is a pure  heavy-fermion-like behavior with In Nd(O₁₋ₓFₓ)BiS₂, specific heat shows a -log T divergence in zero field, we have found a pronounced -log T₁/2 doublet and excited doublets are located above 300 K. At low temperatures in zero field, we have found a pronounced -log T divergence in the specific heat, revealing the presence of strong correlations among 4f magnetic moments. Considering that CeOBiS₂ is a nonmetal, this phenomenon cannot be attributed to the competition between Kondo and RKKY interactions as in usual f-electron-based strongly correlated metals, pointing to an unconventional mechanism working in this material.

In Nd(O₁₋ₓFₓ)BiS₂, specific heat shows a -log T divergence in the similar temperature range but it ends up with a heavy-fermion-like behavior with C/T≈7.4 J/K²mol below 0.3 K. Similar behavior was observed in cuprate superconductor (Nd₂₋ₓCex)CuO₄, where dynamical magnetic coupling between Nd and Cu spins has been discussed as a possible mechanism. A possible role played by the characteristic layered crystal structure is discussed.

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**Tu-A7i, 14:00**

Unconventional 4f-Electron Magnetism in Ln(O,F)BiS₂ Layered Superconductors

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Second order phase transitions and the associated critical phenomena lie at the heart of a wide variety of exciting phenomena in solid state physics. Critical fluctuations are tuned by temperature or non thermal control parameters as e.g. pressure, doping, or magnetic field. Recently, perfectly antisymmetric strain has been suggested as a new tuning parameter for Ising-nematic quantum critical transitions and has shown to be a powerful tool for studying solid state phenomena like nematicity, or superconductivity. Experimentally, however, the concept of strain as a tuning parameter is complicated by the fact that isotropic or anisotropic pressure applied to a solid almost always yields a combination of strain fields of different symmetry.

Here we present a first study decomposing the effect of strain on the coupled nematic/structural transition (Tₙ) of underdoped iron pnictides Ba(Fe₁₋ₓCox)₂As₂ into three orthogonal strain modes of the tetragonal D₄h point group. The decomposition into the two symmetric modes $\epsilon_{A1g,1}=\frac{1}{2}(\epsilon_{xz}+\epsilon_{yy})$, and $\epsilon_{A1g,2}=\epsilon_{xz}$, as well as the antisymmetric mode $\epsilon_{B1g}=\frac{1}{2}(\epsilon_{xz}-\epsilon_{yy})$ is achieved by probing $T_n$ using electrical resistivity under (i) uniaxial pressure, and (ii) hydrostatic pressure as a function of temperature. Combining the results of both techniques we find that the linear response $\frac{\partial \rho}{\partial \epsilon_{A1g,1}}$ is larger and has opposite sign as compared to $\frac{\partial \rho}{\partial \epsilon_{B1g}}$ for all studied Co dopings. In line with a Landau free energy analysis, we also find evidence for a nonlinear variation of $T_n$ as a response to $\epsilon_{B1g}$.

We anticipate that a symmetry decomposition as proposed here offers a great opportunity for extending the insight into various existing and new phase diagrams.

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**Tu-A8i, 14:30**

Strain as tuning parameter for the coupled nematic/structural phase transition in Co doped BaFe₂As₂


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Influence of doped 3d atom on the magnetic order in fourfold NiMnGe:T compounds
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Influence of doped T = 3d metal (Cr, Ti) on the magnetic properties NiMnGe are investigated by powder neutron diffraction ($\lambda = 4.567$ Å). All investigated samples have the helicoidal magnetic structure with the propagation vector $k = (k_x, 0, 0)$.

The data for NiMn$_{1-x}$Cr$_x$Ge for $x = 0$, 0.04, 0.11 and 0.18 indicate magnetic ordering at low temperature. The values of $k_x$ decrease from 2/11 ($x = 0$) by 1/6 (0.04), 1/7 (0.11) to 1/16 (0.18) at 2 K. With increase of the temperature the helicoidal order for $x = 0$, 0.04 and 0.11 is stable up to Néel temperature while for $x = 0.18$ at 150 K the change of the magnetic order to the ferromagnetic one is observed.

The helicoidal ordering is also observed in NiMn$_{0.95}$Ti$_{0.05}$Ge and Ni$_{0.95}$Ti$_{0.05}$MnGe with the components of the propagation vectors equal $k_x = 0.193$ and 0.187. Temperature dependence of the intensity of 000 satellite reflection indicates the change of magnetic structure at 210 K and 190 K, respectively.

The obtained data are analyzed based of the simple model in which the magnetic interactions between Mn/Cr magnetic moments are described by exchange integrals: $J_1 > 0$ for first and $J_2 < 0$ for second neighbouring atoms. Other 3d atoms change the magnetic order from modulated to ferromagnetic. The change of the magnetic structure is connected with the change in the exchange parameters.

This model can also by an explanation for the temperature dependence of the values of components of propagation vector.

These data are compared with the results of the magnetic measurements in the function of pressure.
Nodeless superconductivity and time-reversal symmetry breaking in the noncentrosymmetric superconductor Re₂₄Ti₅

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As possible systems to harbor unconventional pairing symmetries, non-centrosymmetric superconductors (NCSCs) are being intensely studied. Here, a lack of inversion symmetry induces an anti-symmetric spin-orbit coupling (ASOC), which lifts the degeneracy of the conduction-band electrons and induces a superconducting order consisting of a mixture of spin-singlets and triplets. In addition, many NCSCs are known to break the time reversal symmetry (TRS) in the superconducting state, although the role played by SOC is not yet clear.

Here we consider the binary alloy Re₂₄Ti₅ (a NCSC with Tc = 6 K), whose microscopic nature of SC is unknown and whose analog compounds Re₂₄(Zr,Hf) are known to break the TRS in the superconducting state. Hence, Re₂₄Ti₅ represents an ideal case to investigate the occurrence of TRS breaking and unconventional SC in a material with a modified SOC value. By using muon-spin rotation/relaxation (μSR) and tunnel-diode oscillator techniques, we could study the Re₂₄Ti₅ SC properties at a microscopic level. The penetration depth, superfluid density, and electronic heat capacity are all consistent with a single s-wave superconductor with an enhanced gap value. Yet, most notably, below Tc spontaneous magnetic fields revealed by zero-field μSR indicate a TRS breaking and thus the unconventional nature of Re₂₄Ti₅. The similar behavior of Re₂₄Ti₅ with the isostructural Re₂₄(Zr,Hf) compounds hints at a common origin of time-reversal symmetry breaking in this superconducting family and that changes in spin-orbit coupling do not affect the pairing symmetry.


Hydrogenation of intermetallics: A new synthetic route for iron-based superconductors

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Since the discovery of unconventional superconductivity in Fe-based materials in 2008¹, Fe-based superconductors (Fe-SC) have attracted much attention and have been the subject of intense and systematic investigations. To date, high-Tc Fe-SC always contain toxic pnictogen or chalcogen elements (P, As and Se, Te respectively). Besides, they are usually obtained by solid state reaction with possibly the use of high pressure. In this context, we have recently synthesized the new hydride LaFeSiH by solid-gas hydrogenation of the precursor LaFeSi. Preliminary results show that this hydride is isostructural to the 1111 Fe-SC compounds (s.g. P4/nmm), hydrogen atoms being inserted in the [La₄] tetrahedra⁵. Interestingly, LaFeSiH displays superconductivity below 10 K as evidenced notably on the resistivity measurement on single-crystal. This hydride also presents other structural, magnetic and electronic similarities with the previously reported Fe-SC compounds. In particular, LaFeSiH undergoes a transition from tetragonal to orthorhombic structure at low temperature, distortion which is suppressed by an external pressure and re-emerges at higher pressure. In addition, Density Functional Theory calculations have evidenced the quasi-2D character of the Fermi surface with a dominant contribution of the 3d(Fe) orbitals. These calculations also predict the onset of a single-stripe antiferromagnetic order that would explain the orthorhombic distortion. Therefore, LaFeSiH can be considered as the first Fe-SC obtained by solid-gas hydrogenation and free from toxic pnictogen and chalcogen elements.

Beryllium-rich intermetallic compounds have aroused interest due to their manifold structure chemistry. Oxidation resistance at high temperatures, high mechanical strength and low density drove the investigations of beryllium alloys with transition metals and recently they attracted attention as possible neutron multiplying blanket materials for the next generation of fusion reactors. However, many binary systems of beryllium with transition metals are only sparsely investigated and most likely still hold a plethora of undiscovered compounds in store.

The complex intermetallic compound Be$_{21}$Pt$_5$ constitutes a new member in the group of F-centered cubic $\gamma$-brass phases with a lattice parameter $a = 15.90417(3)$ Å. The crystal structure was determined in a combination of synchrotron and neutron powder diffraction and can be described on the basis of 26-atom cluster units. Analysis of the calculated electron density and electron localizability indicator (ELI-D) shows strongly polar and predominantly multi-center bonding. Furthermore, superconductivity was observed below 2 K.

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Multiband systems, which possess a wide parameter space, allow to explore a variety of competing ground states. Bright examples are the iron-based pnictides and chalcogenides, which demonstrate metallic, superconducting, and various magnetic phases. The superconducting state is unconventional and thus the system demonstrates unusual spin response with the spin resonance feature that can be observed in the inelastic neutron scattering experiments. Here we study the spin resonance in the superconducting state having unequal anisotropic gaps on different Fermi surface sheets. We show that due to the indirect nature of the gap entering the spin susceptibility at the nesting wave vector $Q$ the total gap in the bare susceptibility is determined by the sum of gaps on two different Fermi surface sheets connected by $Q$. For the Fermi surface geometry characteristic to the most of iron pnictides and chalcogenides, the indirect gap is either sum of larger and smaller gaps or twice the larger gap scale. We show that the resonance peak shifts to higher frequencies with shifting the ‘center of mass’ of the anisotropic gap. On the contrary, with increasing the gap anisotropy, it shifts to lower frequencies and lose intensity. Comparison with available inelastic neutron scattering data confirms that what is seen is the true spin resonance inherent to the spin-fluctuation mediated $s_{\pm}$ state.

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$^*$This work was supported in part by RFBR (grant 16-02-00098) and “BASIS” Foundation for Theoretical Physics Development.

$^1$also at Siberian Federal University, 660041, Krasnoyarsk, Russia

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Oral
DFT calculations in Half-Heusler systems

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Solid solutions of Half-Heusler (HH) compounds TiNiSn, ZrNiSn, HfNiSn, known as n-type semiconductors, have proven a remarkably high efficiency in thermoelectric conversion of waste heat into electrical power. As a big advantage for thermoelectric optimization, HH compounds offer a tunable electronic structure, which can be modified through (i) doping/substitution/vacancy formation on its three metal sublattices, (ii) engineering of a narrow electronic band gap, and (iii) nanostructuring or (iv) exploiting spinodal decomposition mechanisms. Recent investigations of the corresponding and related ternary systems aided by DFT calculations showed that some HH compounds are characterized by (i) a homogeneity region toward full-Heusler compounds or (ii) an off-stoichiometric composition.

Homogeneity regions of HH TiNi₁₋ₓSn and ZrNi₁₋ₓSn phases toward the corresponding Heusler phases are characterized by a positive change in the calculated heat of formation, however, an accounting of configuration entropy leads to the appearance of the solubility of additional Ni atoms in the 4d vacant site of TiNiSn and ZrNiSn compounds. A formation of the miscibility gap was also predicted in Ti₁₋ₓZrₓNiSn and Ti₁₋ₓHfₓNiSn solid solutions and influences of various substitutions in Ti/Zr/Hf and Sn sites were modeled.

DFT calculations of the HH phase in the Ti-Fe-Sb system showed that it is characterized by off-stoichiometry and the presence of the Ti₁₋ₓFe₁₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋_x solid solutions and influences of various substitutions in Ti/Zr/Hf and Sn sites were modeled.

Thus a DFT modeling of the deviation from the equiatomic composition of some HH phases gives an additional degree of freedom in a discovery of “missed” HH phases and in tuning the thermoelectric properties of already known materials.

Electronic Structure, Magnetic and Electrochemical Properties of Li- and Na-ion Battery Systems in View of KKR-CPA Calculations

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Lithium-ion battery materials are still considered to be the most promising energy converter, due to their excellent electrochemical parameters. However, many efforts have been recently undertaken to find alternative cathode materials conducting for instance Na ions. In this work, the results of electronic structure calculations of operating and potential materials for Li- and Na-ion battery systems, based essentially on AMO₃ compounds (A=Li, Na and M=Mn, Fe, Co, Ni) and their alloys are discussed [1,2]. Noteworthy, theoretical results obtained using the Korringa-Kohn-Rostoker method with the coherent potential approximation (KKR-CPA) allowed to interpret the step-like vs. continuous-like character of the discharge curve in terms of some correlations between electronic structure and electrochemical properties in selected Na- and Li-ion cathode materials, respectively [1,2] as well as to study a novel variant of the well-known cathode material LiₓCo₁₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋_x NiₓMnₓO₂ [3].

Chemical disorder such as Li vacancy defects and Co/Ni/Mn alloying was accounted for the KKR-CPA calculations, which resulted in specific evolution of density of states in the whole range of Li contents and alloy compositions. It was found that electronic structure of LiₓCo₁₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋_x NiₓMnₓO₂ exhibits semiconducting-like, half-metallic-like or metallic-like properties depending on Li content as well as relative concentrations of transition metal elements (Co, Ni and Mn). Moreover, the magnetic moments are found for selected compositions as resulted from the KKR-CPA computations, which affect the overall DOS shape near E_F. Finally, the correlations between electronic structure of LiₓCo₁₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋ₓ₋₀₋_x NiₓMnₓO₂ and its electrochemical properties are discussed.

Longitudinal integration measure in classical spin space and its application to first-principle based simulations of ferromagnetic metals.

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The classical Heisenberg type spin Hamiltonian is widely used for simulations of finite temperature properties of magnetic metals often using parameters derived from first principles calculations. In itinerant electron systems, however, the atomic magnetic moments vary their amplitude with temperature and the spin Hamiltonian should thus be extended to incorporate the effects of longitudinal spin fluctuations (LSF). Although the simple phenomenological spin Hamiltonians describing LSF can be efficiently parameterized in the framework of the constrained Local Spin Density Approximation (LSDA) and its extensions, the fundamental problem concerning the integration in classical spin space remains. It is generally unknown how to integrate over the spin amplitude. Two intuitive choices of integration measure have been used up to date; the Murata-Doniach scalar measure and the simple three dimensional vector measure. Here we derive the integration measure by considering a classical limit of the quantum Heisenberg spin Hamiltonian under conditions leading to the proper classical limit of the commutation relations for all values of the classical spin amplitude and calculate the corresponding ratio of the number of quantum states. We show, that the number of quantum states corresponding to the considered classical spin amplitude is proportional to this amplitude and thus a non-trivial integration measure must be used. We apply our results to the first-principles simulation of the Curie temperatures of the two canonical ferromagnets bcc Fe and fcc Ni using a single-site LSF Hamiltonian with parameters calculated in the LSDA framework in the Disordered Local Moment approximation and a fixed spin moment constraint. In the same framework we compare our results with those obtained from the scalar and vector measures.

Spin model of the Heisenberg antiferromagnet Li₃Ni₂SbO₆:
the relevance of third-neighbor exchanges∗
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The quasi-2D $S=1$ Heisenberg antiferromagnet Li₃Ni₂SbO₆ exhibits a small Weiss temperature of 8 K and a zigzag magnetic ground state below $T_N = 15$ K [1,2]. At the same time, the experiments indicate the presence of a short-range magnetic order up to 80 K [2]. The experimental behavior was rationalized in terms of a honeycomb lattice model with inequivalent nearest-neighbor (NN) exchanges [1]: antiferromagnetic $J_1$ forming dimers and ferromagnetic $J'_1$ ($J_2$ in the notation of [1]) forming chains. Puzzled by the drastic dissimilarity of $J_1$ and $J'_1$, we performed microscopic magnetic modeling and found that both NN exchanges are ferromagnetic. The antiferromagnetism and magnetic frustration are induced by two sizable third-neighbor exchanges, $J_3$ and $J'_3$, that are mediated by the nonmagnetic SbO₆ octahedra in the voids of the honeycomb lattice. The resulting $J_1$-$J'_1$-$J_3$-$J'_3$ model provides a simple and natural explanation for the observed zigzag state. Finally, we will compare the spin model of Li₃Ni₂SbO₆ with that of the nearly isostructural compound Na₃Ni₂SbO₆.


∗This work has been supported by the Austrian Science Fund (FWF) through the Lise Meitner programme, project no. M2050.

Oral
**Tu-B5, 12:30**

**LDA+ DMFT approach to core-level spectroscopy; application to 3d transition-metal compounds**

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We present an application of the local-density approximation (LDA) + dynamical mean-field theory (DMFT) to compute various core-level X-ray spectra of correlated materials. Anderson impurity model including the core states of the studied atom is constructed using the continuous LDA+DMFT hybridization function, which reflects the correlated dynamics of the valence electrons in the crystal. This allows us to obtain the fine structure of the spectra missing in the conventional cluster calculations, which capture only the metal-ligand hybridization. Technically, the calculations are enabled by a new configuration-interaction-based impurity solver. We present a systematic comparison of 2p core-level X-ray photoemission spectra (XPS) of 3d transition-metal oxides MO (M=Ni, Co, Mn, Fe) and M₂O₃ (M=Ti, V, Cr, Fe) to recent high-resolution experiments [1-3]. We find overall a good agreement. We show how the fine structures in the XPS are related to specific microscopic processes. We also present selected examples of application to the L-edge X-ray absorption spectra and L-edge resonant inelastic X-ray scattering.

**Tu-B7i, 14:00**

**Multi-center bonding in γ-brass phases**

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Phases with the crystal structure of γ-brass type (Cu5Zn8 type) are typical representatives of intermetallic compounds. The Pearson Data Base counts up to 70 members of this structure family. From the chemical point of view, these substances are mainly formed by transition metals. The γ-brass-type phases of the main-group elements are rather rare. From the electronic point of view, they are usually interpreted in the first approximation within the jellium model, further using the valence electron concentration approach of Hume-Rothery, developed previously for transition metals, or by application of the cluster orbitals.

Starting with Be$_2$Pt$_5^{11}$, we systematically applied the quantum-chemical techniques in position space to study the atomic interactions in the compounds of the γ-brass family. Employing the quantum theory of atoms in molecules (QTAIM) visualizes the role of the charge transfer in stabilization of the materials of this group, in particular for the compounds of main-group elements. Involving the 2-electron functionals, like Electron Localizability Indicator, for the analysis of the electron pairs’ distribution in the structure space showed the way of the structural organization by means of multi-center bonding, in particular for the transition-metal compounds. For the first time, the new type of interactions – the so-called cage bonds – were observed on this route.

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**Tu-B8i, 14:30**

**Carbodiimides of the Transition Metals: From Basic Research to First Applications**

*Richard Dronskowski*

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Solid-state physics often deals with various studies on “correlated” oxides such as NiO and related stuff. In those, intraatomic e–e repulsion (“correlation”) on the metal competes with chemical bonding (“hybridization”) between metal and O; hence, a plethora of many-body effects results. To modify matter, one may change the metal but also substitute the oxide anion. For example, the N-based pseudo-oxide of CaO is given by CaCN in which the NCN$^2$ carbodiimide anion replaces O$^2$; one might call NCN$^2$ the “divalent nitride” anion. Interestingly, the existence of the transition-metal carbodiimides was established only within the last decade after DFT total-energy calculations predicted their metastability. Subsequently, the “correlated” 3d carbodiimides were synthesized one after the other, namely green MnNCN,[1] black CuNCN,[2] orange CoNCN,[3] light-brown NiNCN,[3] and crimson FeNCN,[4] all binary phases are antiferromagnets. Also, we know the green ferromagnetic Cr(NCN)$_3$[5] plus a growing list of ternaries. And yet, there is new physics and chemistry. Many-body effects dominate CuNCN for which magnetic and mechanical behavior point towards a spin liquid.[6] Likewise, phases such as FeNCN have turned out as excellent anode materials for Li/Na batteries.[7] In addition, Ag$_2$NCN catalyzes photoelectrochemical water oxidation.[8] There is plenty of room at the bottom for N-based pseudo-oxides of the transition metals.

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*This work was supported by the German Research Foundation*

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Tu-B9, 15:00

Mixed Ligand Complexes of Rare Earth Carboxylates with Aminoligands as Precursors for MOCSD of Thin Films

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At present rare earth carboxylates are widely used for synthesis of rare earth oxide and fluoride functional materials by means of Metal Organic Chemical Solution Deposition (MOCSD). The development of the new precursors as well as the study of the formation of complexes in such systems are crucial for the research. Mixed ligand complexes of rare earth trifluoroacetates, pentafluoropropionates and pivalates (Ln(tfa), Ln(pfp), Ln(piv), respectively) with diethylenetriamine and monoethanolamine (deta, mea) were subjects of this work. Solutions of Ln(tfa)+deta in CH₂CN or i-PrOH were used as precursors for rare earth fluoride thin films. Under conditions of controlled hydrolysis, we isolated either polynuclear hydroxo-compounds ([La(OH)(tfa)(deta)(detaH)]·[La(OH)(tfa)(deta)(H₂O)]·H₂O·CH₂CN or La(tfa)(deta)(OH)·H₂O, or mixed ligand complexes (meaH)[Y(tfa)₂·CH₂CN·0.5CH₃CN and [Ln(tfa)(deta)](tfa) (Ln=Dy–Lu, Y). The latter were proven to be suitable precursors for NaYF₃ thin film deposition. Due to the stability of the ([Ln(tfa)(deta)](tfa)), dimers predicted by DFT (B3LYP/TZVP) calculations and confirmed by NMR spectroscopy, we succeeded to obtain the hexagonal β-phase of the fluoride which demonstrates upconverting optical properties. Syntheses of pivalate rare earth complexes led to isolation of La(piv)(deta) molecular mixed ligand complex and partially hydrolysed octahedral clusters Ce₂O(piv)(deta), Pr₂(OH)(piv)(deta);C₂H₅, and Gd(OH)₂O(piv)(deta);2CH₂CN, predicted by DFT calculations. Such LnO₂-based edifices could be used as building blocks for a variety of metal-organic frameworks (MOF).

*The quantum chemical calculations were carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University; this work was supported by Russian Foundation for Basic Research, project no. 16-03-00923.

Tu-B10, 15:15

Joint melt of two p-metals: New approach to synthesis of intermetallic compounds with functional properties*

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T-E intermetallic compounds, where T is a transition metal and E is a main group element, crystallize in more than 34 binary structure types displaying unique structural diversity. Empirical knowledge reveals that different structures are confined within specific ranges of valence electron count (VEC), which is the number of valence electrons per T atom. Exceeding the limits of VEC results in change between structure types. For instance, in the series NiSi₂, CoSi₂, and FeSi₂, gradually decreasing VEC leads to the change from the CaF₂-type of crystal structure for T = Ni, Co to the β-FeSi₂-type for T = Fe³. We take advantage of the fact that the VEC parameter plays a crucial role when determining the stability ranges of T-E intermetallics and put forward a new synthetic approach that enables careful control of VEC through the ratio of two p-metals within their joint melt. The approach is based on the reaction of a transition metal T with a flux E, which contains two metals E₁ and E₂ from different groups of the left side of the p-block. In the chosen ternary system T-E₁-E₂, we restrict the molar ratio of ν(T) : ν(E) = 1 : 50 and gradually change the composition of melt from the pure E₁ element to the pure E₂, thus, scanning possible values of VEC. In our study, we focus on T = Mo and Re searching for new endohedral gallide cluster compounds that are candidates for superconductivity¹. Ternary systems Mo-Ga-Zn, Mo-Ga-Sn, Mo-Zn-Sn, and Re-Ga-Zn were studied systematically. By employing the crystal growth from the high-temperature flux, five new compounds were isolated, four of which belong to the endohedral gallide cluster compounds.

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¹ Inorg. Chem., 2015, 54, 11385–11398

Oral
Tu-B11i, 16:00

High Temperature and High Pressure Synthesis and Magnetic Properties of Arsenic-Based Filled Skutterudite compounds∗

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Filled skutterudite compounds with the general formula RT4X12 (R=rare earth metal or alkaline earth metal, T=transition metal, X=pnictogen) exhibit various physical properties, such as unconventional superconductivity, magnetic ordering, multipole ordering and anomalous metal-insulator transition, depend on combinations of elements. While the physical properties of phosphorus- and antimony-based compounds have been investigated intensively, few studies of arsenic (As)-based filled skutterudite compounds have been conducted. One of the reasons is that the compounds are quite difficult to prepare at ambient pressure. High-pressure synthesis is a powerful technique for preparing As-based filled skutterudite compounds. Recently, new As-based filled skutterudite compounds EuFe4As12 and SrFe4As12 prepared under high pressure, have been reported. The magnetic measurements for EuFe4As12 reveal a ferromagnetic-like behavior below 152 K. The magnetic transition could be related to the interaction of Eu and Fe moments. In this presentation, the high-pressure synthesis technique using a multi-anvil press will be introduced and the magnetic structure of EuFe4As12 will be discussed from the results of magnetoresistance and neutron scattering experiments. Furthermore, itinerant magnetic properties of SrFe4As12 will be also discussed.

∗This work was performed using the facilities of the Institute for Solid State Physics, The University of Tokyo. This work was supported by JSPS KAKENHI Grant Numbers 23340092. This work has been performed under the approval of the Photon Factory Program Advisory Committee (Proposal Nos. 2015G031, and 2013G124).

Tu-B12i, 16:30

Multifunctional phenomena in rare-earth intermetallic compounds with a Laves phase structure

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Simple crystal structure of the Laves phase compounds RT2 (R = rare earth, T = transition metal) and remarkable magnetic properties have ensured a great deal of experimental and theoretical interest during past several decades. We report on the recent progress in the studies of multicomponent RR′R″T2 alloys. Simultaneous substitutions in both the R and 3d-metal sublattices provide a rich array of magnetic phenomena, among which are various spontaneous and field-induced transitions. These together with a complex behavior of lattice parameters allow us to observe large magnetocaloric effect and magnetostriiction at magnetostructural transitions.

Compounds for this study were prepared with the use of high purity metals. Substitutions in (Tb,Dy,R)(Co,Fe)2 (R = Gd, Er, Ho) allowed us to vary the type of magnetic ordering transition (first or second) and tuned continuously the magnetic ordering temperatures. Substitutions of Al for Co in Tb3(Dy0.5Ho0.5)1−x,Co3 increased the Curie temperature (Tc) and changed the transition type from first- to the second-order. Discussion of physical mechanisms behind the observed phenomena is given on the basis of first principles electronic-structure calculations taking into account both the atomic disorder and the magnetic disorder effects at finite temperatures. The advantage of Al-containing materials is that sufficiently high magnetocaloric effect values are preserved at T>Tc.

† Tereshina et al., J. Appl. Phys. 120 (2016) 013901.
Tu-B13, 17:00

**Electronic structure, magnetic, electric transport, and thermal properties of Ce₅PdGe₂**

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From the study of crystallographic structure of the ternary Ce₅MGe₂ compounds (M = Co, Ni, Ru, Rh, Pd, Ir, and Pt) [1] results that the structure depends on metal M. Most of the components of the Ce₅MGe₂ series crystallize in the Y₂HfS₃ structure type (Pnma space group), while Ce₅PdGe₂ compound was reported as Mn₅Si₃-type system with the space group P6₃/mcm [1]. Until now there is no research on this compound except structure investigations. Our X-ray diffraction analysis predicts for Ce₅PdGe₂ the Y₂HfS₃-type structure with symmetry Pnma. Magnetic properties of Ce₅PdGe₂ are studied by combined investigations involving susceptibility, magnetization, heat capacity and electrical resistivity. The comprehensive magnetic research was discussed on the base of the results from band structure calculations. Two magnetic transitions were found in the absence of magnetic field, at 13.8 K and 3.5 K, respectively. The 3.5 K phase is a mixture of ferrimagnetic and spin-glass-like magnetic order. We propose a magnetic H − T phase diagram for the complex magnetic structures of Ce₅PdGe₂, field-induced.


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Tu-B14, 17:15

**Closo-boranes of 3d transition metals, synthesis and characterization**

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Magnesium and 3d transition metals closo-boranes were prepared by mechano-synthesis (ball-milling) of the mixtures Na₂B₁₂H₁₂ + MCl₂ (M = Ti, Cr, Mn, Fe, Co, Cu, Zn, Mg) and CuCl, followed by solvation (water, methanol, ethanol) and drying under dynamic vacuum. The dead mass of NaCl was partly removed by filtration. The crystal structures of solvated and solvent-free closo-boranes have been characterized by temperature-dependent synchrotron radiation X-ray powder diffraction, *ab initio* calculations, thermal analysis and infrared spectroscopy.

Crystal structures of the closo-boranes contain various metal-solvent complexes: octahedral M(H₂O)₆, M(EOH)₆ and M(MeOH)₆, octahedral M(H₂O)₄H₂, square pyramidal or octahedral M(EOH)₃H₃, M(EOH)₃H₃ and M(MeOH)₃H₃, octahedral M(H₂O)₄H₄, and square pyramidal M(EOH)₃H₃, M(EOH)H₄ and M(MeOH)H₄ bridging two closo-borane anions.

Solvent-free manganese, iron, cobalt, nickel and copper closo-boranes were obtained by drying the solvated sample. The compounds crystallize with *hcp* or *bctc* packing of closo-boranes. M²⁺ (Mn, Fe, Co, Ni) is disordered close to the triangular face of the tetrahedral closo-boranes interstice coordinated by H₅ square pyramid or H₆ octahedron, and Cu⁺ is disordered bridging two closo-boranes, and is coordinated by H₆ octahedron. The coordination of the metals was obtained by *ab initio* calculations using ordered structural models.

The solvent free transition metal closo-boranes are stable up to 250-350 °C, and are potentially applicable as insertion electrodes for Li- and Na-ion batteries with closo-borane solid electrolytes.

Oral
Tu-PO1

**Excess conductivity and pseudogap in YBa$_2$Cu$_3$O$_{7-δ}$ nanolayers**

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After thirty years since the high-temperature superconductors (HTSC’s or cuprates) discovery the physics behind the pairing mechanism which allows the Cooper pairs formation at $T>100$K still remains unknown. Importantly, apart from the high $T_c$’s, cuprates possess the so-called pseudogap (PG) which opens below PG temperature $T^\ast$. It is believed at present that the proper understanding of the PG phenomenon has to account for the pairing mechanism both in cuprates and new FeAs-based high-$T_c$ superconductors (pnictides), which is important in view of the search for the room-temperature superconductivity.

A huge amount of various models has been put forward to explain the PG in HTSC’s but the issue as for PG physics also remains rather controversial. We believe the PG to be due to preformed pairs (local pairs (LP’s)) formation but the pairing mechanism is very likely of a magnetic type. Thus, the comprehension of the interplay between superconductivity and magnetism is widely considered to be one of the great challenges of the condensed-matter physics. To clarify the issue, we studied the fluctuation conductivity (FLC) and PG in YBa$_2$Cu$_3$O$_{7-δ}$-PrBa$_2$Cu$_3$O$_{7-δ}$ (YBCO-PrBCO) superlattices (SL’s) and YBCO-PrBCO double-layer films (so-called “sandwiches”, SD’s) with different layer composition, prepared by pulsed lased deposition. Pr$^{3+}$ atoms are known to have an intrinsic magnetic moment, $\mu_{\text{eff}} \approx 3.58\mu_B$ and $\mu_{\text{eff}} \approx 2\mu_B$ in the PrBCO compound. Thus, such compounds are considered to be very promising in studying the change of interplay between superconductivity and magnetism in HTSC’s which is expected to increase with an increase of the number of PrBCO layers $N_p$.

Tu-PO2

**Transport properties and magnetic states in Fe-intercalated titanium dichalcogenides**

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The Fe-intercalated titanium dichalcogenides Fe$_x$Ti$_x$X$_2$ ($X = S, Se$) are an example of quasi-two-dimensional systems in which Fe atoms can form a monoatomic layer between tri-layer nonmagnetic blocks $X$-Ti-$X$. While the compounds Ti$_x$X$_2$ are Pauli paramagnets, the intercalated compounds Fe$_x$Ti$_x$S$_2$, depending on the concentration of Fe atoms, exhibit a spin-glass (at $x \leq 0.20$) or cluster-glass (0.20 < $x$ < 0.40) behavior and show a long-range magnetic order above $x \approx 0.4$. We synthesized the Fe$_x$Ti(S,Se)$_2$ compounds ($x$ up to 0.75) with Se for S substitutions and studied their magnetization, electrical resistivity and magnetoresistance behaviors. It has been observed that in the Fe$_x$Ti(S,Se)$_2$ compounds with $x \leq 0.5$, the change of the electrical resistivity with temperature shows a metallic character with pronounced anomalies around the magnetic ordering temperatures. However, the resistivity of Fe$_x$Ti(S,Se)$_2$ with higher Fe concentrations (above $x = 0.5$) exhibits substantial growth with cooling below the magnetic critical temperature. An additional magnetic contribution to the resistivity which does not vanishes with cooling is ascribed to the appearance of the magnetic-polaron-like states in these compounds due to the partial Fe-Ti mixing in cationic layers. At low temperatures, the application of a magnetic field is accompanied by a giant magnetoresistance ($\Delta \rho/\rho \sim -40$%) in some Fe$_x$Ti(S,Se)$_2$ reflecting the field-induced transformations of their magnetic state. The results obtained indicate the distribution of Fe atoms and vacancies in the cationic layers together with the Fe concentration substantially affects the magnetic and transport properties of Fe$_x$Ti(S,Se)$_2$.

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Tu-PO3

Field Induced Lifshitz Transition in Antiferromagnetic CePd$_2$In$_7^\dagger$

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For the past few years a considerable research effort has been directed towards Ce$_n$T$_m$In$_{n+2m}$ (T = Pd and Pt) system, which exhibits a variety of exciting ground state properties such as superconductivity, heavy-fermion behavior, complex magnetic ordering and proximity to quantum critical point$^{1-5}$. Very recently, superconductivity driven by antiferromagnetic exchange interaction has been discovered$^3$ in Ce$_3$PdIn$_7$ ($n = 1$ and $m = 2$) with two successive magnetic transitions at $T_{N1} = 1.45$ K and $T_{N2} = 1.25$ K. Heat capacity measurements, $C(T)$, carried out in applied magnetic fields, revealed that both transitions shift to lower temperatures with increasing field, hence, elucidating antiferromagnetic nature of the ordering. However, in a critical field of about 4 T, the two transitions suddenly merge into a single first-order type anomaly in $C(T)$ at a temperature $T_{N3}$ that first increases with ramping field up to 5 T, and then decreases. Remarkably, the overall behavior resembles a Lifshitz like transition. Furthermore, the $C/T$ ratio attains an enhanced value of 2.05 J/(mol K$^2$) at 0.4 K hinting towards the formation in CePd$_2$In$_7$ of heavy fermion state.

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Tu-PO4

Magnetic Properties of (1–x)La$_{0.7}$Sr$_{0.3}$MnO$_3$/xGeO$_2$ Composites

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(1–x)La$_{0.7}$Sr$_{0.3}$MnO$_3$/xGeO$_2$ composite samples with $x = 0.1–0.3$ demonstrated the high absolute values of isotropic negative magnetoresistance about 15% at room temperature$^7$. Here we present the investigation of microstructural and magnetic properties of (1–x)La$_{0.7}$Sr$_{0.3}$MnO$_3$/xGeO$_2$ composite materials for $x = 0$, 0.15, 0.2. For the preparation of composites the GeO$_2$ was added in the stoichiometric mixture of La$_2$O$_3$, SrCO$_3$, Mn$_2$O$_3$ at the percolation threshold. The additional GeO$_2$ leads to the decreasing of the absolute value of the magnetization and $T_C$ of composite materials in respect to pure La$_{0.7}$Sr$_{0.3}$MnO$_3$ (Fig. 1). The changing in magnetic properties of these samples can be connected with magnetic inhomogeneity that proofs by the two lines in the electron spin resonance spectra of (1–x)La$_{0.7}$Sr$_{0.3}$MnO$_3$/xGeO$_2$.

$^7$Yu. V. Kabirov et al., Technical Physics Letters 42, 278 (2016)
Effects of vanadium or nickel substitutions on the crystal structure and properties of Fe$_{7-y}$M$_y$Se$_8$.

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The magnetic behavior of the ferrimagnetic compound Fe$_7$Se$_8$ with a layered superstructure of the NiAs type is strongly dependent on the distribution and ordering of vacancies in cationic layers and substitutions. In the present work, the compounds Fe$_{7-y}$M$_y$Se$_8$ (M = V, Ni) have been prepared by an ampoule synthesis method in the whole concentration range (0 ≤ y ≤ 7) and studied by means of X-ray diffraction, magnetic susceptibility, magnetization, electrical resistivity and thermal expansion measurements. All the synthesized samples are observed to exhibit a layered crystal structure of the NiAs type. The substitution of vanadium or nickel for iron leads to anisotropic changes in the crystal lattice. Thus, the V for Fe substitution is found to expand the crystal lattice in the direction perpendicular to the layers, however, the average intra-layer distance slightly decreases with increasing V content. In the Fe$_{7-y}$Ni$_y$Se$_8$ system, the replacement of Fe by Ni atoms reduces an average interlayer distance by about 7% with an increase in the nickel concentration up to y = 7, while the interatomic distances within layers remain almost unchanged. In both the Fe$_{7-y}$V$_y$Se$_8$ and Fe$_{7-y}$Ni$_y$Se$_8$ systems the magnetic ordering temperature and the resultant magnetization shows are observed to decrease with increasing content of substituting elements. Below y < 4, the Fe$_{7-y}$M$_y$Se$_8$ compounds (M = V, Ni) exhibit a ferrimagnetic order as the non-substituted compound Fe$_7$Se$_8$; the magnetic state of Fe$_{7-y}$M$_y$Se$_8$ with 4 < y < 6 seems to be non-homogeneous and of a spin cluster glass type; while at y > 6, they show a Pauli paramagnetic behavior.

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Magnetic Properties of Copper-Based Ludwiges

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Here we present the investigations of structural and magnetic properties of Cu-based compounds of the ludwigite family: Cu$_2$AlBO$_5$, Cu$_2$GaBO$_5$ and Cu$_{2.5}$Mn$_{0.5}$BO$_5$. These single crystals were synthesized by the flux method in the form of orthogonal prisms (Fig. 1a inset). The synthesized samples have a monoclinic symmetry and belong to the P2$_1$/c space group.

The important peculiarity of Cu$_{2.5}$Mn$_{0.5}$BO$_5$ compared Cu$_2$GaBO$_5$ is the presence of two Jahn-Teller cations in the structure. Because of the strong distortions of the nearest surroundings of Mn and Cu ions the original magnetic structure is expected. The typical feature of these compounds is a presence of quasi-low dimensional elements - ribbons, ladders, zigzag walls. The significant difference between Cu$_2$GaBO$_5$/Cu$_2$AlBO$_5$ and Cu$_{2.5}$Mn$_{0.5}$BO$_5$ magnetic structures is manifested in temperature dependencies of magnetic susceptibility presented in Fig.1, where we can see the magnetic phase transition in Mn-containing ludwige and difference in absolute values of magnetization between Mn-containing and non-containing ludwigites.

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The intercalation of niobium diselenide by 3d-metal atoms leads to suppression of the transition to the superconducting state and results in the appearance of the structural and magnetic transitions. Along with the intercalation of 3d elements which occupy positions between tri-layer blocks of Se-Nb-Se, it is of great interest to introduce additionally hydrogen atoms into NbSe₂ since hydrogen predominantly occupies the positions inside the block around the Nb ions. In the present work, the Cr₃NbSe₅ compounds intercalated with Cr atoms up to x = 0.33 were synthesized by a solid-state reaction method, and the synthesized samples were hydrogenated using a Siverts-type apparatus at hydrogen pressures up to 16.5 MPa for 7 hours at temperature 630 K. Intercalation of hydrogen and 3d-metal (Cr) into NbSe₂ matrix was carried out for the first time. The HₓCrₓNbSe₂ samples (0 ≤ x ≤ 0.33) with co-intercalated chromium and hydrogen were studied by X-ray, magnetization and electrical resistivity measurements. The hydrogenation of NbSe₂ is observed to increase the unit cell volume by about 3 %, while the Cr-containing samples (x = 0.05, 0.1) show a lower change in the unit cell volume (∆V ~ 1%). It has been found, that an increase in the intercalant content in CrₓNbSe₂ above x = 0.1 prevents the formation of a stable hydride. The CrₓNbSe₂ compounds exhibit various magnetic states from spin glass at low Cr concentrations to a long-range ferromagnetic order at x ≥ 0.25. The intercalation of hydrogen into CrₓNbSe₂ is observed to increase the spin-glass freezing temperature from 3 K up to Tₓ=6 K, however, the hydrogenation process does not influence the magnetic properties of the CrₓNbSe₂ compounds with increased Cr content (x ≥ 0.33). The results obtained show that the effect of hydrogenation on the structure and properties of intercalated transition metal dichalcogenides depends on the type and concentration of intercalated atoms.

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We report on the synthesis and physical properties of polycrystalline R₃NiSi₃ (R= La and Ce) which crystallizes in orthorhombic (Space group Immm) structure. A detailed study of physical properties has been performed by means of electrical resistivity ρ(T), magnetic measurements and heat capacity measurements which suggest that Ce₃NiSi₃ orders antiferromagnetically below T�试=6.2 K. ρ(T) data of Ce₃NiSi₃ resembles with that observed in usual Ce based Kondo lattice/ heavy fermion(HF) compounds. An enhanced value of Sommerfeld coefficient (~260mJ/mol K²) strongly indicates HF behavior of Ce₃NiSi₃ which is a rare example of a Ce-based compound exhibiting HF behavior in the presence of magnetic ordering in the system.
Tu-PO9

Antiferromagnetism and Related Phenomena in Non-centrosymmetric UIrSi3

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We have grown a UIrSi3 single crystal and measured the AC susceptibility magnetization, specific heat, electrical resistivity, magnetoresistance, and magnetostriiction as functions of temperature, external magnetic field and hydrostatic pressure.

The results provide clear evidences of antiferromagnetism below $T_N = 41.7$ K with strong uniaxial anisotropy.

The AF ordering is suppressed by a metamagnetic transition (MT) at the critical magnetic field $H_c (= 7.3$ T at 2 K) applied along c whereas the a-axis magnetization shows only weak linear response to the field up to 14 T. At low temperatures (< 28 K) the MT is a first-order transition manifested by a step in magnetization and all the other measured properties.

The pronounced field hysteresis of MT is attributed to slow relaxations of the spin arrangement from the metamagnetic state to a complex ground-state AF structure. $H_c$ decreases with increasing $T$ whereas the hysteresis becomes rapidly reduced and vanishes above 25 K. At $T < T_N (H=0)$ the MT is of second-order type. The point of change of the order of transition at $T_{M} ~ 28$ K and $\mu_0 H_{M} ~ 5.9$ T in the $H$-$T$ magnetic phase diagram is tentatively suggested to be a tricritical point. $T_N$ and $T_{M}$ increase with applying hydrostatic pressure whereas $H_c$ and $H_{M}$ decrease which has interesting consequences in the evolution of MTs at $T$ above 28 K temperatures with varying hydrostatic pressure.

The temperature dependencies of the a- and c-axis paramagnetic susceptibility, respectively, are crossing at ~ 93 K. The Weiss temperatures $\Theta^a_c ~ -60$ K and $\Theta^c_c ~ +38$ K obtained from modified-Curie-Weiss-law fits point to competing ferromagnetic and antiferromagnetic interactions which are apparently responsible also for the low $H_c$ values in comparison to the rather high $T_N$.

Tu-PO10

Quasi-binary System CeCoC2–CeNiC2: Crystal Structure and Physical Properties

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Ternary compounds CeTC2 ($T =$ Co, Ni) crystallize in two original structure types: orthorhombic CeNiC2-type, space group Amm2 and monoclinic CeCoC2-type, space group Cc'. These carbides are interesting for their complex magnetic and electric properties.1 In the present study, we report on crystallographic characteristics, magnetic properties, heat capacity and electrical resistivity of a series of solid solutions CeCo1–xNixC2 (x = 0, 0.33, 0.5, 0.67, 0.83, 1). The samples were prepared by arc-melting stoichiometric amounts of the constituent elements and annealed at 1073 K for 4 weeks. Co richer solid solutions CeCo1–xNixC2 (0 ≤ x ≤ 0.5) crystallize in the monoclinic CeCoC2-type structure; $a = 5.4073(4)$ Å, $b = 7.4873(5)$ Å, $c = 5.4075(4)$ Å, $\gamma = 102.1311(6)^\circ$, $V = 213.90(5)$ Å3 for x = 0.5. Ni rich CeNi1–xCoxC2 with y = 0.17 and 0 are isotopic with the orthorhombic CeNiC2-type structure, $a = 3.8563(7)$ Å, $b = 4.5534(8)$ Å, $c = 6.1601(1)$ Å, $V = 108.17(6)$ Å3 for y = 0.17. In the region 0.5 < x < 0.83 two phases CeCo1–xNixC2 and CeNi1–xCoxC2 coexist. The non-isoelectronic substitution of Ni by Co in the solid solution CeNi1–xCoxC2 causes a continuous reduction of Néel temperature and finally results in a paramagneticresh Kondo-lattice ground state of CeCoC2.

Tu-PO11

Effect of (Zr,Mn) co-doping on structural, electronic and magnetic properties of zinc sulphide by first-principles studies

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Electronic and optical properties of (Zr, Mn) co-doped ZnS were investigated by using FP-LAPW method with LSDA and LSDA+U approximations. The lattice parameter of undoped ZnS was found in a good agreement with the experimental work; it was increased by doping ZnS with Zr and Mn impurities. In this work, we showed the semi-conducting behavior of doping ZnS from the band structure and density of states calculations. The band gap of ZnS was found to be decreased by co-doping with Zr and Mn elements. Furthermore, to calculate the correct exchange couplings d-d and sp-d of Mn-doped ZnS, we have applied the Hubbard U parameter on Mn-d states. The influence of this Hubbard U parameter on the optical, electronic and magnetic properties of ZnS:(Zr,Mn) is investigated. (Zr,Mn) co-doping leads to the formation of magnetism in ZnS. Zinc sulphide has an absorption peak in UV region. Hence, (Zr, Mn) co-doping leads to an optical peak at about 395nm. This material can be one of the most promising materials for optoelectronic devices

Tu-PO12

Extended phase diagram of RNiC2 family: linear scaling of the Peierls temperature

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The ternary rare earth nickel carbides RNiC2 (R-rare earths) have recently attracted much interest due to intriguing physical properties, i.e. charge density waves (CDW), antiferromagnetic or ferromagnetic ordering and superconductivity are ideal candidates to study the competition/coexistence between the CDW state and magnetism. So far, the CDW state was reported for seven compounds of RNiC2 family (R = Ce, Pr, Nd, Sm, Gd, Tb and Ho) within temperature range 89 K - 317 K.

Physical properties for the late lanthanide based RNiC2 (R = Dy, Ho, Er and Tm) ternary compounds will be presented here. The results of the transport and galvanomagnetic properties confirm a charge density wave state at and above room temperature with transition temperatures T_{CDW} = 284 K, 335 K, 366 K, 394 K for DyNiC2, HoNiC2, ErNiC2 and TmNiC2, respectively. As a conclusion, an extended phase diagram for RNiC2 family (including R = Dy, Ho, Er, Tm and Lu) with linear scaling of Peierls and lock-in transition temperatures will be shown here as well.

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Tu-PO13

Antiferromagnetic-Weak Ferromagnetic Transition in Bi$_{1-x}$Ae$_x$Fe$_{1-x}$Ti$_x$O$_3$ Multiferroics

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Magnetoelectric multiferroics exhibit the simultaneous existence of spin and electric dipole ordering, making them promising for future technological applications. While BiFeO$_3$ is the most thoroughly studied magnetic ferroelectric compound, the properties of its solid solutions remain a matter of intensive debate. In this paper we show how variation in the chemical composition of Bi$_{1-x}$Ae$_x$Fe$_{1-x}$Ti$_x$O$_3$ ($Ae$=Ca, Sr, Ba) perovskites affects their crystal structure and magnetic behavior. In particular, our research demonstrates that Ca/Ti and Sr/Ti substitutions suppress the cycloidal antiferromagnetic structure specific to the parent compound, thus stabilizing a weak ferromagnetic ferroelectric state. The Ba/Ti-doped solid solutions retain the magnetic behavior characteristic of the pure BiFeO$_3$. The composition-driven changes in the magnetic properties of the Bi$_{1-x}$Ae$_x$Fe$_{1-x}$Ti$_x$O$_3$ compounds correlate with the evolution of lattice parameters, thus confirming the existence of a tight coupling between the magnetic and structural/electric dipole order in these materials.

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Tu-PO14

Magnetopiezoelectric effects in easy-plane ferroborates

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Rare-earth borates with formula RFe$_3$(BO$_3$)$_4$ (R = Y; La-Nd; Sm-Er) are popular object of study because they are rare-earth borates which combine magnetically ordered and ferroelectric media properties. This is why ferroborates belong to the family of multiferroics 2

Since ferroborates belong to noncentrosymmetric class 32, the direct piezoelectric effect (PE) is allowed in these crystals. We have investigated the piezoelectric properties of SmFe$_3$(BO$_3$)$_4$ and NdFe$_3$(BO$_3$)$_4$ single crystals using the acoustic method 3

It was found that in those compounds, the value of the piezoelectric modulus e$_{11}$ in the paraelectric phase ($\approx 1.4$ C/m$^2$) was almost an order of magnitude higher than that of the α-quartz, and, therefore, such compounds may be recommended for technical applications.

In addition to the above-mentioned direct PE in multiferroics the indirect PE may exist. It consists in the joint action of the magnetoelastic and magnetoelastic mechanisms. Due to magnetoelastic deformation changes the state of magnetic variables and through the magnetoelastic coupling excites the electric field (and vice versa). This effect was first discovered in samarium ferroborate 4

In NdFe$_3$(BO$_3$)$_4$, direct renormalization of the piezoelectric interaction in a magnetically ordered phase is observed 4


Tu-PO15

Field Induced Phase Transitions and Magnetic Phase Diagrams Revisited in DyIG*

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The far-infrared spectra of magnetic excitations have been studied recently on dysprosium iron garnet (Dy3Fe5O12 or DyIG) single crystals and a connection with the changes of the static dielectric constant and magnetic susceptibility has been found [1]. A peculiar behavior was revealed under a low critical magnetic field $H_C$ for $H$ applied along the <100> direction and a magnetic phase diagram (MPD) was established on the basis on the values of $H_C < 0.38 T$ below a critical temperature $T_C = 16 K$ where the so-called angular <uvv> phases occur at $T_{SR} = 14.5 K$ [2]. Few works have been devoted to the study of the field induced phase transitions (FIPTs) predicted from the Néel theory of ferrimagnets and the related complicated MPDs depending of the H direction in a wide range of T well below the magnetic compensation temperature $T_{comp} = 218.5 K$ [3]. Only the Faraday rotation measured up to ~ 25 K under ultra-high magnetic fields up to 200 T and applied along the easy axis of magnetization <111> has revealed the separation of the canted phase in two parts [4]. Using spherical single crystals of DyIG, the MPD is reinvestigated by means of magnetization measurements in DC fields up to 16 T applied along the three mean crystallographic directions in the 1.5-300 K temperature range. Far away $T_{comp}$, FITPs related to the end of the rotation of the easy axis of magnetization from <111> toward the hard directions <100> and <110> of $H$ are observed at a critical field $H_{C1}$. Below 150 K, a significant anisotropy appears between the two lines $H_{C1}$ which increase with decreasing of $T$ up to $T_{SR}$ where a third critical field $H_{C0}$ ~ 1 T is observed for $H//<111>$. Boundaries of the MPD stability regions are specified in the (H-T) plane.


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Tu-PO16

Anomalous Behavior of the Magnetic Structure in YbIG at Low Temperature*

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The magnetic structure in ytterbium iron garnet Yb3Fe5O12 or YbIG has been studied using powder neutron diffraction (NPD) in the 1.5-130 K temperature range. Two types of reflections, {hkkl} and {hkkl}* are observed in the NPD pattern at 1.5 K. They are indexed with the same general extinction rule of the cubic space group $I4_3d$ No. 230, (h + k + l = 2n) with the propagation vector, $k = [000]$. The first set of fundamental reflections {hkkl} such {(211), (220), (321), (400), (420), (332), (422), (431), (521), (440), (532), (611), (620) and (541)} are due to the contribution of the collinear ferrimagnetic ordering of the Néel model along the easy axis <111> below room temperature. Whereas the intensities of the reflections (211) and (321) decrease slowly up to 80 K, the reflection (220) increase between 1.5 and 80 K and shows an inflection point near 14 K. They tend to an independent plateau-like in the 80-130 K temperature range. The lines (200)* and (110)* constitute the second set of reflections {hkkl}* They are considered as the superstructure reflections forbidden by the nuclear space group. The line (200)* was observed previously at 1.5 K [1] whereas (110)* appears for the first time. It is interestingly to mention that the superstructure lines (222)* and also (622)* which have not been given special attention before [1, 2] are absent in the whole temperature range. The results which are in favor with the signature of a “double umbrella” of the Yb* moments at 1.5 K are also compared with those found with the $^{57}$Fe NMR measurements carried out on Yb0.1Y2.9G [3] and discussed on the basis of the experimental and theoretical works of Belov [4] who predicted a low-temperature point $T_B$ estimated close to 14 K.


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Tu-PO17

Large magnetocaloric effect in Ni(en)$_2$Ni(CN)$_4$ induced by a crystal-field anisotropy

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Experimental studies of the thermodynamic properties of Ni(en)$_2$Ni(CN)$_4$, (en = C$_2$H$_8$N$_2$) commonly known as NENC, revealed that the compound can be considered as an $S = 1$ antiferromagnetic Heisenberg chain with strong planar $D/k_B = 6.3$ K and weak in-plane anisotropy $E/k_B = 0.9$ K with $D/|E| = 7.5$ [1]. Electron-spin-resonance studies have shown the existence of single-ion bound states in NENC [2]. NENC crystallizes in the monoclinic space group $P2_1/n$, $a = 7.104$ Å, $b = 10.671$ Å, $c = 9.940$ Å. The structure is built up of infinite electroneutral $\text{-}[\text{NC-Ni(1)-(CN)}_2\text{-CN-Ni(2)-(en)}_2]_\infty$ chains parallel to the $c$ axis. The Ni(1) atom is square-planarly coordinated by four cyano groups, thus it is diamagnetic. The paramagnetic Ni(2) atom is placed in the center of the deformed octahedron, where four N atoms of the two $en$ molecules are in the basal plane, while two N atoms from the cyano groups are in apical positions. Magnetocaloric studies of a single crystal of NENC weighing 0.42 mg have been performed in the magnetic field up to 5 T applied along the crystallographic $b$ axis in the temperature range from 2 K to 10 K. The isothermal magnetization curves have been measured in a commercial Quantum Design SQUID magnetometer. In the first approximation, the magnetocaloric effect in NENC has been theoretically calculated within a simple model of a spin 1 paramagnet with energy levels split by a crystal field described by $D$ and $E$ parameters. Large conventional magnetocaloric effect was found around 3.5 K ($\Delta S_{\text{max}} = 12$ J/kg K for 5 T). Temperature dependence of the isothermal entropy change under different magnetic fields is in good agreement with theoretical predictions from crystal electric field parameters.


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Tu-PO18

Effect of hydrogen on the structure, magnetic and magnetocaloric properties of Laves phase type-compounds R(Fe$_{0.25}$Co$_{0.75}$)$_2$H$_{y}$ with $R = \text{Er, Ho and y = 0, 1.5 and 3.5}$

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In the present work, the effects of hydrogen atom insertion in the crystal structure and overall magnetic properties of R(Fe$_{0.25}$Co$_{0.75}$)$_2$H$_{y}$ series were analyzed. The metal compounds synthesized using the cold crucible HF melting technique, were found single phase of cubic Laves phase C15 type. Then, resulting metal hydrides with various hydrogenation levels, which synthesis was controlled using a PCI apparatus, were received as well as C15 type compounds. Both parent systems were analyzed for their magnetic susceptibility and magnetization behaviors versus temperature and magnetic field strength. The impact of hydrogen insertion on the cell parameter, the Curie temperature $T_C$ and the magnetization saturation were determined. All compounds and hydrides are ferrimagnets, the magnetic moment of R and 3d elements being opposite since Ho and Er belong to the 2$^{nd}$ raw of rare earth elements. Depending on the formula, a typical compensation point was noticed. The 2$^{nd}$ character of the ferri- ↔ paramagnetic transition was determined using the Arrots’ plots method. Magnetic isotherms plotted vs magnetic field have allowed quantify the strength and thermal range of magnetic entropy variation applying the Maxwell relation.

Hydrogen has revealed as a very interesting lever arm, to increase the MCE of the starting material, with a fine adjustment of the Curie temperature by controlling the hydrogen content. However increasing y leads to decrease both $T_C$ and the potential application range to lower and lower temperatures, e.g. cryogenic uses.
Tu-PO19

Extension of the IrIn3 Structure Type Family: New Members with 7th Group Metals and Theirs Thermoelectric Properties

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Nowadays various intermetallic compounds are being widely investigated as prospective thermoelectric materials. Among them are compounds of the IrIn3 structure type. For instance, Zn or Sn substituted RuIn3 possess a high figure-of-merit $ZT = 0.8$. It is known that compounds with the IrIn3 structure type are formed by combination a transition metal from either the group 8 or 9 on the one hand and $p$-metal, Ga or In, on the other hand, and the number of valence electron ranges between 17 and 18. Owing to strong hybridization of $d$- and $p$-orbitals of a transition metal and $p$-metal, respectively, a gap opens near the Fermi level, and for 17 electron compound this level may fall into the gap causing semiconductor properties. Tuning the Fermi level by the substitution into $d$- or $p$-sublattices affects the transport properties, which make these compounds promising thermoelectric materials.

Until recently, only one IrIn3 structure type’s member has been known in which the group 7 metal is contained in the $d$-sublattice under normal conditions. This is Fe$_{1+x}$Mn$_x$Ga$_3$ solid solution. In our work, new Fe$_{1+x}$Re$_x$Ga$_3$ solid solution was synthesized. In addition, the low and high-temperature thermoelectric properties of the Fe$_{1+x}$Mn$_x$Ga$_3$ and Fe$_{1+x}$Re$_x$Ga$_3$ solid solutions in comparison to each other were investigated.

Furthermore, we obtained first IrIn3 structure type member, in which the $d$-sublattice consists entirely of the group 7 element - rhenium. The peculiarities of crystal structure, composition and thermoelectric properties of new compounds will be presented in this report.

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Tu-PO20

Magnetic and magnetocaloric properties of the Gd-rich melt-spun Gd$_{75}$M$_{25}$ alloys: the role of 3d metal

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The aim of this work is to study the impact of the transition metal atoms on magnetic and magnetocaloric properties of amorphous alloys with a high content of gadolinium. Amorphous Gd$_{75}$M$_{25}$ ($M=$ Fe, Co, Ni) samples were prepared by liquid quenching. The glass forming ability of these alloys is observed to decrease with increasing Fe content. Magnetization measurements were performed using a SQUID-magnetometer MPMS-7EC-XL (Quantum Design, USA) in magnetic fields up to 70 kOe and in temperature range 2 K – 350 K. The amorphous Gd$_{75}$M$_{25}$ ($M=$ Fe, Co, Ni) alloys are found to exhibit a soft ferrimagnetic behavior unlike the crystalline Gd$_3$Co and Gd$_3$Ni compounds which are antiferromagnets. The substitution of Co and Ni for Fe in the melt-spun Gd$_{75}$M$_{25}$ alloys leads to an increase of the magnetic ordering temperature from 172 K and 118 K up to 244 K. The average values of the magnetic moment per transition metal atom, obtained from saturation magnetization measurements, are found to be of about 1.6 $\mu_B$, 1.2 $\mu_B$ and 1.1 $\mu_B$ for the melt-spun Gd$_{75}$Co$_{25}$, Gd$_{75}$Ni$_{25}$, and Gd$_{75}$Fe$_{25}$, respectively. The variations of the Curie temperature and magnetization in Gd$_{75}$M$_{25}$-type amorphous alloys ($M=$ Fe, Co, Ni) are discussed bearing in mind a possible noncollinearity of magnetic moments of 3d metal atoms. The maximal values of the isothermal magnetic entropy change ($\Delta S_m$) are observed to exhibit the Fe-poor alloys. The results obtained in the present work have shown that the change in the concentration of 3d-metal of different types in amorphous Gd$_{75}$M$_{25}$ alloys with a constant gadolinium content makes it possible to vary both the magnetocaloric effect and the operating temperature range.

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Phase transitions and magnet properties of BiNb$_{1-x}$Fe$_x$O$_{4-\delta}$

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The magnetic susceptibility and ESR of iron-containing solid solutions BiNb$_{1-x}$Fe$_x$O$_{4-\delta}$ of triclinic and orthorhombic modifications synthesized by the ceramic method have been studied$^1$. The X-ray diffraction analysis and magnetic dilution allowed us to establish that the phase transition of the polycrystalline compact samples of BiNb$_{1-x}$Fe$_x$O$_{4-\delta}$ from the orthorhombic modification to the triclinic modification is reversible and is a result of prolonged calcination at 750 °C. The doping of BiNbO$_4$ with iron atoms stabilizes the solid solution structure and prevents the reversibility of the phase transition. During the phase transition from the triclinic modification to the orthorhombic modification, the magnetic susceptibility decreases significantly and the complicated system of lines typical for the triclinic modification disappears in the range of 80–300 mT of the ESR spectra.

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Tu-PO22

Slow magnetic relaxation in the presence of the optical phonon modes in KEr(MoO$_4$)$_2$ $^*$

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Slow magnetic relaxation in the lanthanide f-element based single ion magnets (f-SIMs) have been studied intensively during last 15 years$^1$. Effects of slow relaxation with respect to electron energy levels have been successfully understood. Other degrees of freedom that can potentially affect slow magnetic relaxation are low-lying optical phonon modes. KEr(MoO$_4$)$_2$ represents a system with very well described electron energy levels and optical phonon energy levels. The ground state of a free Er$^{3+}$ is $^4$I$_{15/2}$ multiplet, which is split into 8 Kramers doublets with the energies $E_{11}/k_B = 18.7$ K and $E_{21}/k_B = 45.4$ K above the ground doublet $E_{01,02}$. Recently, the energies of two optical phonon modes have been reported, $S_{1a}/k_B = 24.5$ K and $S_{1b}/k_B = 37.5$ K$^2$. It was shown that the application of the external magnetic field along the medium axis c splits the electron doublets and two crossing points between electron and phonon energy levels appear in the fields $B_{c1} = 0.8$ T ($E_{12}$ and $S_{1a}$) and $B_{c2} = 1.8$ T ($E_{11}$ and $S_{1a}$). Previous thermodynamic studies of KEr(MoO$_4$)$_2$ indicated a presence of magnetic correlations described by a model of a two-dimensional array of $S = 1/2$ ferromagnetic Ising chains with an intrachain coupling, $J_1/k_B \approx 0.85$ K and an interchain antiferromagnetic coupling, $J_2 \approx 0.2 |J_1|$. Long-range magnetic ordering of Er$^{3+}$ moments in zero magnetic field was observed at $T_C = 0.95$ K$^3$. While experimental study of AC susceptibility in the paramagnetic phase $T \geq 2$ K in zero magnetic field did not indicate any magnetic relaxation, slow magnetic relaxation appears in the magnetic field applied along the c axis up to $B_{c2}$. The frequency dependence of the out-of-phase component, $\chi''$, and corresponding Cole-Cole diagrams point at the existence of multiple separate relaxation processes with a different time scale. Different types of magnetic relaxation found in the three regions of the magnetic fields $0 < B < B_{c1}$, $B = B_{c2}$ and $B_{c1} < B < B_{c2}$ are discussed.

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Tu-PO23

Lanthanide-based MOFs built on silicon-containing carboxylate ligands: Synthetic strategies and properties evaluation

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This study shows that using two different polycarboxylate ligands: bis(p-carboxyphenyl)diphenylsilane and tri[p-carboxyphenyl]phenylsilane, in combination with control of synthetic parameters such as solvents, temperature and metal ions (f-block elements) could lead to new porous materials with interesting structures and properties (figure 1). Such compounds show excellent structural properties due to the special arrangement of the polynuclear clusters (SBUs) resulting in a diversity of structural motifs as single crystal X-ray diffraction analysis revealed. The presence of the silicon atom with a higher polarizability could confer several advantages compared with their carbon analogues, the most important being the properties associated with the increased processability and solubility. The conformational flexibility of such ligands due to longer bond lengths than carbon analogues has been shown to have a great impact on the final architecture of the structure.

Figure 1. X-ray structures of MOFs based on bis(p-carboxyphenyl)diphenylsilane (a) and tri[p-carboxyphenyl]phenylsilane (a) and Pr(III) (a) and Eu(III) ions (b)

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Tu-PO24

Indication of Unconventional Superconductivity in β-Bi2Pd Studied by Resistivity under Pressure

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We have studied pressure effect on superconducting and normal state properties of β-Bi2Pd sample (Tc ≈ 4.98 K at ambient pressure) by electrical resistivity. In addition, we have performed heat capacity measurements in the temperature range 0.7 - 300 K at ambient pressure. In superconducting state we have focused on the influence of pressure on superconducting transition temperature Tc, upper critical field (Hc2), and coherence length (ξ). Recent calculations of electronic DOS, electron-phonon interaction spectral function α2F(ω) and phonon density of states of β-Bi2Pd [1], were examined by our experimental results. A simplified Bloch-Grüneisen model with one Einstein phonon mode was used to analyze the pressure effect on the temperature dependence of normal state resistivity. The obtained results point to a decrease of the electron-phonon coupling parameter λ and to shift of phonon frequencies to higher values with pressure. Moreover, the temperature dependence of normal-state resistivity follows a Tβ dependence above Tc up to about ~25 K. Together with the enhanced value of Sommerfeld coefficient γ=13.23 mJ.mol−1.K−2 and the decrease of ρ0 with pressure these results point to significant role of the electron-electron interaction in superconducting pairing mechanism in β-Bi2Pd.

Tu-PO25

**Transition metal compounds in devitrified high-entropy and usual metallic glasses**

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The formation of transition metal compounds (TC) in selected devitrified high-entropy (HE) and conventional metallic glasses (MG) has been studied by using X-ray diffraction (XRD) and magnetic susceptibility ($\chi$) measurements. The alloys selected were Al$_{0.5}$TiZrPdCuNi [1], (TiZrNbL)$_{1-x}$M$_x$ (L = Cu, Ni; M = Fe, Co, Ni, Cu) [2] HEMGs, as well as conventional binary and ternary MGs containing early (TE) and late (TL) transition metals, such as the Ti, Zr, Hf – L [3] and Zr-Cu-Al alloys. Such study provides a comparison between the crystallization patterns in TE-TL HEMGs and these in conventional MGs with the same constituents, which can help to understand the differences in glass forming ability (GFA) between HEMGs and conventional MGs [2,3]. The measurements of $\chi$ on both as-cast and crystallized alloys provide an insight into the changes of electronic structure (ES) accompanying transition from amorphous to crystalline (TCs) state, which seem to determine GFA of TE-TL alloys [3]. Further, the values of $\chi$ for crystallized alloys, $\chi_C$, enable in principle the determination of $\chi_L$ values corresponding to particular TCs. These $\chi_C$ (TC) values in addition to giving an insight into contribution of given TC to ES also enable the determination of the fractions of TCs in a given alloy. This is important for a quantitative analysis of the phase contents in alloys in which the crystalline texture make the determination of phase contents from XRD less accurate. Wherever possible we compare and combine our data with the results from literature.

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Tu-PO26

**Magnetic Properties of Kyanites $M_2$GeO$_5$ ($M$=Cr and V)**

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The polymorph Al$_2$SiO$_3$ is known as a geophysically important mineral having three structures of kyanite (space group $P\overline{1}$), andalusite ($Pnnm$), and sillimanite ($Pnma$). Natural minerals generally contain more than one transition element but their content cannot be controlled. Therefore, the interpretations of magnetism for such minerals are difficult and the synthesis of pure 3d substituted systems is required for magnetic investigations. In this paper, we report the synthesis and magnetism of polycrystalline materials $M_2$GeO$_5$ ($M$=Cr and V) with kyanite structure. In each system, the edge-shared $MO_6$ octahedra construct chains running parallel to the triclinic $c$ axes and these chains are two-dimensionally connected by the remaining $M$ atoms. Thus, the presence of two-dimensional layered magnetic network is expected in $M_2$GeO$_5$.

From the results of magnetization and specific heat measurements, we identify that Cr$_2$GeO$_5$ undergoes the transition from the paramagnetic phase to the antiferromagnetic phase at the transition temperature $T_N$ = 60 K. The magnetization curves of Cr$_2$GeO$_5$ observed below $T_N$ show spin-flop like behavior around 8 T. This indicates that the quasi-two-dimensional magnetic interactions predicted from the layered magnetic network are dominant in Cr$_2$GeO$_5$. On the other hand, for V$_2$GeO$_5$ small anomaly indicating the antiferromagnetic phase transition was observed around 36 K in magnetization and specific heat measurements. We will discuss in detail the difference of magnetism between Cr$_2$GeO$_5$ and V$_2$GeO$_5$.

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Electrodynamic response of YbMnBi$_2$: a type II Weyl semimetal candidate

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Weyl fermions play a major role in quantum field theory but have been quite elusive as fundamental particles. Materials based on quasi two-dimensional bismuth layers were recently designed and provide an arena for the study of the interplay between anisotropic Dirac fermions, magnetism and structural changes, allowing the formation of Weyl fermions in condensed matter. Here, we present results of an optical investigation of YbMnBi$_2$, a representative type II Weyl semimetal, and contrast its excitation spectrum with the optical response of the more conventional semimetal EuMnBi$_2$[1]. Our data cover a vast spectral range extending from the far infrared up to the ultraviolet and were collected at different temperatures. Our comparative study allows us disentangling the optical fingerprints of type II Weyl fermions. While our findings are in broad agreement with the most recent theoretical predictions, they also challenge the present understanding of the electrodynamic response in Weyl semimetal.


Drumhead surface states in topological nodal line semimetals

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Nodal-line semimetals are characterized by one-dimensional nodal rings in the bulk protected by symmetry. Projection of these nodal rings onto the surface of a three-dimensional topological semimetal leads to a new class of topological surface states known as drumhead surface states. Materials hosting these exotic features are expected to exhibit several quantum phenomena along with unusual transport characteristics and hence are promising candidates for device application and quantum information. Our research aims at verifying the existence and stability of the drumhead surface states in noncentrosymmetric semimetals.
**Tu-PO29**

**Electron Spin Resonance Study of Anomalous Magnetism of Pr in PrCoAsO**

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We report on an investigation of the itinerant ferromagnet PrCoAsO performed by means of electron spin resonance (ESR) spectroscopy in a broad temperature range between 4 and 300 K. Detailed magnetization and magneto-transport measurements showed that Co moments in PrCoAsO exhibit weakly itinerant ferromagnetic (FM) Co spins ordering at below 80 K with a small magnetic moments of \(\sim 0.12 \mu_B/\text{f.u.}\). ESR study demonstrates that Pr exhibits anomalous behavior in PrCoAsO, as the same though magnetic but still behaves more closely with non magnetic La counterpart LaCoAsO than the magnetic RE comprising Sm/Nd/GdCoAsO. In FM phase, due to delocalization of electrons in presence of low external magnetic fields, conductivity increases quadratically as this is the case of paramagnetic phase. We suppose that RE ions influence the FM phase only via the induced structural shrinkage without involving any active role from the electronic \(f\) degrees of freedom, which are only giving a sizable magnetic contribution at much lower temperatures \(^1\).


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**Tu-PO30**

**Investigation of structural, elastic, mechanic and thermodynamic properties of \(K_{1-x}Na_xFeF_3\)(x=0, 0.25, 0.5, 0.75) alloy: an ab-initio calculation**

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We employed first principles calculations to predict the structural and thermodynamic properties of of \(K_{1-x}Na_xFeF_3\)(x=0,0.25, 0.5, 0.75) alloy using the pseudopotential method with the plane wave (PP) in the context of the functional theory of the DFT density. The structural properties are obtained by minimization of energy in function of volume. Elastic constants \(C_{11}, C_{12}\) and \(C_{44}\) and mechanical properties as shear modulus \(G_{\text{VRH}}\), Young’s modulus , Poisson coefficient \(v\), compressibility \(\mu\) and Lame’ are calculated. The thermodynamic proprieties (thermal expansion, bulk modulus, heat capacity and the Debye temperature) in function of pressure and temperature are obtained using the quasi harmonic Debye model.
Tu-PO31

Half-metallic compensated ferrimagnetism in the Mn-Co-V-Al Heusler alloys

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We show detailed theoretical and experimental investigations on the electronic and magnetic properties of the Mn2xCo1-xVAl and Mn2-Co1-xVAl Heusler compounds. The electronic band structure calculations performed using the Korringa-Kohn-Rostoker (KKR) Green’s function method show the possibility to obtain half-metallic fully compensated ferrimagnets (HMFi) in these Mn2-type of Heusler compounds. The theoretical investigations show different ground state spin configurations of the Mn atoms in these Heusler compounds. The experimental investigations for Mn2xCo1-xVAl with L21 structure show a decrease of the Curie temperature with Co content, between 771 K (x = 0) and 289 K (x = 1). The magnetic moments on the Mn and V atomic sites are very small in the MnCoVAl compound (x=1) with L21 structure, as deduced from the Mn 3s and V 3s core level spectra by X-ray photoemission spectroscopy investigation, with negative consequences on the applicability of the L21-type Heusler compounds in spintronic devices. On the other hand, the band structure calculations for Mn2-Co0.5V0.5Al show half-metallic behavior and increased values of the individual spin moments. An almost compensated ferrimagnetic behavior with a measured Curie temperature of 671 K was found for the Mn2-Co0.5V0.5Al compound, with possible applications in the spintronic devices.

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Tu-PO32

Does Ag doping in ZnO lead to a stable p-type ZnO: A First-Principles Investigation

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The main issue in ZnO related materials and devices, is the existing difficulty to achieve stable and high quality p-type conductivity. In this investigation, first principles calculations within the hybrid functional method are employed to address the electronic properties and possible p-type conductivity in Ag-doped ZnO. We demonstrate that at low Fermi levels required for p-type conduction the potential acceptor defects AgZn and VZn are thermodynamically rare and cannot contribute to the hole generation even at the assumed O-rich condition. We also show that an exothermic reaction between VO and AgZn defects results in VO-2AgZn complex defect, which is shown to be a less effective donor center, compared to single preexisting VO. The formation of this less electronically effective complex defect makes it possible to describe the conductivity instabilities in the silver doped zinc oxide.
Tu-PO43

A stepwise theoretical approach to study hydrogen diffusion in disordered Ti-V-Cr alloys
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Study of hydrogen site solubility and diffusion pathways is of major interest in the overall understanding of fundamental properties of metal-hydrogen systems. Although ordered metal-hydrogen systems have been extensively studied both experimentally and theoretically, a theoretical description of disordered metal hydrides remains still challenging. The main difficulties arise from the correctness of a disorder representation. Ti-V-Cr alloys have proved to be promising materials for hydrogen storage, as they demonstrate good hydrogen sorption kinetics and absorption capacity up to 3.7 w%. In this contribution we propose a theoretical approach to study hydrogen diffusion in disordered Ti-V-Cr alloys. The approach comprises the following steps: to create a supercell with a random distribution of metallic atoms; to calculate hydrogen site solubility energies $E_{sol}$ for a given hydride; using the calculated $E_{sol}$ values and applying Fermi-Dirac statistics to create a model of the hydride with hydrogen distribution over possible interstitial sites; to calculate activation energy for the most probable diffusion pathways using the NEB method accounting for phonon contribution. The calculations have revealed that the hydrogen diffusion path in the fcc TiV₀.₈Cr₁₂H₁.₇₅ hydride from one T-site to another lies near an intermediate O-site. Both the activation energy (0.158 eV) and the diffusion coefficient (3.6 x 10⁻¹¹ m²/s) calculated within this approach are in good agreement with the experimental data. Although the modeling has been done for a particular TiV₀.₈Cr₁₂-hydride we anticipate that the present results can be generalized to the other fcc Ti-V-Cr-hydridses of the series.

¹ All the calculations were carried out using computational facilities provided by Resource Center «Computer Center of SPbU» (http://cc.spbu.ru/en).

Tu-PO33

Structure and Thermodynamics of Mg-Ti-H Films deposited by Microwave Plasma-Assisted Co-Sputtering
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With a hydrogen-uptake of 7.6w% Mg is a challenging material for solid state hydrogen storage. However, the direct formation of MgH₂ operates extremely slowly and both nano-structuration and addition of transition metal “so-called catalysts” were demonstrated effective when processed under certain conditions. The activation mechanism remains a much discussed topic and a large number approaches via electronic structure calculations have tentatively completed the many experimental ones. Recently, Mg-Ti thin film composites have bring a better enlightening of their subsequent H-sorption reaction by Vermeulen et al. [1].

For the first time, a direct synthesis of Mg-Ti-H films with various Ti contents was successfully operated by microwave plasma assisted co-sputtering. The films were systematically analyzed for their structure up to nano-structure by using XRD, FESEM, HRTEM, STEM-HAADF. A peculiar entanglement of stable $\beta$-MgH₂, metastable $\gamma$-MgH₂ and a new hexagonal h-Mg-Ti-H type, was revealed in proportions, structures, textures, grains morphology etc, markedly dependent on the combined amount of Ti (0.15 to 19.5 metal at.%) at synthesis. Desorption/absorption procedures were applied to the hydrogenated films in various conditions using TGA, DTA and mass spectrometry analyses, as well as here above structural techniques. Interestingly the medium Ti containing films (2 to 9 at.%) operate markedly fair reactivity with a desorption temperature for 4.8 at.% Ti occurring 150°C lower than for pure $\beta$-MgH₂. Discussion of the completed results will be made on the basis of initial and final characteristics, (after H-desorption and re-absorption), underlining the peculiar robustness of the new h-Mg-Ti-H, which was demonstrated here surprisingly stable up to ~500°C.


Poster
Structural, Microstructural and Magnetic Properties of Nanocrystalline Ni50Ti50

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In the present work, the influence of milling time on morphological, structural and magnetic properties of Ni50Ti50 powder mixture prepared by high-energy planetary ball milling have been studied. In-depth Qualitative and quantitative phases analysis was performed using Maud program; both structural and microstructural parameters have been refined. It was found that, during the first stage of milling (typically 1 h), the structure consisted of a Ni solid solution [FCC-Ni (Ti)], Ti solid solution [HCP-Ti (Ni)] and amorphous phase (~22 wt. %). For longer milling time, an amorphous phase was obtained followed by the formation of nanocrystalline NiTi-martensite (B19) and NiTi-austenite (B2) phases. The effect of milling time on the evolution of crystallite size, microstrain and dislocations density shows a decrease in crystallite size down to the nanometer scale (~50nm), and increasing of both microstrain and dislocation density. Magnetic measurements of the milled Ni50Ti50 powder mixture exhibit a soft ferromagnetic character where the magnetic parameters are found to be very sensitive to the milling time mainly due to the particle size refinement as well as the formation of amorphous phase. Both the saturation magnetisation (Ms) and coercivity (Hc) were found to decrease with milling time, attaining the values of Ms = 2.8 emu/g and Hc = 48 Oe after 24 h of milling.

Tu-PO35

Relation between the Co-O bond lengths and the spin state of Co in layered Cobaltates using synchrotron radiation: a high-pressure study

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Layered perovskites $A_2$BO$_4$ with a K$_2$NiF$_4$-type structure have been intensively investigated owing to their unique properties, such as high-temperature superconductivity in cuprates, spin-triplet superconductivity in ruthenates, spin/charge stripes in nickelates and manganeseites. Recently, Sr$_2$IrO$_4$ with low-spin (LS) Ir$^{4+}$ has attracted much attention because of the insulating behavior resulting from the strong spin-orbit interaction, while Sr$_2$CoO$_4$ exhibits a metallic behavior because of its intermediate-spin (IS) Co$^{4+}$ coming from both the negative charge-transfer energy and the tetragonal distortion. In this study, the pressure-response of the Co-O bond lengths and the spin state of Co ions in a hybrid 3d-5d solid-state oxide Sr$_{2.5}$Co$_0.5$Ir$_0.5$O$_4$ with a layered K$_2$NiF$_4$-type structure was studied by using hard X-ray absorption and emission spectroscopies. The Co-$K$ and the Ir-$L_3$ X-ray absorption spectra demonstrate that the Ir$^{5+}$ and the Co$^{3+}$ valence states at ambient conditions are not affected by pressure. The Co $K\beta$ emission spectra, on the other hand, revealed a gradual spin state transition of Co$^{3+}$ ions from a high-spin (S = 2) state at ambient pressure to a complete low-spin state (S = 0) at 40 GPa without crossing the intermediate spin state (S = 1). This can be well understood from our calculated phase diagram in which we consider the energies of the low spin, intermediate spin and high spin states of Co$^{3+}$ ions as a function of the anisotropic distortion of the octahedral local coordination in the layered oxide. We infer that a short in-plane Co-O bond length (< 1.90 Å) as well as a very large ratio of Co-O$_{ap}

Poster
Tu-PO36

Correlations and dynamics of spins in an XY-like spin-glass (Ni_{0.4}Mn_{0.6})TiO_{3} single crystal system


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Elastic and inelastic neutron scattering (ENS and INS) experiments were performed on a single crystal of (Ni_{0.4}Mn_{0.6})TiO_{3} (NMTO) to study the spatial correlations and dynamics of spins in the XY-like spin-glass (SG) state. Magnetization measurements reveal signatures of SG behavior in NMTO with a freezing temperature of T_{SG} ~ 9.1 K. The ENS experiments indicated that the intensity of magnetic diffuse scattering starts to increase around 12 K, which is close to T_{SG}. Also, spin-spin correlation lengths (\xi) at 1.5 K are approximately 21.05\pm0.6 and 72.99\pm1.6 Å in the interlayer and the in-plane directions, respectively, demonstrating that magnetic correlations in NMTO exhibit quasi two-dimensional-like antiferromagnetic order. In addition, critical exponent (\beta) is determined to be approximately 0.37\pm0.02 from the intensity of magnetic diffuse scattering confirms the XY-like SG state of NMTO. INS results show quasi-elastic neutron scattering (QENS) profiles below T_{SG}. The life-time of dynamic correlations, \tau ~ h/\Gamma_{q}, obtained from the half width at half maximum of the Lorentzian (\Gamma_{q}) QENS profiles, are approximately 16.27\pm0.8 and 15.88\pm1.9 psec at 10 K for two positions (0.00, 0.00, 1.52) and (0.01, 0.01, 1.50), respectively. Therefore, our experimental findings demonstrate that short-range-ordered antiferromagnetic clusters with short-lived spin correlations are present in the XY-like SG state of NMTO at a temperature of approximately T_{SG}.

Tu-PO37

The comparison of magnetic structures of low-dimensional spin frustrated PbMnTeO_{6}

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In the quasi-two-dimensional magnets with acentric (chiral) crystal structure and a triangular lattice of magnetic atoms in a layer, the competition between exchange interactions, frustrations and anisotropy can revolutionary affect the fundamental mechanisms of ordering and the corresponding phase transitions. Low-dimensional spin frustrated systems assume noncollinear incommensurate spin orderings in order to reduce the degree of their spin frustration. The PbSb_{2}O_{6}-type materials (general formula, ABB'O_{6}) exhibit a layered structure (centrosymmetric space group, P31m).\textsuperscript{1,2} We have discovered and synthesized a compound PbMnTeO_{6} with a similar layered trigonal structure. Previously, the compound of this composition was studied with symmetry group P62m.\textsuperscript{3} Our sample was characterized by Rietveld analysis of the neutron powder diffraction patterns. A magnetic ordering model of PbMnTeO_{6} was constructed.

\textsuperscript{1}The reported study was funded by RFBR according to the research project № 16-02-00260-a.
\textsuperscript{1}Journal Of Solid State Chemistry 71, 12-18 (1987)
\textsuperscript{2}Inorganic Chemistry, 56, 9019–9024 (2017)
\textsuperscript{3}Inorganic Chemistry, 55, 1333–1338 (2016)
Tu-PO38

Addressing the nature of the giant magnetostriction of Galfenol-polyurethane composite by nuclear resonance scattering of synchrotron radiation

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The giant magnetostriction of the Galfenol (Gallium-Ferrum alloy) can be applied and tuned with Galfenol-polymer composites towards further enhancement of its functional magnetoactive response. The performance of the polymer filled with metal particles composites depends on a wealth of parameters as composition, size, morphology, shape and spatial distribution of the grains, polymer matrix, interaction between particles, and properties of the particle-polymer interface. Our recent studies [1-2] showed that, for some specific particles-to-polymer volume concentration, the magneto-deformational effect of the Galfenol-polyurethane composites can be increased up to threefold by an arrangement of the particles in continuous chains. To reveal the mechanisms of the effect, and to use this effect for optimization of the composite properties we used nuclear resonance scattering of synchrotron. Namely, we applied small-angle nuclear resonance scattering to probe the size and shape of the magnetic domains in the particles, and time-domain Mössbauer spectroscopy to monitor the value and direction of the hyperfine magnetic field. The size of the studied particles was about 1 μm. The angular distributions of small-angle electronic and nuclear scattering, and the time spectra of nuclear scattering were analyzed for samples with various particles-to-polymer compositions and particles-in-polymer orientations relative to the synchrotron radiation beam, and for various values of the external magnetic field. The results reveal that the decisive role in the formation of material’s properties belongs to the internal structure and shape anisotropy of the Galfenol particles.


Tu-PO39

Thermoelectric performance of Nb-doped SrTiO3 enhanced by reduced graphene oxide and Sr deficiency cooperation

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Oxide materials are of current interest as high-temperature thermoelectrics in the automotive and manufacturing energy-harvesting sectors due to high chemical robustness, low toxicity and low cost. Driven by a need to improve the thermoelectric performance of n-type oxides to the level of p-type analogues, ceramics and composites based on donor-doped SrTiO3 are considered as a promising material. Here Nb-doped SrTiO3 with Nb content of 10 and 15 % as well as Sr/(Nb+Ti) ratio of 1.00 and 0.98 was mixed with 0.6 wt. % of graphene oxide (GO) prepared by Hummer-based method and conventionally sintered in atmosphere of H2/N2 to reduce both Nb-doped SrTiO3 and GO. Addition of reduced GO in combination with introduction of Sr vacancies provides the best synergistic effect of fastening charge transport and thereby increasing electrical conductivity σ and suppressing the thermal conductivity κ. These factors, together with a moderate Seebeck coefficient S, result in a high power factor PF = S^2σk up to ~1.98 mW/(K m) and thermoelectric figure of merit ZT = PF/κ up to 0.29. These findings offer further prospects for seeking high performance SrTiO3-based thermoelectrics by modification with reduced GO.

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Tu-PO40

Structural stability of the ZrMM’ (M = Ti, V and M’ = Ni, Co, Cu) compounds and related hydrides studied by neutron diffraction and electronic structure calculation

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AB2 Laves phases crystallise with three types of crystal structure: Cubic C15 (MgZn2) Hexagonal C14 (MgCu2) and double Hexagonal C36 (MgNi2). The structural stability of the Laves phases depends on geometric factor (t_{aA}/t_{aB}) and electronic factor (electronegativity difference and valence electron number). Most, ZrM2 compounds show relatively high hydrogen uptake and fast sorption kinetics. However, many hydrides reveal too stable at RT e.g. ZrV2H3, ZrMn2H6, ZrCrH3.4, to develop reversible storage applications. Besides, multi-component Ti/Zr-based Laves phase compounds have retained attention as material electrodes. The present work aims point out chemical and structure parameters expected having a significant impact on the performances in terms of reversible absorption capacity. The crystal structure of the ternary compounds ZrVC, ZrVN, ZrTiNi, ZrTiCo and ZrTiCu and their related hydrides (deuterides) was investigated by neutron diffraction. The microstructure the materials was checked by SEM/EDX analysis. The crystal structure refinement allows confirm the stability of the C14 Laves-type in a large extend of formula. Neutron diffraction experiments performed on the corresponding ZrMM’ hydrides indicate that after hydrogen (deuterium) absorption the crystal structure remains unchanged, except for ZrTiNi. Electronic calculations based on the Korring Kohn Rostoker method with Coherent Potential Approximations (KKR- CPA) were carried out allowing to check the peculiarities of the DOS and total energy for the various ZrMM’ and their hydrides.

Tu-PO41

Proton motion in hydrated layered perovskite-like H2La2Ti3O10

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Layered perovskite-type oxides are considered as promising materials for photocatalytic water decomposition under sunlight irradiation for further hydrogen storage. Moreover, they exhibit rather high mobility of interlayer cations and ability to intercalate water and other molecules. Properties of these compounds strongly depend on the composition (cations, number of perovskite layers, stacking mode). Compounds may be converted into their protonated forms, which exhibit interesting properties, including proton conductivity and photocatalytic activity, affected by the mobility of protons and intercalated molecules. From this perspective a comprehensive study of the proton state and its mobility in the interlayer space is highly required.

Nuclear magnetic resonance (NMR) is a unique tool to study hydrogen motion, first due to a rather wide timescale, and second due to its non-invasive nature that does not perturb thermodynamics of the studied system. NMR is very effective to study both hydrogen diffusivity, and its motional characteristic, like the jump frequency and the activation energy, as well. In this contribution, we report on the results of various NMR techniques applied to study hydrogen motion parameters in a fully hydrated three-layered perovskite-type oxide H2La2Ti3O10.

The evolution of 1H NMR spectra recorded at magic angle spinning (MAS) conditions makes evident that with temperature increasing not only reorientational motion of intercalated water molecules increases but translational as well. This suggests a possibility of the Grothuss mechanism, for which molecular rotations of H2O* is a part of translational diffusion, and which may take place in layered perovskite-like oxides. The asymmetric temperature dependence of the 1H spin-lattice relaxation time and its flattening in the low-temperature region indicate that H2La2Ti3O10 should exhibit high protonic conductivity.

3 The NMR studies were carried out at the Centre for Diagnostics of Functional Materials for Medicine, Pharmacology and Nanoelectronics of Saint Petersburg State University.

Poster
Our work on new superconductors in recent years has concentrated on materials with interesting chemical and crystallographic characteristics, and, in particular, on intermetallic compounds of the transition elements. I will describe some of that work in this talk and put it in context with previously known intermetallic superconductors. The work I will describe has primarily been done by students and postdoctoral fellows in my research group - in particular by Elizabeth Carnicom, Fabian von Rohr, and Karoline Stolze, and also through our collaborations with professors Weiwei Xie at Louisiana State University, Tomasz Klimczuk at the Gdansk Technical University, and Liling Sun at the Institute of Physics in Beijing, and their graduate students and postdoctoral fellows.

The talk will concentrate on two superconducting materials systems. The first system is of interest due to its unusual crystallographic symmetry. In a non-centrosymmetric superconductor the standard superconducting state, where electrons with opposite momenta form pairs on the Fermi surface, is not possible. A handful of such materials is known; they display different degrees of influence of the lack of inversion symmetry on their superconducting properties. The effect of crystal structure chirality on the properties and applications of superconductors, on the other hand, is little discussed. I will describe our recent finding of two new non-centrosymmetric chiral superconductors. The second superconducting system is based on high entropy alloys (HEA), one of which we find maintains its superconductivity to pressures equivalent to that of earth’s outer core, and the second of which, made from combining both early and late transition elements, has a crystal structure of the CuAu type.

The discovery of ferroarsenide superconductors in 2008 immediately attracted attention to functional properties of various compounds of iron. In this paper, we will present and discuss several different compounds of iron with intriguing properties that appear owing to strong electron correlations. We will first focus on layered complex tellurides structurally resembling ferroarsenide superconductors but displaying a framework of short Fe–Fe contacts that evoke metallic properties and peculiar magnetic behavior including a sizable magnetocaloric effect. We will compare these tellurides with intermetallic iron semiconductors rich in $p$-metals, such as FeGa₂. They are promising thermoelectric materials, which properties are governed by strong $d$–$p$ interactions between iron and a $p$-element that open a band gap in the electronic structure near the Fermi level. As an intermediate between these two opposites we will bring to consideration iron germanides that possess atypically complicated antiferromagnetic structures due to comparable contribution of $d$–$d$ and $d$–$p$ interactions to their electronic structure. We will discuss the underlying physics of these properties and the unique role of iron in them.
Recent Progress in Itinerant Magnetism and Spin Fluctuations in Intermetallics and Compounds

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In these several decades, a lot of important theoretical and experimental approaches have been performed for understanding the itinerant-electron magnetism. Among them epoch-making was the great success of the spin-fluctuation theory for weak itinerant ferro- and antiferromagnets based on the self-consistent renormalization of spin fluctuations to magnetic free energy since 1973. Afterwards, the spin fluctuation theory has been developed toward the unified theory between the weakly itinerant ferro- and antiferromagnetic regime and the localized moment regime in metallic magnets by a phenomenological method. Furthermore, the itinerant-electron theory of spin fluctuations has been developed and rearranged in a quantitative way as well as by utilizing different approaches, by which we can compare the experiments and spin-fluctuation theories quantitatively by means of a set of spin-fluctuation parameters [1].

Meanwhile the novel superconductors have been discovered in the strongly correlated electron systems, such as heavy-fermion compounds and intermetallics, the organic compounds, the high-\textit{Tc} cuprates, pyrochlore compounds, Co oxides with triangular lattices, Fe pnictides, and so on. Therefore, the correlations and interplays between the itinerant magnetism and the novel superconductivity, called exotic superconductivity, have been one of the most important problems in the solid-state sciences. In high-\textit{Tc} cuprates and exotic superconductors, microscopic experiments have shown that the magnetic excitations were crucial, leading to the possible mechanism involving magnetic interaction-mediated Cooper pairs [1].

Together with discoveries of exotic superconductors, a lot of interesting itinerant-electron magnets have been discovered around them such as 2D itinerant ferromagnetic compounds, LaOCoAs, LaOCOP, LaCoAs\textsubscript{2}, LaCo\textsubscript{2}P\textsubscript{2}, etc. In this talk, the essence of recent developments in experiments on newly discovered itinerant magnets and theories of itinerant-electron magnetism will be introduced and explained in terms of spin fluctuations [1].


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The puzzling Ru: A synchrotron journey in the electronic properties of some ruthenium oxides

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We recently developed on the material and magnetism beamline I16 at Diamond the capability to investigate the behavior of ruthenium based system by measuring resonant diffraction at the L\textit{2}\textsubscript{3} and L\textit{3} Ru edges. Ruthenium is a fascinating element as it presents an almost infinite variety of behaviors when forming oxides, depending on the compound structure and the Ru electronic configuration [1]. This abundance is reflected in the extremely different behavior of Ru in the hexagonal perovskites and in the Ruddlesden Popper (RP) phases. Sr\textsubscript{2}(Li,Na)RuO\textsubscript{3} are extremely insulating, with high magnetic ordering temperature [2]. Using XRS, neutron and lab characterization we fully characterized the magnetic ground state and we theoretically understood the stabilization mechanism as resulting from tiny effect in the free energy development in Sr\textsubscript{2}(Li,Na)RuO\textsubscript{3} [2]. A completely different behavior is observed in the RP family [3], where the only compound to present an insulating behavior below 365 K is Ca\textsubscript{2}RuO\textsubscript{3}. In this Mott insulator the low temperature phase is characterized by the presence of an orbital ordering and two competing magnetic ground states. Interestingly all the other known Ru based RP systems are metallic with Sr\textsubscript{2}RuO\textsubscript{4} in particular widely studied for its unconventional superconductivity. Ca\textsubscript{2}RuO\textsubscript{4} under the application of an extremely small electric field can be driven through the insulator to metal transition at room temperature [4]. Using XRS we review the currently accepted picture of the magnetic ordering and we investigated the behavior of the orbital and magnetic ordering under an external field.


Oral
**We-A3i, 12:00**

**Vibron quasi-bound states in Ce intermetallics**

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The tetragonal CeTX2 and CeT'X2 compounds, T = d-metal and X = p-metal, have been investigated for a variety of exotic ground state properties. Recently, inelastic neutron scattering experiments on CeCuAl1 and CePd2Al2 powder samples revealed energy spectra containing three CEF-like peaks [1,2] although only two CEF excitations are expected for a Kramer’s Ce3+ ion in a tetragonal point symmetry. The energy spectrum has been interpreted as evidence of a vibron quasi-bound state originating from strong interaction between crystal field excitations and phonons. Such has been proposed for the cubic CeAl2 earlier [3]. Our recent studies on mainly single crystals confirmed the presence of three excitations in the energy spectrum of CeCuAl3. The polarized neutron scattering experiment showed that all three peaks are of magnetic origin and the collected data allowed separating the individual components of the magnetization [4]. Moreover, we investigated the effect of Cu-Al and Al-Ga substitutions on the energy schemes of CeCuAl3 and CePd2Al2 [5,6]. Results of our studies will be discussed and compared to investigations conducted by other groups.

[4] M. Klicpera, et al., to be submitted (recent results)

**We-A4, 12:30**

**Disordered and Frustrated Magnetization in Coated MnFe2O4 Nanoparticles Prepared by Microwave Plasma Synthesis**

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Disordered and frustrated magnetization of different surface coated (CoO, Cr2O3, ZrO2, and SiO2) MnFe2O4 nanoparticles have been studied by using SQUID-magnetometer and analyzed with theoretical simulations. In nanoparticles, it is most important to control their surface functionalization for different applications. The magnetic core anisotropy get different preferential direction as it approaches to the nanoparticle’s surface. Therefore surface spins experience different exchange interactions as compared to core spins. This surface disorder and frustration can lead to the formation of surface spin-glass behavior nanoparticles. Magnetic measurements such as ZFC/FC, temperature dependent M-H loops, AC susceptibility, etc. gave evidence of surface spin-glass behavior. ZFC/FC curves were also compared with numerical simulation. Frequency dependent AC susceptibility was analyzed by using Neel-Arrhenius law, Vogel-Fulcher law and dynamic scaling law to further confirm the spin-glass behavior. It is observed that the strength of surface spins disorder and frustration strongly depends upon the type of coating material. All these analysis signify the presence of disordered and frustrated surface magnetization in MnFe2O4 nanoparticles, which greatly depends upon the type of surface coating materials and are useful for controlling the nanoparticle’s magnetism for different practical applications.

*This work was supported by Higher Education Commission of Pakistan.
We-A5, 12:45

Magnetic properties of multicomponent Al\textsubscript{x}FeNiCrCo High Entropy Alloys*  
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High-entropy alloys (HEA) have become attractive systems due to various technological applications but interpretation of their physical properties is still challenging for condensed matter physics. The specific character of chemical disorder occurring in the multicomponent magnetic alloys yields complex electronic and magnetic interactions on one hand, but allows stabilizing simple crystal structures (bcc, fcc) on the other one. It is known that high configurational entropy tending to lower free energy of the system is an important factor in crystal stability in HEA materials.

The effect of the relative change in Al content with respect to other elements on observed phase coexistence in Al\textsubscript{x}FeNiCrCo alloy has already been experimentally evidenced, using XRD, neutron diffraction and EDX measurements and supported by electronic structure calculation results, especially total energy analysis. However the magnetic properties of the system were not analyzed in view of coexistence of phases with different stoichiometries.

In this work, magnetic properties of particular phases were investigated using VSM technique (magnetization measurements vs field and temperature) as well as Mossbauer measurements. In parallel, the electronic band structure calculations were performed using KKR and KKR-CPA methods, the latter being especially well-adapted to treat chemical disorder systems. Due to large number of elements constituting different crystal structures and compositions in detected phases, various models of disorder have been proposed and discussed. Special attention was paid on analysis of local magnetic moments variation vs. composition and the phase preference. Calculated average hyperfine fields and average magnetic moments of Al\textsubscript{x}FeNiCrCo well correspond to those determined experimentally for various Al concentrations.

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We-A6i, 14:00

Local peculiarity of the crystal structure of hexagonal pnictides of Fe\textsubscript{2}P type impacting the stability of the magnetic structure and the MC effect apart the ordering temperature  
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For more than 40 years the MM'X series of ternary MM'X transition metal phosphides, arsenides, silicides… (orthorhombic, hexagonal and tetragonal polytypes) has retained our attention owing to their very peculiar structural and magnetic properties. One of the most complicated behaviours in the MM'X compounds was found with the MnFeP\textsubscript{1-x}As\textsubscript{x} system, isotype to the hexagonal Fe\textsubscript{2}P type (itself sharing evidence of magnetic instabilities of electronic origin). In fact the magnetic structure can be considered having a net 2D character with successive Mn and Fe (001) sheets, those atoms selectively occupying pyramidal (CN5) and tetrahedral (CN4) X-coordinated sites. Furthermore the magnetic long-range ordering supported by F and AF competing exchange interactions, the 1\textsuperscript{st} and 2\textsuperscript{nd} order character of the magnetic order-disorder transition and the paramagnetic correlations, were established critically dependant of the level of the magnetic polarisation at the tetrahedral site (Fe mainly).

Later, at the ferro–paramagnetic magnetic transition, a markedly strong magnetocaloric effect (MCE) was evidenced for this type of compounds and then MnFeP\textsubscript{1-x}Si(Ge)\textsubscript{x} parents. From a systematic analysis on parent magnetic compounds such as Fe\textsubscript{2-x}Ru\textsubscript{x},P, CrMnAs, Mn\textsubscript{2-x}Fe\textsubscript{x}P\textsubscript{1,5}Si\textsubscript{y}, MnM'X (M' = Ru, Rh, X = P, As)…, a structure-chemical bonding index A was demonstrated to impact the tetrahedral site, which anisotropy governs the local electronic polarisation and correspondingly the overall magnetic trends of the compounds, namely those related to the MCE behaviour.
Many Faces of a Single Cuboctahedron: Structure and Bonding of Group 10 – Main Group Metal Cu₃Au-type Intermetallics and Derivatives

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Ordered intermetallic compounds are a fascinating object of studies both due to their structural diversity and the variety of physical properties. The very fact of their existence in itself is worth explaining, however, they also often feature complicated structure motifs and convoluted bonding patterns, as well as sometimes unique and potentially useful properties and complicated structure-property relationships. Furthermore, if a 3D intermetallic system is diluted with a typical non-metal, the situation becomes even less straightforward. This concept is showcased well using transition metal-rich mixed group 10 – group 13 chalcogenides and pnictides.

The focus of our research is TM₃M intermetallics of the Cu₃Au or related type (where TM = Ni, Pd, Pt; M – main-group metal) as parent compounds for complex ternary phases. The structural unit of such intermetallics is a main-group metal-centered cuboctahedron of transition metal atoms. The packing of these units may vary, depending on the type of constituents, but the units remain the same. We have produced and characterized a series of ternary chalcogenides and pnictides based on the TM₃M-type fragments with structures varying from 2D linear intergrowth structures to open-framework to 3D ones. To gain more insight into their principles of formation and stability, we have studied electronic structures and bonding, both in orbital (COHP) and direct (ELF, ELI-D) space, in ternary compounds and their parent binaries based on the DFT calculations. Along with common features in electronic structures and bonding, the differences in bonding patterns, depending on the type of transition metal, are revealed and discussed.

This work was supported by Russian Science Foundation (Grant No. 14-13-01115). The use of the resources of MSU Supercomputer Center is acknowledged.

Modification of Magnetism of Cr₁₀ wheel molecules on metallic (111) surfaces and bulk

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We report on the magnetic properties of {Cr,}₁₀ wheels (Cr,(OMe)₃, (OCCMe)₃) [1] UHV-sublimated on Cu(111) and Au(111) single-crystals investigated by means of by XAS & XMCD, SQUID magnetometry and STM. We discuss the magnetic anisotropy and magnetic moment field-dependence of the grafted {Cr,} molecules, as a function of the metallic substrate and layer thickness, and compare it with bulk material. Our results demonstrate that evaporated molecules show negligible anisotropy and weak dependence with the substrate. A combination of XMCD and SQUID magnetometry show that Mono- and Multi-layer {Cr,} samples exhibit a magnetic behavior stemming from a S = 9 ground state, ruling out some previous results [1]. Monte Carlo simulations show that the magnetic bulk ground state can be explained by {Cr,} molecules magnetically consisting of two semicrowns containing 4 Cr ions interacting ferromagnetically, separated by 2 Cr ions with antiferromagnetic interactions, giving rise to the ground S = 9 state, in agreement with previous EPR data in literature [2]. Evaporation of {Cr,} onto a substrate producing subtle structural changes induce strong changes in the Cr-Cr interactions and distinct magnetic behavior from the bulk, probably stabilizing S = 0 ground state.

Magnetic properties of FeO$_2$ and FeO$_2$H possible constituents of Earth’s lower mantle

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The recent discovery\textsuperscript{†} of FeO$_2$, which can be an important ingredient of the Earth’s lower mantle and which in particular may serve as an extra source of oxygen and water at the Earth’s surface and atmosphere, opens new perspectives for geophysics and geochemistry, but this is also an extremely interesting material from physical point of view. We found that in contrast to naive expectations, its properties are very different from the well-known pyrite FeS$_2$. FeO$_2$ turned out to be metallic with Fe ions nearly 3+, while FeS$_2$ is an insulator with Fe ions having 2+ oxidation state. Moreover, while FeS$_2$ is diamagnetic, FeO$_2$ is magnetic, with nontrivial temperature dependence of the magnetic susceptibility\textsuperscript{‡}. Doping, which is most likely to occur in the Earth’s mantle, makes FeO$_2$ much more magnetic. The fact that FeO$_2$ lies “in between” the usual dioxides and peroxides makes it also an extremely interesting material for physics and solid state chemistry.

\textsuperscript{*This work was supported by Russian Science Foundation, project 17-12-01207

We-A10i, 16:00

Magnetic Properties and Thermal Conductivity of Layered Borides

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Borides have yielded interesting systems for solid state chemistry and physics investigations \cite{1}. Layered REAlB$_4$ for example, has attracted attention with phenomena such as multiple magnetic anomalies in α-TmAlB$_4$ below the Neel temperature indicated to be due to building defects \cite{2}. It was discovered that the building defect formation could be controlled by counter-intuitive crystal growth conditions \cite{3}. Spin glass-like behavior was discovered in α-HoAlB$_4$ and ErAlB$_4$ \cite{4}. The building defects were also demonstrated to have large effect on the thermal conductivity from TD-TR measurements of microcrystals \cite{5}. Furthermore, the thermal conductivity of AlB$_2$ was discovered to be lower in-plane (≈60 Wm$^{-1}$K$^{-1}$) parallel to the graphitic (graphene-like) structure, compared to cross-plane (≈100 Wm$^{-1}$K$^{-1}$) \cite{5}. This was attributed to the different bonding of borides compared to carbon, i.e. graphite-related material. PrRh$_{4.8}$B$_2$ takes an interesting layered crystal structure, where PrRh$_3$B$_2$ blocks are separated by metal Rh honeycomb layers. The existence of the Rh layers enhances the ferrimagnetic transition temperature. From area-selective picosecond thermoreflectance, the cross-plane thermal conductivity of PrRh$_{4.8}$B$_2$ is estimated to be 1.39 Wm$^{-1}$K$^{-1}$, much lower than other known layered borides. Judging from the fine crystal structures obtained by TEM, phonon conduction is considered to be depressed due to random dispersion of Rh vacancy sites and two-dimensional nature of PrRh$_{4.8}$B$_2$ \cite{6}. The interesting magnetism and thermal conductivity of layered borides will be discussed and presented.


Oral
We-A11i, 16:30

Unusual order in the new compound Ce$_2$Rh$_2$Ga
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The new ternary intermetallic compound Ce$_2$Rh$_2$Ga and its nonmagnetic analogue La$_2$Rh$_2$Ga were found to form in a derivative of the La$_2$Ni$_3$ crystal structure type, with orthorhombic space group Cmce ($\#64$). Each of the atoms occupy a unique site in the unit cell. The Ce atom has six Rh nearest neighbours (2.968 – 3.100 Å) and four Ga nearest neighbours (3.344 – 3.391 Å). The most closely spaced Ce atom pair is separated by 3.432 Å. A striking feature with strong temperature dependence and thermal hysteresis in physical and magnetic properties occurs at $T^* = 128$ K. From Curie-Weiss behaviour below room temperature according to the full free-ion Ce$^{3+}$ effective moment, the magnetic susceptibility deviates and peaks sharply at $T^*$. The electrical resistivity as well as thermal resistivity both pass through a discontinuous jump upward upon cooling through $T^*$. The specific heat rises to a peak value of 440 J/mol.K at $T^*$ which is more than three times the Dulong-Petit value for this compound. We discuss various scenarios that may be responsible for the unusual phase transition found in Ce$_2$Rh$_2$Ga.

$^1$ JHN Van Vucht, and KHJ Buschow, J. Less-Common Met., 46 (1976) 133

We-A12i, 17:00

Crystal Chemistry of Ternary Rare Earth Transition Metal Carbides: Recent Studies
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A brief critical overview will be presented on ternary rare earth – transition element – carbon systems and their compounds. Main attention will be devoted to recent studies of crystal structure peculiarities of ternary carbides. More than 400 ternary phases have been found up to now, 45 of which in past 10 years. In total, they represent a variety of 50 structure types. Three species of carbon arrangement occur in these structures: isolated C atoms, C$_2$ pairs and C$_3$ chains. All known structure types of these ternary carbides are classified into two groups: metal-rich carbides (intermetallics) and carbometalates. Conditional division into these groups is performed depending on the carbon content and the M/C ratio (M = metal atoms). In the latter group, complex anions $[T,C_n]^{y-}$ forming clusters of different dimensionality are identified as the key structure building elements of these compounds. The presence of covalent T–T interactions in $[T,C_n]^{y-}$ clusters was recently confirmed by $^{57}$Fe Mössbauer spectra of R$_3$Fe$_8$C$_{25}$ compounds.

Two series of novel compounds, R$_2$Mn$_2$C$_3$ and R$_2$CoC$_2$, with novel structure-types as well as new representatives of earlier known structure types have been investigated in this work. From the analysis of crystal structure data we estimate some physical properties and the valence states of elements in these compounds. Crystal structure relations with chemical reactivity are discussed. The broad diversity of unusual topologies has rendered these compounds of great interest for experimental as well as theoretical chemistry, and also with respect to their electronic and physical properties.

We-B1i, 11:00

Probing the topological nature of SmB$_6$ by dynamical mean field theory

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Experiments on the presumptive topological insulator SmB$_6$ remain controversial and hotly debated, with largely conflicting physical interpretations. We present reliable density functional theory plus dynamical mean field theory (DFT+DMFT) calculations that yield a mixed valence (4f$^{5.5}$) state with a tiny bulk band gap and a $\Gamma_1+\Gamma_8$ ground state. The bulk states and the emerging topological surface states well agree with angular resolved photoemission spectra (cf. Figure). Strong electronic correlations and the mixed valency severely modify the simple topological Kondo insulator picture, and explain, among others, the unusual spin texture of the topological surface states.

Topological surface states. Left: DFT+DMFT spectrum at the Fermi level vs. momenta perpendicular to the surface (including the spin structure in the left part of the panel). Right: experiment [courtesy of J. Denlinger et al., JPS Conf. Proc. 3, 017038 (2014)].

$^*$This work was supported by the European Research Council under the European Union’s Seventh Framework Program (FP/2007-2013) through ERC grant agreement n. 306447.

We-B2i, 11:30

Multiscale study of itinerant magnetism based on first principles

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The rich variety of magnetic systems acts as a gold mine both for basic research and technological applications. First principles calculations are helpful to explore the underlying physics controlling the formation and dynamics of magnetic structures. I will give an introduction to our theoretical approach based on a fully relativistic implementation of the density functional theory within the local spin-density approximation. The magnetism of itinerant systems can be studied either by means of ab initio spin-dynamics relying on the so-called constrained density functional theory or by mapping the first principles total energy onto a Heisenberg like Hamiltonian to be treated via Monte Carlo simulations or real-time spin-dynamics simulations. The relativistic treatment of the electronic structure allows for a full account of the magnetic anisotropy, of the anisotropic exchange interactions and of the chiral Dzyaloshinsky-Moriya (DM) interactions$^\dagger$.

Among the many studies we performed in the past years I will concentrate on low-dimensional systems in which several novel and challenging consequences of the DM interactions have been explored due to breaking of inversion symmetry. These include homochirality of domain walls$^\ast$, the chiral asymmetry of spin waves$^\ddagger$, the formation of long range magnetic patterns and skyrmionic states in ultrathin films$^\ddagger$, as well as the exchange bias effect at spin-flop coupled antiferromagnet-ferromagnet interfaces$^\ddagger$. 

$^\ddagger$L. Udvardi and L. Szunyogh, Phys. Rev. Lett. 102, 207204 (2009)
Mixed-pairing superconductivity in 5d Mott insulators with antisymmetric exchange

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We study the symmetry of the potential superconducting order parameter in 5d Mott insulators with an eye toward Sr\textsubscript{2}IrO\textsubscript{4}. We investigate the potential existence of a superconducting phase in hole doped Sr\textsubscript{2}IrO\textsubscript{4}, as an example of the new class of Mott insulators. Currently, remarkable attentions have been attracted to exotic physics driven by the interplay of the spin-orbit coupling and electronic correlations. Particularly, in 5d transition metals neither the spin-orbit coupling nor the Coulomb interaction can merely lead to the insulating behaviour. A very interesting question is whether these materials with very similar properties to the cuprates can clarify the essential microscopic physics of high Tc superconductivity? Using a mean-field method, a mixed singlet-triplet superconductivity, d+p, is observed due to the antisymmetric exchange originating from a quasi-spin-orbit-coupling. Our calculation on ribbon geometry shows possible existence of the topologically protected edge states, because of nodal structure of the superconducting gap. These edge modes are spin polarised and emerge as zero-energy at bands, supporting symmetry protected Majorana state, verified by evaluation of winding number and Z2 topological invariant. At the end, a possible experimental approach for observation of these edge states and determination of the superconducting gap symmetry are discussed based on the quasi-particle interference (QPI) technique \cite{1}.

\cite{1} M.H. Zare, M. Biderang, A. Akbari, Phys. Rev. B 96, 205156 (2017).

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DFT+Dynamical Mean-Field Theory Approach to Crystal-Field Splitting in Hard-Magnetic Rare-Earth Intermetallics

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The single-ion anisotropy of rare-earth ions is crucial for the high coercivity of hard-magnetic intermetallics. This anisotropy is determined by an interplay of the spin-orbit coupling with the crystal and exchange fields acting on the localized rare-earth 4\textit{f} shell. A quantitative prediction of magnetic properties for these technologically-important materials thus requires a robust \textit{ab initio} evaluation of these crucial quantities. The crystal field splitting represents a particular challenge due to its generally small value and sensitivity to the details of theoretical treatment of the 4\textit{f} shells.

We propose \cite{1} a first-principles density functional theory+dynamical mean-field theory framework to evaluate the crystal-field splitting on rare-earth sites. An atomic (Hubbard-I) approximation is employed for local correlations on the rare-earth 4\textit{f} shell and self-consistency in the charge density is implemented. We reduce the density functional theory self-interaction contribution to the crystal-field splitting by properly averaging the 4\textit{f} charge density before recalculating the one-electron Kohn-Sham potential. We also suppress the 4\textit{f} contribution to magnetization density to avoid a double-counting for the rare-earth exchange field. The approach is applied to hard-magnetic intermetallics of the \textit{RCo}_5 and \textit{RFe}_{12}X families (\textit{R} =Nd, Sm and \textit{X} =N, Li or empty site). In \textit{RCo}_5 we find a good quantitative agreement of the theoretical crystal-field splitting and 4\textit{f} wavefunctions with experimental neutron-scattering results and refine previous estimates for the crystal-field parameters.

Applying the same approach to \textit{RFe}_{12}X compounds we obtain, in particular, a large positive value of the crystal field parameter \( A^0_2(r^2) \) in NdFe\textsubscript{12}N resulting in a strong out-of-plane anisotropy observed experimentally. The sign of \( A^0_2(r^2) \) is predicted to be reversed by substituting N with Li, leading to a strong out-of-plane anisotropy in SmFe\textsubscript{12}Li. We discuss the origin of this strong impact of N and Li interstitials on the crystal field splitting on rare earth sites.


Oral
Spin-triplet superconducting phase of ferromagnetic UGe$_2$: An example of Hund metal

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UGe$_2$ possesses unique magnetic properties with a number of ferromagnetic phases and critical points$^*$ that have been explained recently in a semiquantitative manner within the Anderson-lattice model (ALM).$^\dagger$ Additionally, the superconducting phase appears principally only in one of the magnetic phases (FM1), $i.e.$, that with lower magnetic moment. We extend the previous approach to include the Hund’s rule coupling within the orbitally-degenerate version of the model and obtain an excellent agreement with experiment for both the ferromagnetic and spin-triplet paired phases, treated on the same footing – the orbitally degenerate ALM. The source of the pairing originates from a combination of the Hund’s rule coupling and strong interelectronic correlations among $f$-electrons due to $U$. The results provide the first complete phase diagram of UGe$_2$ based on a single microscopic model. The situation for other compounds of this family (URhGe, UCoGe, and UIr) will be briefly characterized. Technical details are presented as a poster.$^\ddagger$ This work was supported by MAESTRO Grant No. DEC-2012/04/A/ST3/00342 from the Narodowe Centrum Nauki (NCN).

$^*$C. Pfleiderer, Rev. Mod. Phys. 81, 1551 (2009).


$^\ddagger$E. Kądzielewa-Major, M. Fidrysiak, and J. Spałek, this conference.

Coexistent ferromagnetic-superconducting phases
in the renormalized mean-field theory: Application to UGe$_2$*

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We have analyzed in detail the orbitally degenerate Anderson-lattice model (ALM) within the modified version of the renormalized mean-field approximation, $i.e.$, the statistically consistent Gutzwiller approximation. This model is an extension of the non-degenerate version applied successfully to the description of ferromagnetic properties of UGe$_2$. Here we include in the analysis the spin-triplet pairing to discuss coexistence of the magnetism with the superconductivity. The model encompasses the two ferromagnetic phases: FM2 and FM1 with high- and low- moment states, respectively, and paramagnetic phase (PM), all separated by discontinuous transitions, which compare very well with the experimental data. The description also provides the values of the moments in each of the phases. Those results are supplemented with the spin-triplet $A_1$ phase (with only one equal-spin gap component $\Delta_{\uparrow\downarrow}$ nonzero), which appears in FM1 phase, in accordance with experiment. Other superconducting states of $A_2$ and $A$ type appear in very narrow regimes near the boundaries FM2/FM1 and FM1/PM, respectively. In this manner, our approach reproduces the complete phase diagram for UGe$_2$ with the pairing induced by the combined effect of the Hund’s rule coupling and strong electronic correlations.

$^*$This work was supported by MAESTRO Grant No. DEC-2012/04/A/ST3/00342 from the Narodowe Centrum Nauki (NCN).


$^\ddagger$C. Pfleiderer, Rev. Mod. Phys. 81, 1551 (2009).
We analyze the pair- (PDW) and charge- (CDW) density-wave states within the single-band t-J-U and Hubbard models of the copper-based high-temperature superconductors. In order to take into account the correlation effects to a proper precision, we use the approach based on the diagrammatic expansion of the Gutzwiller wave function (DE-GWF), that goes beyond the renormalized mean field theory (RMFT) in a systematic manner. For the case of the t-J-U model with the parameters, for which selected principal properties of the superconducting phase in the cuprates have been reproduced, a stable coexistent CDW+PDW phase appears below δ ≈ 0.18, i.e., close to the optimal doping. This rationalizes the experimental findings corresponding to the CDW phase appearance in the copper-based materials. The situation is slightly different for the case of the Hubbard model, where a narrow stability regime of a precursor nematic phase sets in preceding the formation of the modulated CDW+PDW state, when reducing the hole doping. The modulation vector of both CDW and PDW in the coexistent phase is $Q = (2\pi/3, 0)a$ ($a$ is the lattice constant) and reflects one of the two simultaneously measured modulations in the experiment.

*This work was supported by the National Science Centre (NCN) of Poland through Grant MAESTRO, No. DEC-2012/04/A/ST3/00342.


‡W. Tabis et al., Nat. Com. 5, 5875 (2014).

Superconductivity in an \(f^2\) System with the \(\Gamma_3\) crystalline electric field ground state

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The \(\Gamma_3\) cubic crystalline electric field (CEF) state is an ideal state to investigate multipole physics, since it does not have dipole but has higher-order multipoles such as quadrupole and octupole. In addition, superconductivity has been observed in Pr compounds with the \(\Gamma_3\) CEF ground state [1]. To approach these phenomena theoretically, we consider a model composed of \(f\) electrons with the total angular momentum \(j = 5/2\). The \(j = 5/2\) states split into \(\Gamma_7\) and \(\Gamma_8\) orbitals under a cubic CEF. When we assume an antiferromagnetic interaction between the \(\Gamma_7\) and \(\Gamma_8\) orbitals, the \(f^2\) ground state is the \(\Gamma_3\) state as long as the level splitting between these orbitals is small. Thus, we employ this model as one of the simplest models to describe the \(\Gamma_3\) state. From this model, we have derived multipole interactions for the \(\Gamma_3\) systems [2].

In the present study, we investigate superconductivity in the same model. In multiorbital systems, we can expect anisotropic superconductivity originated from the orbital anisotropy. For example, we obtain a \(d\)-wave spin-triplet state in a model for \(c_9\) orbitals on a square lattice [3]. We apply random phase approximation for superconductivity in a multiorbital system [4] to the present model. Then, we have obtained a \(d\)-wave spin-singlet state. This pairing state is naturally expected from the \(f^2\)-\(\Gamma_3\) CEF ground state. To stabilize such a superconducting state, we do not need characteristic momentum dependence in fluctuations in contrast to the single orbital Hubbard model on a square lattice where superconductivity is expected to be mediated by antiferromagnetic fluctuations. Indeed, multipole fluctuations are weak in the parameter region where the superconductivity takes place. Thus, such superconductivity may stable against external perturbations.

Planar Hall Effect and Chiral Anomaly in Half-Heusler Antiferromagnet DyPdBi

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Half-Heusler phases form an outstanding group of multifunctional materials. One of their fascinating properties is topological non-triviality of electronic band structure. It has recently been discovered that different topological phases may exist within this family. Several non-magnetic half-Heusler compounds have been predicted and confirmed experimentally to be topological insulators, while antiferromagnetic GdPtBi has recently been discussed as a Weyl semimetal that exemplifies the concept of antiferromagnetic topological insulators.

Here, we report on electronic transport properties of half-Heusler single-crystalline phase DyPdBi, grown from bismuth flux. This compound orders antiferromagnetically at low temperatures, as evidenced by means of magnetic susceptibility, heat capacity, neutron diffraction and electrical resistivity measurements. Character of its electrical resistivity behaviour changes from semiconducting-like at high temperatures to metallic-like at low temperatures. Magnetoresistance of DyPdBi is very large and negative at low temperatures. Remarkably, there occurs distinct Shubnikov – de Haas oscillations, which may originate from Dirac states located in the vicinity of the Fermi energy. Most remarkably, DyPdBi clearly demonstrates two characteristic features of Weyl semimetals: planar Hall effect and chiral anomaly in longitudinal magnetotransport.

Finite-temperature dynamics of $d = 3$ antiferromagnets near quantum criticality: The case of TlCuCl$_3$

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Recent detection of the magnetic amplitude (or Higgs) mode in spin-dimer compounds TlCuCl$_3$ and KCuCl$_3$ near the pressure-induced quantum phase transition calls for a quantitative study of dynamical properties of three-dimensional antiferromagnets (AF) close to quantum criticality. The specific puzzle that emerges from experiments is that the width to mass ratios of the paramagnons at high temperatures ($k_B T \approx$ excitation energy) are comparable with that of the amplitude mode at the lowest available $T$. The latter implies unexpected robustness of magnetic modes to thermal damping.

Here we propose a unified framework to study dynamical properties of $D = 3 + 1$ AF that is based on the effective $\varphi^4$ theory approach. We employ hybrid renormalization group (RG) scheme that combines the Callan-Symanzik and Wilson thermal RG methods. The latter approach is applicable both at $T = 0$ and $T > 0$ and thus, with a single set of fitting parameters, can be compared with experiment across the entire pressure-temperature phase diagram.

We identify the mechanism protecting paramagnons from thermal damping as a non-pertubative reorganization of the paramagnon decay processes and a substantial downward renormalization of the magnon-magnon coupling by thermal fluctuations. We argue that the latter leads to the linear scaling between the width to mass ratios of the high-temperature paramagnons and that of the low-temperature amplitude mode, with the proportionality factor of the order of unity. Masses and widths of the magnetic excitations are computed across the quantum- and classical-transition points and compared with the data for TlCuCl$_3$. Quantitative agreement is demonstrated for available range of pressures and temperatures.

This work was supported by MAESTRO Grant No. DEC-2012/04/A/ST3/00342 from the Narodowe Centrum Nauki (NCN).

References:

1. This work was supported by the National Science Centre (Poland) under research grant no. 2015/18/A/ST3/00057.

We-B11, 16:30

Finite-temperature dynamics of $d = 3$ antiferromagnets near quantum criticality: The case of TlCuCl$_3$

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Recent detection of the magnetic amplitude (or Higgs) mode in spin-dimer compounds TlCuCl$_3$ and KCuCl$_3$ near the pressure-induced quantum phase transition calls for a quantitative study of dynamical properties of three-dimensional antiferromagnets (AF) close to quantum criticality. The specific puzzle that emerges from experiments is that the width to mass ratios of the paramagnons at high temperatures ($k_B T \approx$ excitation energy) are comparable with that of the amplitude mode at the lowest available $T$. The latter implies unexpected robustness of magnetic modes to thermal damping.

Here we propose a unified framework to study dynamical properties of $D = 3 + 1$ AF that is based on the effective $\varphi^4$ theory approach. We employ hybrid renormalization group (RG) scheme that combines the Callan-Symanzik and Wilson thermal RG methods. The latter approach is applicable both at $T = 0$ and $T > 0$ and thus, with a single set of fitting parameters, can be compared with experiment across the entire pressure-temperature phase diagram.

We identify the mechanism protecting paramagnons from thermal damping as a non-pertubative reorganization of the paramagnon decay processes and a substantial downward renormalization of the magnon-magnon coupling by thermal fluctuations. We argue that the latter leads to the linear scaling between the width to mass ratios of the high-temperature paramagnons and that of the low-temperature amplitude mode, with the proportionality factor of the order of unity. Masses and widths of the magnetic excitations are computed across the quantum- and classical-transition points and compared with the data for TlCuCl$_3$. Quantitative agreement is demonstrated for available range of pressures and temperatures.

This work was supported by MAESTRO Grant No. DEC-2012/04/A/ST3/00342 from the Narodowe Centrum Nauki (NCN).

References:

1. This work was supported by the National Science Centre (Poland) under research grant no. 2015/18/A/ST3/00057.

Oral
We-B13, 16:45

Electronic structure, magnetic and response properties of B20 $A_{1-x}B_x$Ge alloys ($A, B = Mn, Fe, Co, Rh$)

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The composition-dependence of the electronic structure and magnetic properties, e.g. isotropic exchange ($J_{ij}$) and Dzyaloshinskii-Moriya interaction (DMI) ($\vec{D}_{ij}$), of Mn$_{1-x}$Fe$_x$Ge, Mn$_{1-x}$Rh$_x$Ge, Mn$_{1-x}$Co$_x$Ge and Fe$_{1-x}$Co$_x$Ge B20 alloys have been investigated by first-principles calculations using the relativistic multiple scattering Korringa-Kohn-Rostoker (KKR) formalism. It was demonstrated a strong dependence on the composition of the $D_{ij}^{\alpha\beta}$ ($\alpha = x, y, z$) elements of the DMI tensor, changing sign at $x \approx 0.85$ in Mn$_{1-x}$Fe$_x$Ge and at $x \approx 0.5$ in Fe$_{1-x}$Co$_x$Ge, in line with previous theoretical calculations as well as with experimental results. The calculated exchange coupling parameters have been used in Monte Carlo simulations to investigate the ground state magnetic structure of the alloys and its finite temperature behaviour. The spin-orbit torque (SOT), anomalous and spin Hall conductivities (AHC and SHC, respectively) of Mn$_{1-x}$Fe$_x$Ge alloys have been investigated. A sign change at $x \approx 0.5$ is predicted for the Fermi sea contribution to the SOT, as this is closely related to the DMI. In the case of anomalous and spin Hall effects it is shown that the calculated Fermi sea contributions are rather small and the composition-dependence of these effects are determined mainly by the electronic states at the Fermi level. The spin-orbit-induced scattering mechanisms responsible for both effects are suggested to cause the minimum of the AHC and the sign change of the SHC.

We-B14, 17:00

Electronic structure mediated vitrification of transition metal alloys$^*$

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When a molten alloy is cooled, the formation of a metallic glass (MG) competes with that of intermetallic compounds (ICs). This competition determines the glass forming ability (GFA) of a given alloy and in binary alloys the GFA can be expressed in terms of the formation enthalpies of the MG and the competing ICs [1]. More recently we have shown that the GFA in Cu-Hf, Zr alloys is enhanced [2] because the electronic structure, ES, represented by the density of states (DoS) at the Fermi level, $N(E_F)$, of competing ICs is similar to that of the MG. In particular, we found that the small differences between the $N(E_F)$-dependent properties, such as the magnetic susceptibility ($\chi$) and Sommerfeld coefficient ($\gamma$), of as-cast and crystallized MGs reflect an enhanced GFA. Combining our results for $N(E_F)$ and $\chi$ with those in the literature, we show here that this correlation holds in all binary (Cu, Ni-Ti, Zr, Hf) and ternary (Cu-Hf-Ti, Cu-Zr-Al) alloys of early (TE) and late (TL) transition metals for which relevant data exist. The correlation between ES and GFA shows up best in all Cu-Zr and NiZr$_2$ alloys for which data regarding changes in $N(E_F)$ upon crystallization is available. The applicability of this correlation, between glass forming ability and electronic structure, to all TE-TL alloys is supported by photoemission studies and low temperature specific heat measurements [3] which show similar composition dependences irrespective of the number of components in the alloy.

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Oral
We-B15, 17:15

Single crystal of URhGa in ambient and hydrostatic pressure
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Weak metallic ferromagnets became center of research due to their phase diagrams predicted by BKV theory.¹ One of theoretical phase diagrams exhibit discontinuous transition where second order phase transition changes into first order one at tricritical point (TCP). First order transition is then tuned into quantum phase transition. Also at TCP metamagnetic transition appears characterized by critical endpoint (CEP). With further increase of tuning parameter metamagnetic transition is suppressed into quantum critical point. In UCoAl², URhAl³ and UCoGa⁴ this phase diagram, or part of it was observed. All mentioned compounds belong to same family of UTX compounds crystallizing in ZrNiAl structure, which makes this family interest of research. Even more, effect of value of Tc and spontaneous magnetic moments on TCP can be determined while keeping origin of magnetism same in UTX family.

One of the compounds belonging in UTX family is URhGa. Polycrystalline sample was reported as ferromagnet with Tc = 41 K.⁵ We present magnetic, electric transport and thermal properties of single crystal of URhGa in ambient and applied hydrostatic pressure. Phase diagram of URhGa is compared to other members of UTX family which has similar Tc but smaller spontaneous moment.

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The discovery of a new ternary alloy is a great challenge for the solid state chemists. The Mg-rich part of the RE-TM-Mg diagram (RE = Rare-Earth, TM = Transition metal) is reinvestigated and a lot of new compounds are highlighted. According to the low weight and cost of magnesium and also of the possible improvement of the corrosion resistance due the RE, such compounds could be of great interest in term of applications such as: hydrogen storage, structural materials...

The focus will be done on 4 new compounds: LaCuMg[1], Gd3Ni5Mg[2], NdNiMg2[3] and NdNiMg12[3]. LaCuMg[1] crystallizes in the La2Mg17 structure type (S.G. P63/mmc) with the lattice parameters a = 10.1254(2) Å and c = 10.0751(2) Å. For Gd3Ni5Mg[2] the determination of the structural parameters is more complex because of the difficulty to obtain a well-crystallized sample. From initial XRD analysis, an average cubic structure with lattice parameter a = 4.55 Å could be assumed. The subsequent TEM analysis shows a possible modulation along both a* and b* axis. Relationship between crystallinity and properties will be established.

NdNiMg2[3] crystallizes with an unusual structural type (S.G : Cmcm, a = 4.4799(2), b = 9.9827(3), c = 13.7854(10) Å). Its structure is made of infinite layers of Mg atoms which form blocks stacked along the c axis. These blocks, with a close-packed array of Mg atoms, are separated by infinite NiNd layers and connected through short Mg-Mg bonds. In the NiNd layer the Ni and Nd atoms form an ordered graphite-type network. The structure and the properties of NdNiMg12 will be presented and discussed for the first time. Composites material Mg – NdNiMg12 will be investigated in term of corrosion resistance and mechanical properties.

Hydrogen sorption properties will be presented and also the first mechanical and corrosion resistance tests will be presented. A clean way for hydrogen production based on hydrolysis will be also presented. The coupling with a fuel cell as well as the adaptation to an electrical assisted bike will be demonstrated.


Oral

Hydrogen desorption for Mg/MgH2 modified thin films *

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Magnesium hydride (MgH2) is one of the most promising hydrogen storage materials because it is directly formed from the reaction of Mg metal with gaseous hydrogen and reaches a high mass capacity (7.6 wt %). However, the sorption reaction is too slow for practical use and needs higher temperature than 573 K for hydrogen sorption reactions. The H storage properties can be tailored by addition of small amount of transition metals (Ti, V, Fe, Co, Ni, Cu and Pd), transition metal oxides (TiO2, CeO2), halides (FeF3) or borides (TiB2). We have used both, theoretical and experimental approach to study reaction mechanism in powder and thin films material.

In fact, processes taking place during hydrogen desorption from Mg/MgH2 thin films upon modification either by TiO2 capped layer or by ion irradiation were investigated. Irradiation was used to produce exact quantity of point defects within well-defined depth distribution. It was shown that the size, shape, and concentration of Mg nuclei formed during hydrogen desorption from MgH2 thin films depend on the characteristics and distribution of the induced defects. In non-irradiated samples the shape of Mg nuclei is spherical, while in irradiated samples it is highly irregular. Variations in sample color were observed during hydrogen desorption and before the creation of Mg nuclei. DFT calculations showed that the observed variations in the optical properties of samples can be explained by changes in MgH2 electronic structure and the appearance of an H-vacancy band within the MgH2 energy gap. On the other hand, the modification induced by capping with TiO2 does not affect the shape of nuclei. The shape is rather spherical and do not depend on film thickness. The size and concentration of nuclei is related to the thickness of films. Both modifications (addition of additives or point defects) lead to reduction of temperature onset for desorption and improved kinetics.

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Oscillating behavior of physical and mechanical properties of alloys at hydrogenation  
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This work provides an overview of experimental results revealing unique phenomenon – as stochastic changes of local composition and transition metal elements ordering within the alloys. A necessary and sufficient condition for the manifestation of this phenomenon is the presence of hydrogen in the structure of the materials. Interestingly the stochastic changes are observed at room temperature after a rather long rest time from the initial insertion of hydrogen. Changing positions and environments of the metal elements yield changing the phase compositions. As a result, specific properties e.g. the mechanical ones, are pointed out. Reproducibility the same effect in a given alloy as well as its occurrence in various states of the matter e.g. in amorphous and crystallized alloys leads question the fundamental basis of the phenomenon. The present analysis aims underline the difference between the stochastic oscillating behavior and the well-known “hydrogen induced atomic rearrangements” (HIA) that could go along hydrogenation of alloys. The steady occurrence of the phenomenon was investigated using various experimental techniques such as XRD, UPS, AES.

In terms of applications, the phenomenon can lead to critical changes e.g. in the structure of low-temperature electrodes used to deliver high purity hydrogen made of platinum group as well as of type alloys.

Transition metal induced bcc phase magnesium  
as issue for fast hydrogen sorption kinetics and low stability of MgH2  
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Among many metals and alloys reacting with hydrogen magnesium, due to its high hydrogen storage capacity and low cost, appears as one of the most promising metal for practical hydrogen storage systems. However, rather high MgH2 enthalpy of hydrogen desorption, slow hydrogen absorption and desorption kinetics, and noticeable reactivity toward oxygen essentially limit its applications. Numerous studies have established that hydrogen sorption kinetics of magnesium can be improved by different processes, e.g. by ball-milling magnesium or magnesium hydride with small amount of transition metals (TM) or their oxides and fluorides. However, up to now the impact of TM additives on hydrogen sorption kinetics of magnesium is not completely understood. Experimental studies of Mg/Nb thin films and micro-sized particles revealed that Nb act not as a true catalyst but as a gateway for hydrogen transportation. As it was shown first theoretically and then confirmed experimentally Nb interfacing Mg layers can stabilize the bcc structure of magnesium. Recent studies have revealed that upon hydrogenation hcp Mg-Ti thin films, a cubic fluorite Mg1.7Ti0.3H8 phase promotes favorable hydrogen sorption kinetics. Furthermore, Mg-Ti nanoparticles of 10-20 nm size demonstrate essentially lower hydride formation enthalpy.

Here we review on the most recent studies of Mg-TM systems for hydrogen storage focusing on the role of TM additives in formation of bcc Mg and fluorite MgH3 structures. In our opinion this acts as a driving force significantly improving the hydrogen sorption kinetics and modify the thermodynamics stability of MgH2.

References:

Oral
Alkali and transition metal fluoride-phosphates as perspective cathode materials for metal-ion batteries

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The ever-growing demand for portable energy in various fields puts forward new challenges to rechargeable battery technologies in improving specific energy and power, life and safety. The battery performance is critically governed by the properties of the cathode material. Fluoride-phosphates of transition metals with A₃MPO₄F (A = Li, Na, K; M = V, Fe, Co) formula take several advantages over existing oxide cathode materials: a substantial increase of operating voltages and much faster kinetics. A distinctive structural feature of these materials is a presence of dangling oxygen atoms (bonded to P and alkaline cations, but not included into the octahedral coordination of transition metals). These oxygen atoms can determine the mechanism of the structure transformation during charging and even trigger the undesirable cation intermixing. Different activities of the alkali positions surrounded by a distinct number of the dangling oxygen atom can explain the striking difference between desodiation mechanisms in Na-ion and Li-ion cells of a layered Na₃FePO₄F cathode material. Its counterpart, Li₂FePO₄F, was found to undergo a severe cation intermixing during charging to compensate a strong underbonding of the dangling oxygen atoms upon removal of the Li⁺ cations from their coordination sphere.

We designed and prepared a new vanadium-based AVPO₄F (A = Li, K) cathode material adopting a KTP-type framework with excellent rate capability. The material showed remarkable capacity retention in Li-ion cells at 40°C maintaining more than 75% of the initial specific capacity. It can also reversibly incorporate Na⁺ and K⁺ ions unveiling rapid kinetics and preserving the host structure. The alkali ion diffusion coefficients measured using the PITT technique were the lowest for Li⁺ (10⁻⁸ – 10⁻¹² cm²/s) and highest for K⁺ (10⁻¹¹ – 10⁻¹² cm²/s) making AVPO₄F a promising candidate for metal-ion batteries.

Our current activities on transition metal fluoride-phosphates based cathode materials for metal-ion batteries will be reported with a particular focus on the interrelation between crystal structure peculiarities and electrochemical properties.

Overstoichiometric Lithium and Lithium-magnesium Manganese Oxide Spinels Synthesis Using Hydride Intercalation Method

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Overstoichiometric oxide spinels of the Li-Mg-Mn-O system possess the significant prospect as a functional materials for lithium- and hybrid lithium-magnesium-ion batteries as well as for catalysts. Promising opportunities for synthesis of spinel-structure materials offer the usage of metal intercalation approaches, but up-to-date methods are either limited with the concentrations of inserted metal or assume the usage of organic or organometallic reagents and therefore can not provide the convenient synthesis of materials with reproducible properties. Major shortcomings of these technologies are due to the chemical nature of intercalating agents. The new method providing the synthesis of overstoichiometric spinels with high preset content of intercalated Li or Mg in mild conditions using the corresponding metal hydrides as intercalating agents have been proposed. Synthesis procedure includes mechanochemical treatment of a stoichiometric host spinel LiMn₂O₄ and corresponding metal hydride, LiH or MgH₂ with desired Li/Mg:Mn ratio. Resulting mechanocomposites then are being consistently calcinated in the high purity argon atmosphere (523-573 K, 1-1.5 h) and air/oxygen (573-773 K- increased with the content of intercalating metal, 1-1.5 h). Resulting products are single phase spinels and do not contain hydrogen. Thus, the hydride intercalation method provides the synthesis of impurity-free, homogenous single phase overstoichiometric spinels with high preset content of intercalated metal, increasing that when traditional methods are being used. Adjacent phase equilibria have been also studied.

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How nano-composites influence physical, mechanical and thermal properties of high ZT-skutterudites

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Skutterudites are known as excellent thermoelectric (TE) materials because they can be produced fast from cheap starting materials; they can be used in a wide temperature range and besides an excellent TE quality they also show long term stability and a good mechanical performance. Although filled Sb-based skutterudites already have a high figure of merit, ZT, a successful route to further increase ZT is the incorporation of homogeneously dispersed nanoparticles into the thermoelectric matrix and this way to reduce the lattice thermal conductivity leaving electrical resistivity and Seebeck coefficient practically unchanged. In this paper we give a critical summary of literature data concerning the change of ZT in skutterudite composites with oxides, metals, intermetallics, antimonides, nitrides, borides, tellurides, silicides and carbon based materials. As good mechanical properties are substantial for all TE applications, the influence of dispersed nanoparticles, on the hardness, elastic moduli, fracture toughness, compressive and flexural strength are discussed and compared to other thermoelectric materials. For a long-term durability of TE modules, matching coefficients of thermal expansion of each leg-type material in the temperature gradient used are essential. In case of skutterudites, it is well known that p-type skutterudites have generally a higher thermal expansion coefficient (CTE) than their n-type counterpart. We show that dispersed borides can reduce the CTE of p-type and enhance the CTE of n-type skutterudites.

Effect of substitutions on the thermoelectric and magnetic properties of half-Heusler alloys – HfNiGe and ZrNiSn variants

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The wide range of compositional flexibility offered by Heusler alloys in general leads to a variety of electronic properties ranging from local magnetism to topological insulators. Hence in the present work new and also variants of known half-Heusler alloys have been synthesized and their thermoelectric and magnetic properties investigated in detail. The low temperature thermoelectric and magnetic properties of HfNiGe, an orthorhombic half-Heusler alloy have been studied in detail. The alloy exhibits a metallic behavior with the resistivity varying from 1.0 mΩcm to 2.5 mΩcm while the Seebeck coefficient exhibits a maximum of -11 µVK⁻¹ at ~ 150 K. Although the alloy exhibits a n-type characteristic, a significant contribution of minority carriers to carrier transport is present leading to reduced Seebeck coefficient due to bipolar conduction. The alloy exhibits a paramagnetic behavior but with strong local ferromagnetic correlations. The magnetization exhibits not only a saturation tendency but also a clear hysteresis even at 300 K.

The n-type half-Heusler alloy ZrNiSn has a high power factor but it is coupled to high thermal conductivity which renders it a low thermoelectric figure-of-merit. In order to reduce the thermal conductivity alloy scattering strategy has been used. Both the sp-element and the transition metal substitutions have been incorporated to investigate their effect on power factor and thermal conductivity. Partial substitution of the sp-element has been found to retain the high power factor while a combination substitutions results in the largest reduction of thermal conductivity. The ZrNiSn₀.₉₅Ge₀.₀₅ alloy has the highest power factor of 2.9 mWm⁻¹K⁻² while the Zr₀.₇₅Ti₀.₂₅NiSn₀.₉₇Si₀.₃ alloy exhibits a lowest thermal conductivity of 3.2 Wm⁻¹K⁻¹. The high power factor of Ge-substituted alloy results in a high figure-of-merit for the alloy.

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Oral
Th-A9, 12:15

Anisotropic heat and charge transport in the cubic clathrate Ba$_8$Au$_{6-x}$Ge$_{40+x}$

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A good thermoelectric material exhibits, in addition to large thermopower, low phonon thermal conductivity and high electrical conductivity. Type-I clathrates, which show promise for thermoelectric application, exhibit remarkably low phonon thermal conductivities, and there is wide consensus that the cage-like crystal structure is of central importance to this phenomenon. The type-I clathrate Ba$_8$Au$_{6-x}$Ge$_{40+x}$ possesses six tetrakaidecahedra and two dodecahedra cages per unit cell, and each cage encapsulates a weakly-bonded Ba atom. This material is particularly interesting for phonon transport studies because the rattling motion of Ba is associated with a very low characteristic energy [Pierre-François Lory et al., Nat. Commun. 8, 491 (2017)].

In this presentation we report electrical and thermal transport properties of single-crystalline Ba$_{7.81}$Au$_{5.35}$Ge$_{40.67}$. Remarkably, both the electrical resistivity and the phonon thermal conductivity show pronounced anisotropy. We observed a reduced electrical conductivity but an enhanced phonon thermal conductivity along the [110] direction. Electronic band structure calculations reveal pronounced anisotropy for the same direction. We suggest that strong electron-phonon coupling is at the origin of the observed phenomena.

Th-A10, 12:30

Low temperature synthesis of intermetallics for energy

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Intermetallic compounds are widely used as materials for energy conversion and storage, from nuclear fuels to hydrogen tanks, from permanent magnets in wind mills to thermoelectric devices... Their attractiveness for such applications is mainly based on their low heat capacity and high effusivity, the specificity of the metallic bonding or the easy synthesis by classical fusion-solidification processes.

The last argument can become a strong drawback for the production of non-congruently melting phases (e.g. La(Fe$_3$Si)$_{13}$, Nd$_3$Fe$_4$B), for high vapor pressure element containing intermetallics (e.g. Mg$_2$Ni, CoSn$_3$) or for powderized highly ductile samples (e.g. γ-U(Mo), high entropy alloys).

In order to overcome these problems, but also to discover new properties, alternative synthesis routes operating below the melting temperature have to be developed. The HDDR process applied to the production of finely divided Nd$_3$Fe$_4$B, or the preparation of high purity γ-U(Mo) alloy powders by magnesiothermy are typical examples of such syntheses. This motivated us to apply some "low" temperature (typically from 1000 K down to room temperature) reactions to prepare some intermetallics for energy in order (i) to shorten the annealing duration and decrease its temperature, (ii) to obtain high purity and highly homogeneous materials and (iii) to discover new phases and/or new properties.

We will present our results on the synthesis, (micro)structural characterization and physical properties investigation of thermoelectric and magnetocaloric materials.

The Density Functional Theory (DFT)-based Disordered Local Moment Theory of magnetic materials and its quantitative description of the temperature and field dependence of magnetic properties will be discussed [1-3]. The intricate interplay between itinerant and more localised spin degrees of freedom in many transition metal materials leads to temperature dependent spin-polarised electronic structure and transport properties. The theory can be applied to materials with quenched static compositional disorder traversing first-order magnetic phase transitions such as nearly stoichiometric Fe-Rh alloys[2] and Mn-antiperovskites [4]. The theory accounts quantitatively for magnetic phase diagrams and caloric effects [2] and in the case of FeRh reveals a compositional hypersensitivity. Results will also be presented for the magnetic properties of rare earth - transition metal permanent magnets such as SmCo5 [5] focussing on their ferrimagnetism and how to describe their intrinsic temperature dependent magnetic anisotropy.


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Th-S2i, 09:30

**LDA+Hubbard-I approximation for modelling of f-electrons systems**

Alexander B. Shick

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Surface supported single magnetic atoms, the so-called ”single-atom magnets”, open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate, and Dy atom on graphene/Ir(111). We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combination of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED). The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized.
Impact of finite temperatures on the response functions of magnetic solids

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A computational scheme is presented that allows to account for thermal lattice vibrations as well as spin fluctuations when calculating response quantities in solids. The approach is based on the alloy analogy model using the CPA (Coherent Potential Approximation) to deal with disorder and the description of the electronic structure via multiple scattering theory (KKR). Various models to deal with spin fluctuations are discussed concerning their impact on the resulting temperature-dependent longitudinal as well as transversal charge and spin conductivities, and Gilbert damping parameter. Separate calculations accounting for the thermal effect due to either lattice vibrations or spin fluctuations show that they give comparable contributions to the conductivity or Gilbert damping. However, comparison to results accounting for both thermal effects demonstrates violation of Matthiessen’s rule, showing the non-additive effect of lattice vibrations and spin fluctuations. As will be demonstrated by various examples, corresponding results obtained for the pure ferromagnets as well as alloy systems and compounds are found in general in rather good agreement with available experimental data.

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Temperature-Dependent Magnetic Anisotropy from First Principles*

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Thermal spin fluctuations, which are present in equilibrium in all magnetic materials, interact with electronic quasiparticles and induce temperature-dependent changes in such observables as the spectral densities, magnetocrystalline anisotropy, and transport properties. These effects can be studied using first-principles calculations, treating the spin fluctuations within the disordered local moment (DLM) model. We will discuss the calculations of the magnetic anisotropy in ferromagnetic (Fe-Co)\textsubscript{2}B [1] and antiferromagnetic Mn-Pt [2] alloys and the electronic mechanisms leading to the spin reorientation transitions and other anomalies in its temperature dependence. These mechanisms include the temperature-dependent changes in band filling, suppression of spin-orbit hot spots by disorder broadening, and competition of contributions from different electronic states. We will also discuss the case of Fe\textsubscript{2}P-based alloys, where DLM calculations reveal [3] a two-dimensional character of the exchange interaction at elevated temperatures and offer a natural explanation for the observed sharp enhancement of the Curie temperature by alloying with multiple elements.

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**Th-S5i, 11:30**

**The spin-disorder resistivity: the disordered local moment approach**

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The spin-disorder resistivity (SDR) of transition metal ferromagnets including bcc-Fe at the Earth’s core conditions, ordered magnetic alloys, rare-earth metals, and chosen Heusler alloys is determined from first principles. We identify the SDR at the Curie temperature with the residual resistivity of the corresponding system evaluated in the framework of the disordered local moment (DLM) model which has the zero spin-spin correlation function. The underlying electronic structure is determined in the framework of the tight-binding linear muffin-tin orbital method which employs the coherent potential approximation (CPA) to describe the DLM state. The DLM fixed-spin moment technique is used in the case when the DLM moment collapses while the electronic structure of rare-earths metals is determined using the open core approach. The Kubo-Greenwood method is employed to estimate the resistivity. For bcc-Fe and Ni<sub>2</sub>MnSn alloy we shall also estimate the temperature-dependent of resistivity below the Curie temperature using a semiempirical approach. Calculations are compared with the supercell Landauer-Büttiker approach developed recently as well as with available experimental data and overall good agreement is obtained. We will also briefly discuss the limitations of the approach.

*In collaboration with V. Drchal, I.Turek, and S.K. Khmelevskii

**Th-P1, 13:30**

**Magnetic Ordering in Cerium-based Kondo Semiconductors**

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Kondo semiconductors based on rare-earth elements possess a narrow gap in the renormalized density of states. They attract renewed interests as candidates for correlated materials with nontrivial topology [1]. The ground states remain nonmagnetic due to strong hybridization of the 4f state with conduction bands. However, Kondo semiconductors CeT<sub>2</sub>Al<sub>10</sub> (T = Ru, Os) order antiferromagnetically (AFM) at a rather high temperature T<sub>N</sub> ≅ 28 K [2-5]. The mechanism was thought to be related with the lack of inversion symmetry at the Ce site, which allows on-site hybridization of the 4f state with 5d state [6]. Our systematic studied of the effects of dilution and electron/hole doping on the magnetic and transport properties, electron tunneling, and spin-gap formation revealed that the hybridization gap is indispensable for the unusual AFM order [7-10]. We also found anisotropic dependence of the AFM transition on uniaxial pressure. Under uniaxial pressure P//b and hydrostatic pressure, T<sub>N</sub> depends linearly on the b-axis parameter [11]. This relation supports the model that a kind of CDW developing along the b axis far above T<sub>N</sub> induces the AFM order in these systems [12].

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Orbital-selective effects in transition metal compounds

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Close to Mott transition several novel states can appear\(^1\). In particular, molecular clusters can be formed in the solid, such as dimers, trimers, etc.\(^2\). Especially important for these phenomena is the role of different d-orbitals, which leads to different orbital-selective effects. In my talk I will formulate the main ideas and will illustrate such phenomena, especially dimer formation, on many examples (pyroxenes; spinels; VO\(_2\) and MoO\(_2\); systems with 4d and 5d electrons such as Li\(_2\)RuO\(_3\) and Li\(_2\)IrO\(_3\)). The concept of orbital-selective Peierls transitions will be proposed and justified\(^3\)\(^4\). In systems containing structural metal dimers there may exist in the presence of different orbitals a special state with partial formation of singlets by electrons on one orbital, while others are effectively decoupled and may give e.g. long-range magnetic order or stay paramagnetic. Similar situation can be realized in dimers spontaneously formed at structural phase transitions, which can be called orbital-selective Peierls transition\(^5\). Yet another consequence of this picture is that for odd number of electrons per dimer there exist competition between double exchange mechanism of ferromagnetism and the formation of singlet dimer by electron on one orbital. Such molecular states can strongly reduce and effectively suppress double exchange ferromagnetism. I will discuss some implications of these phenomena, and consider examples of real systems, in which orbital-selective phases are realized. Especially important can be these effects in 4d and 5d systems, for which also spin-orbit coupling (SOC) can play an important role. In my talk I will also discuss some effects connected with the interplay of orbital degrees of freedom and spin-orbit coupling, in particular a nontrivial interplay of SOC and Jahn-Teller effect.

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\(^1\) D.I. Khomskii, Transition Metal Compounds, Cambridge University Press, Cambridge 2014
\(^3\) Sergey V. Streltsov, Daniel I. Khomskii, Phys. Rev. B 89, 161112(R) (2014)
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