SCIENTIFIC PROGRAM

Study of Matter at Extreme Conditions

March 30 - April 06, 2019
Conference Center, Celebrity Equinox

&

BOOK OF ABSTRACTS

Sponsors:
Sapienza University of Rome
High Pressure Society of America (HIPSSA)
Organizers:

Naurang L. Saini  
Sapienza University of Rome  
e-mail: Naurang.Saini@roma1.infn.it

Jiuhua Chen  
Florida International University  
e-mail: chenj@fiu.edu

James J. Hamlin  
University of Florida  
e-mail: jhamlin@ufl.edu

Richard G. Hennig,  
University of Florida  
e-mail: rhennig@ufl.edu

Arun Bansil  
Northeastern University  
e-mail: ar.bansil@northeastern.edu

Advisor

Surendra K. Saxena  
Emeritus, Florida International University  
e-mail: surendrasaxena8@gmail.com
Symposiums & organizers:

Symposium 1: High pressure chemistry: Theory and experiments (Artem R. Oganov, Skolkovo Institute of Science and Technology & Alexander F. Goncharov, Carnegie Institute) - merged into Symposium 9

Symposium 2: Multifunctional metal hydrides for energy storage: developments and perspectives (Torben R. Jensen, Arhus University; Craig Buckley, Curtin University of Technology & Hai-Wen Li, Kyushu University)

Symposium 3: Materials for energy applications (Rajeev Ahuja, Uppsala University & Yaroslav Filinchuk, Universitet Catholique de Louvain)

Symposium 4: Quantum emergent matters: materials & phenomena driven via extreme conditions (Changqing Jin, Chinese Academy of Sciences) - merged into Symposium 6

Symposium 5: Unconventional superconductivity in Fe-based materials under extreme conditions (Christoph Meingast and Frederic Hardy, Karlsruhe Institute of Technology)

Symposium 6: Recent development in topological and correlated materials (Arun Bansil and Swastik Kar, Northeastern University & Humberto Terrones, Rensselaer Polytechnic Institute)

Symposium 7: Emerging layered superconductors and related materials (Naurang Saini, Sapienza University of Rome & Takashi Mizokawa, Waseda University)

Symposium 9: High pressure earth and planetary science (Jiuhua Chen and Surendra Saxena, Florida International University)

Symposium 10: Two-dimensional materials: graphene and beyond (Andreia Luisa da Rosa and Renato Borges Pontes, Federal University of Goias & Erika Nascimento Lima, Universidade Federal de Mato Grosso)

Symposium 11: Operando methodologies: applications to batteries and beyond (Giuliana Aquilanti, Elettra Sincrotrone Trieste & Fabrizio Bardelli, CNR-Nanotec, Roma, Italy) – merged into Symposuims 2,3

Symposium 12: 50 years of high-pressure superconductivity research (Richard G. Hennig and James J. Hamlin, University of Florida)
Celebrity Equinox, March 30 – April 6, 2019

Saturday March 30, 2019

15:00-17:30  Registration – Conference center, Celebrity Equinox
17:30-18:30  SMEC Reception & Welcome Party – Sky Lounge
## PROGRAM AT A GLANCE

### Sunday March 31, 2019

<table>
<thead>
<tr>
<th>Time</th>
<th>Activity</th>
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</thead>
<tbody>
<tr>
<td>8:30-10:30</td>
<td>Opening &amp; Plenary Session</td>
</tr>
<tr>
<td>10:30-11:00</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>11:00-12:30</td>
<td>Symposium 6, <em>Recent developments in topological and correlated materials.</em></td>
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<tr>
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<td>Symposium 7, <em>Emerging layered superconductors and related materials.</em></td>
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<td>Symposium 2, <em>Multifunctional metal hydrides for energy storage.</em></td>
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<td>Symposium 3, <em>Materials for energy applications.</em></td>
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<tr>
<td>12:30-14:00</td>
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<td>Symposium 6, <em>Recent developments in topological and correlated materials.</em></td>
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<td>16:00-16:30</td>
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### Monday April 01, 2019

<table>
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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>8:30-10:30</td>
<td>Symposium 6, <em>Recent developments in topological and correlated materials.</em></td>
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<td>Symposium 7, <em>Emerging layered superconductors and related materials.</em></td>
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<td>Symposium 2, <em>Multifunctional metal hydrides for energy storage.</em></td>
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<td>Symposium 3, <em>Materials for energy applications.</em></td>
</tr>
<tr>
<td>10:30-11:00</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>11:00-12:30</td>
<td>Symposium 6, <em>Recent developments in topological and correlated materials.</em></td>
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<tr>
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<td>Symposium 7, <em>Emerging layered superconductors and related materials.</em></td>
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<td>12:30-14:00</td>
<td>Lunch Break</td>
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<tr>
<td>14:00-16:00</td>
<td>Symposium 6, <em>Recent developments in topological and correlated materials.</em></td>
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<td>Symposium 7, <em>Emerging layered superconductors and related materials.</em></td>
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</table>
**Tuesday April 02, 2019**

<table>
<thead>
<tr>
<th>Time</th>
<th>Events</th>
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</thead>
</table>
| 08:30-10:00 | Symposium 6, *Recent developments in topological and correlated materials.*  
             | Symposium 3, *Materials for energy applications.*                        |
| 16:30-18:30 | Symposium 12, *50 Years of high pressure superconductivity research.*  
             | Symposium 7, *Emerging layered superconductors and related materials.*   |

**Wednesday April 03, 2019**

<table>
<thead>
<tr>
<th>Time</th>
<th>Events</th>
</tr>
</thead>
<tbody>
<tr>
<td>08:30-09:30</td>
<td><strong>Graduate Students Session – I</strong></td>
</tr>
<tr>
<td>16:30-18:30</td>
<td><strong>Graduate Students Session – II &amp; Posters</strong></td>
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**Thursday April 04, 2019**

<table>
<thead>
<tr>
<th>Time</th>
<th>Events</th>
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<tbody>
<tr>
<td>08:30-10:30</td>
<td>Symposium 5, <em>Unconventional superconductivity in Fe-based materials under extreme conditions.</em></td>
</tr>
<tr>
<td>10:30-11:00</td>
<td><strong>Coffee Break</strong></td>
</tr>
</tbody>
</table>
| 11:00-12:30| Symposium 5, *Unconventional superconductivity in Fe-based materials under extreme conditions.*  
             | Symposium 9, *High pressure planetary and earth sciences.*             |
| 12:30-14:00| **Lunch Break**                                                        |
| 14:00-16:00| Symposium 5, *Unconventional superconductivity in Fe-based materials under extreme conditions.*  
             | Symposium 9, *High pressure planetary and earth sciences.*             
| 16:00-16:30| **Coffee Break**                                                       |
| 16:30-18:30| Symposium 5, *Unconventional superconductivity in Fe-based materials under extreme conditions.*  
             | Symposium 6, *Recent developments in topological and correlated materials.*  
             | Symposium 4, *Quantum emergent matters: materials & phenomena driven by extreme conditions.* |
| 19:30-20:30| **Get Together Party - Sky Lounge**                                    |

**Friday April 05, 2019**

<table>
<thead>
<tr>
<th>Time</th>
<th>Events</th>
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</thead>
<tbody>
<tr>
<td>08:30-10:30</td>
<td>Symposium 7, <em>Emerging layered superconductors and related materials.</em></td>
</tr>
<tr>
<td>17:00-19:00</td>
<td>Symposium 10, <em>Two-dimensional materials: graphene and beyond.</em></td>
</tr>
<tr>
<td>18:00-19:00</td>
<td><strong>Closing &amp; Concluding Remarks</strong></td>
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</tbody>
</table>
## Detailed Scientific Schedule

### Sunday March 31, 2019

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Location</th>
<th>Chair(s)</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>08:30-09:30</td>
<td>Opening Plenary Session&lt;br&gt;Chairs: S. Saxena, R. Hennig</td>
<td>Room 1</td>
<td></td>
<td>H. K. Mao,&lt;br&gt;Recent advances in high-pressure physics, materials, and geoscience.</td>
</tr>
<tr>
<td>09:30-10:30</td>
<td>A. Bansil,&lt;br&gt;Raising the bar toward a first-principles description of stronger correlations: Novel superconductors to topological materials.</td>
<td>Room 1</td>
<td></td>
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<tr>
<td>10:30-11:00</td>
<td>Coffee Break</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>11:00-11:30</td>
<td>K. Tanigaki,&lt;br&gt;Single crystal thin films of three-dimensional topological insulators via non-catalytic vapor phase epitaxial crystal growth.</td>
<td>Room 1</td>
<td>A. Bansil, X. X. Xi</td>
<td>C. J. Webb,&lt;br&gt;The use of oxides to kinetically enhance the sorption properties of MgH₂ at high pressure.</td>
</tr>
<tr>
<td>11:30-12:00</td>
<td>T. H. Choudhury,&lt;br&gt;Controlling epitaxial growth of transition metal dichalcogenides by gas source CVD.</td>
<td>Room 2</td>
<td>C. Jensen, Reversible Hydrogenation of Magnesium Boride and Magnesium Boranes to Magnesium Borohydrate.</td>
<td></td>
</tr>
<tr>
<td>12:00-12:30</td>
<td>Z. Mao,&lt;br&gt;Layered magnetic topological semimetals and their unusual interlayer quantum transport.</td>
<td>Room 1</td>
<td>T. R. Jensen, Hydrogen storage and battery materials - new types of materials.</td>
<td></td>
</tr>
<tr>
<td>12:30-14:00</td>
<td>Lunch Break</td>
<td></td>
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<tr>
<td>Time</td>
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<tr>
<td>14:00–14:30</td>
<td>Qi Li, <em>Topological Surface States and Inducing Superconductivity in Bi$_2$Te$_3$ Nanotubes.</em></td>
<td>C. Zlotea, <em>Multi-principal-element alloys as new materials for hydrogen absorption.</em></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15:00–15:30</td>
<td>S. Y. Matsushita, <em>Quantum hall effect and thermoelectric properties of surface Dirac states in Sn-Bi$<em>{1.1}$Sb$</em>{0.9}$Te$_2$S crystal.</em></td>
<td>Y. Filinchuk, <em>Non-equilibrium Kr adsorption in nanoporous γ-Mg(BH$_4$)$_2$ by in situ synchrotron powder diffraction.</em></td>
<td></td>
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<tr>
<td>15:30–16:00</td>
<td>I. Dasgupta, <em>Realization of Spin-Orbital Liquid State in Iridates.</em></td>
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</table>

**Coffee Break**

<table>
<thead>
<tr>
<th>Time</th>
<th>Room 1</th>
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<tbody>
<tr>
<td>16:00–16:30</td>
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<tr>
<td>17:00–17:30</td>
<td>T. Schmitt, <em>Evolution of the spin, orbital and charge excitations upon tuning the local lattice environment of Sr$_2$IrO$_4$.</em></td>
<td>M. Heere, <em>Complex metal hydrides investigated by fast neutron powder diffraction.</em></td>
</tr>
<tr>
<td>18:00–18:30</td>
<td>O. Eriksson, <em>DMFT coupled to DFT: Case of some complex oxides.</em></td>
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</tbody>
</table>
### Monday April 01, 2019

<table>
<thead>
<tr>
<th>Time</th>
<th>Room 1</th>
<th>Room 2</th>
</tr>
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<tbody>
<tr>
<td>09:00-9:30</td>
<td>M. Shi, <em>ARPES on topological quantum materials: from topological Kondo insulator to Weyl semimetal.</em></td>
<td>L. Stievano, <em>The sodiation-desodiation mechanism of Sb-based electrode materials revealed by operando spectroscopy assisted by chemometric data analysis.</em></td>
</tr>
<tr>
<td>09:30-10:00</td>
<td>J. -F. He, <em>Angle-resolved photoemission studies on strongly correlated materials.</em></td>
<td>M. Heere, <em>Neutron diffraction for energy storage and conversion in metal hydrides.</em></td>
</tr>
</tbody>
</table>

<table>
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<tr>
<th>Time</th>
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<tbody>
<tr>
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<td>Room 1</td>
<td>Room 2</td>
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</table>
### S-8

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title and Abstract</th>
</tr>
</thead>
<tbody>
<tr>
<td>08:30-09:00</td>
<td>X. X. Xi</td>
<td><em>Nature of the metal-insulator transition in few-unit-cell-thick LaNiO$_3$ films.</em></td>
</tr>
<tr>
<td>09:00-09:30</td>
<td>B. Barbiellini</td>
<td><em>Identification of ferrimagnetic orbitals preventing Jahn-Teller distortions in Li$_x$Mn$_2$O$_4$ cathodes.</em></td>
</tr>
<tr>
<td>09:30-10:00</td>
<td>S. H. Lee</td>
<td><em>New Materials for Next Generation Printable Solar Cells.</em></td>
</tr>
</tbody>
</table>

### Coffee Break

### S-9

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title and Abstract</th>
</tr>
</thead>
<tbody>
<tr>
<td>16:30-17:30</td>
<td>W. Pickett</td>
<td><em>How Compressed Hydride Superconductors Produce Room Temperature Superconductivity.</em></td>
</tr>
<tr>
<td>17:30-18:00</td>
<td>E. Zurek</td>
<td><em>Computational Discovery of Novel Superconducting Hydride Phases Under Pressure.</em></td>
</tr>
<tr>
<td>18:00-18:30</td>
<td>T. Shibauchi</td>
<td><em>High-$T_c$ superconducting phases of FeSe-based materials at high pressure.</em></td>
</tr>
</tbody>
</table>
### S-10  
**Room 1**  
**Graduate Students Session-I**  
**Chairs:** M. Polanski, C. E. Buckley  

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Topic</th>
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<tbody>
<tr>
<td>08:30-08:45</td>
<td>M. Jørgensen</td>
<td>Weakly coordinating anions in solid state electrolytes.</td>
</tr>
<tr>
<td>08:45-09:00</td>
<td>J. B. Grinderslev</td>
<td>Extreme Hydrogen Densities in Ammonium Metal Borohydrides.</td>
</tr>
<tr>
<td>09:00-09:15</td>
<td>M. Pęska</td>
<td>Magnesium – Lithium alloys as hydrogen storage materials.</td>
</tr>
<tr>
<td>09:15-09:30</td>
<td>J. Vodeb</td>
<td>Correlated Configurational States and a Quantum Charge Liquid in Layered Metallic Dichalcogenides.</td>
</tr>
</tbody>
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**16:00-16:30**  
**Coffee Break**

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### S-11  
**Room 1**  
**Graduate Students Session-II**  
**Chairs:** N. L. Saini, K. Kudo  

<table>
<thead>
<tr>
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<th>Topic</th>
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<tbody>
<tr>
<td>16:45-17:00</td>
<td>P. Nautiyal</td>
<td>Graphene Foam for Engineering Ultra-Stiff, Tough and Impact-Resistant Structural Composites.</td>
</tr>
<tr>
<td>17:00-17:15</td>
<td>J. T. Paul</td>
<td>Materials Informatics Search for Strongly Correlated 1D Materials.</td>
</tr>
<tr>
<td>17:15-18:30</td>
<td></td>
<td>Poster Presentations (Pugliese, Stramaglia, Shinzato, Karczewski, T.R. Jensen)</td>
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</table>
### Iron-based Superconductors - 1

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<tr>
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<th>Speaker</th>
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<tbody>
<tr>
<td>08:30-09:00</td>
<td>P. Hirschfeld</td>
<td>Pairing mechanism in iron-based superconductors: variations on the s+/- theme.</td>
</tr>
<tr>
<td>09:00-09:30</td>
<td>Y. Li</td>
<td>Spin-orbit coupling and “preferred” magnetic excitations in iron-based superconductors.</td>
</tr>
<tr>
<td>09:30-10:00</td>
<td>R. Hackl</td>
<td>Microscopic origin of Cooper pairing in Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and CaKFe$_4$As$_6$.</td>
</tr>
<tr>
<td>10:00-10:30</td>
<td>F. Hardy</td>
<td>Nodal Superconductivity in FeSe single crystals from heat capacity.</td>
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### Coffee Break

<table>
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<tr>
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<tbody>
<tr>
<td>10:30-11:00</td>
<td>S-13A</td>
<td>Iron-based Superconductors - 2</td>
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<tr>
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<td>Chairs: P. Hirschfeld, F. Hardy</td>
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<tr>
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<td></td>
<td>Chairs: J. Chen, S. Saxena</td>
</tr>
<tr>
<td>11:00-11:30</td>
<td>B. M. Andersen</td>
<td>Multi-orbital effects and the role of spin-orbit coupling in iron-based superconductors.</td>
</tr>
<tr>
<td>11:30-12:00</td>
<td>B. Buechner</td>
<td>Orbitals and Nematicity in La-1111 Single Crystals.</td>
</tr>
<tr>
<td>12:00-12:15</td>
<td>A. P. Dioguardi</td>
<td>$^{75}$As NMR under uniaxial pressure in BaFe$_2$As.</td>
</tr>
<tr>
<td>12:15-12:30</td>
<td>M. He</td>
<td>Ubiquitous dichotomy between the in-plane uniform magnetic susceptibility and resistivity anisotropies in iron-based superconductors.</td>
</tr>
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### High Pressure Earth & Planetary Sci.

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<tbody>
<tr>
<td>11:00-11:30</td>
<td>Han Hsu</td>
<td>Iron spin crossover in the Earth and planetary interiors: A perspective from computational materials physics.</td>
</tr>
<tr>
<td>11:30-12:00</td>
<td>M. Hou</td>
<td>Temperature-induced amorphization in CaCO$_3$ at high pressure: implication for recycled CaCO$_3$ in subduction zones.</td>
</tr>
<tr>
<td>12:00-12:15</td>
<td>W. L. Mao</td>
<td>Hydrogen-bearing iron peroxide in Earth's lowermost mantle.</td>
</tr>
<tr>
<td>12:15-12:30</td>
<td>W. L. Mao</td>
<td>Hydrogen-bearing iron peroxide in Earth's lowermost mantle.</td>
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### Lunch Break

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<tr>
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<td>Lunch Break</td>
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<tr>
<td>Time</td>
<td>Room 1</td>
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</tr>
<tr>
<td>14:00-14:30</td>
<td>T. Shibauchi, <em>Novel electronic nematicity in</em> <em>(Ba,Rb)Fe2As2</em></td>
</tr>
<tr>
<td>15:45-16:00</td>
<td>C. Meingast, <em>Intertwined and vestigial electronic phases in hole-dopes Sr1-xNa2Fe2As2.</em></td>
</tr>
</tbody>
</table>

16:00-16:30 [Coffee Break]

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<tr>
<td>16:30-17:00</td>
<td>V. Taufour, <em>Pressure dependence of the superconducting upper critical field in KFe2As2 and related materials.</em></td>
<td>P. Vashishta, <em>Reactive molecular dynamics simulations and machine learning.</em></td>
</tr>
</tbody>
</table>

19:30-20:30 [Get Together Party – Sky Lounge]
### S-16

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
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<tbody>
<tr>
<td>08:30-09:00</td>
<td>K. Tanigaki</td>
<td>Electron-phonon and electron-electron interactions in electron doped aromatic carbon materials viewed from electrical transport.</td>
</tr>
<tr>
<td>09:00-09:30</td>
<td>S. Tsuchiya</td>
<td>Development of optical pump probe spectroscopy under uniaxial pressure: Application to strongly correlated superconductors.</td>
</tr>
<tr>
<td>09:30-10:00</td>
<td>K. Park</td>
<td>Projected BCS theory for the unification of antiferromagnetism and strongly correlated superconductivity.</td>
</tr>
<tr>
<td>10:00-10:30</td>
<td>S. Feng</td>
<td>Autocorrelation of quasiparticle spectral intensities and its connection with quasiparticle scattering interference in cuprate superconductors.</td>
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ABSTRACTS
March 31, 2019
Recent advances in high-pressure physics, materials, and geoscience
H.K. Mao\textsuperscript{1}, B. Chen\textsuperscript{1}, C. Ji\textsuperscript{1}, Y. He\textsuperscript{1}, M.Q. Hou\textsuperscript{1}, Q.Y. Hu\textsuperscript{1}, F. Ke\textsuperscript{1}, D.Y. Kim\textsuperscript{1}, B. Li\textsuperscript{1}, J. Liu\textsuperscript{1}, L.X. Yang\textsuperscript{1}, W.G. Yang\textsuperscript{1}, B. Li\textsuperscript{1}, Z.D. Zeng\textsuperscript{1}

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High-pressure science has made major progresses in multidisciplinary frontiers. In high-pressure physics, the natures of hydrogen phases III and IV are finally unveiled. X-ray diffraction up to 254 GPa shows solid molecular hydrogen crystallizes in hexagonal-close-packed (hcp) structure throughout the I-III-IV transitions. The precipitous drop of \(c/a\) ratio in phase IV associated with drastic changes of Raman and infrared spectra reveals a new type of electronic topological transition. In materials research, novel pressure-induced bonding changes and interesting new properties have been observed and quenched in crystalline, amorphous, and two-dimensional carbon. In deep Earth studies, unexpected iron superoxides and superionic hydrogen are discovered in reactions of mineral with water under the deep lower mantle conditions, leading to revolutionary new understanding of the Earth’s deep process. The progresses demonstrate the power of coordinated, integrated efforts of high-pressure science and technology.
Raising the bar toward a first-principles description of stronger correlations: Novel superconductors to topological materials

Arun Bansil

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I will discuss how advanced density functionals are enabling new insights into the electronic structure, phase diagrams and magnetism of a wide variety of materials that have until now been considered to be so strongly correlated as to lie outside the scope of first-principles treatment. A spectacular example is provided by the cuprate high-Tc superconductors in which the density functional theory fails to correctly predict the half-filled parent compounds to be insulators. In sharp contrast, however, the recently constructed SCAN functional [1] not only reproduces the insulating character and magnetism of the half-filled cuprates, but also captures the transition to the metallic state with doping without invoking any free parameters such as the Hubbard U. [2-4] I will also comment on the opportunities for a new generation of predictive modeling in correlated materials more generally, including the topological phases of quantum matter, which are drawing intense current interest [5], and the possibilities for more robust modeling of high-pressure phases. Work supported by the U.S. Department of Energy.

Single crystal thin films of three-dimensional topological insulators via non-catalytic vapor phase epitaxial crystal growth

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Topological insulators (TIs) have currently been attracting much attention from the viewpoint of contemporary materials science generating new electronic states of helical massless Dirac fermions on the two-dimensional (2D) surface or the one-dimensional (1D) edge. The existence of such special energetic states on the topological surface states (TSS) has been confirmed by surface sensitive measurements of angle and spin resolved photoemission spectroscopy. Although many theoretical approaches suggest exotic physical properties as well as novel applications of TIs, clear observation of such physical properties is experimentally not feasible because itinerant carriers thermally generated from the bulk bands are frequently involved in experimental observations. In order to unveil the intrinsic physical properties of TSS in 3D-TIs, it is required to minimize the contribution of the bulk carriers by tuning the Fermi level ($E_F$) inside the bulk gap using large band gap materials and grow high quality ultra-thin films to sufficiently reduce the bulk contribution. The $E_F$ of 3DTIs is known to be engineered in synthesis by the concept of charged defects control. In the phase diagram of tetradymites consisting of V$^{\text{th}}$(Sb,Bi)-VI$^{\text{th}}$(Se,Te) elements are most frequently studied for 3D-TIs. Bi$_2$Se$_3$ and Bi$_2$Te$_3$ are known to be n-type 3D-TIs, while Sb$_2$Te$_3$ is p-type one although Sb$_2$Se$_3$ is still debated as to whether this is trivial or nontrivial as 3D-TIs. Since it has been difficult to observe the intrinsic TSS properties, ternary (Bi,Sb)$_2$Te (BST) or (Bi,Sb)$_2$Se$_3$ (BSS) are frequently studied by molecular beam epitaxy crystal growth. Highly bulk insulating quaternary tetradymites 3D-TIs of (Bi,Sb)$_2$(Te,Se)$_3$ (BSTS) and Sn-(Bi,Sb)$_2$(Te,S)$_3$ (Sn-BSTS) are recently proposed for 3D-TIs with larger band gaps and are intensively studied. We have been focusing on BSTS by non-catalytic vapor phase epitaxial (VPE) growth and Sn-BSTS via the exfoliation (EXF) technique by plastic tapes widely used for graphene. These techniques provide large-size thin films with high quality and can be transferred to various kinds of substrates. In this presentation, I will describe our recent advancement in BSTS and Sn-BSTS 3D-TIs [1-5].

Controlling epitaxial growth of transition metal dichalcogenides by gas source CVD

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¹2D Crystal Consortium-Materials Innovation Platform, ²Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA USA

Monolayer transition metal dichalcogenides (TMDs, MoS₂, WSe₂, etc.) possess a range of intriguing optical and electronic properties including direct bandgap, high exciton binding energies, valley polarization, etc. Our research is aimed at the development of an epitaxial growth technology for layered dichalcogenides, like that which exists for III-V and other compound semiconductors, based on gas source chemical vapor deposition (CVD). We are focused on understanding the factors at play for coalesced monolayers as well as site-specific growth. Our initial studies have focused on the uniform epitaxial growth of binary TMD monolayers including MoS₂, WS₂, WSe₂ and MoSe₂ using metal hexacarbonyl and hydride chalcogen precursors to deposit on 2” sapphire wafers in a cold-wall CVD reactor. A multi-step precursor modulation growth method was developed to independently control nucleation density and the lateral growth rate of monolayer domains on the sapphire substrate [1]. Using this approach, uniform, coalesced monolayer and few-layer TMD films were obtained on 2” sapphire substrates at growth rates on the order of ~1 monolayer/hour. In-plane X-ray diffraction demonstrates that the films are epitaxially oriented with respect to the sapphire with narrow X-ray full-width-at-half-maximum indicating minimal rotational misorientation of domains within the basal plane [2]. Growth of (Mo,W)S₂ alloy monolayers was also achieved over the entire composition range by controlling the inlet gas phase ratio of Mo and W hexacarbonyl precursors. In addition to the wafer-scale growth, efforts at understanding the role of metallic seeds in controlling the nucleation sites is also underway. These metallic particles act as separate nucleation sites only when a considerable seed separation is achieved. Given the interest in 2D heterostructures, the role of defects in controlling the nucleation and growth of WS₂ on epitaxial graphene is also being investigated. The nucleation sites can be modulated by the bonding between the epitaxial graphene buffer layer and the underlying SiC substrate. The observations and challenges of this technique for the different approaches will be discussed.

The authors acknowledge financial support of the U.S. National Science Foundation through the Penn State 2D Crystal Consortium – Materials Innovation Platform (2DCC-MIP) under NSF cooperative agreement DMR-1539916 and EFRI 2-DARE Grant EFRI-1433378.


Layered magnetic topological semimetals and their unusual interlayer quantum transport
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Recent discoveries of three dimensional topological semimetals have generated immense interests since they represent new topological states of quantum matters. In this talk, I will first give a brief introduction to this emerging direction and then present our recent studies on topological semimetals [1-4], which are focused on Dirac/Weyl fermions generated by square lattices in layered compounds. I will report on our discoveries of new magnetic Dirac semimetals (Sr/Ba)$_{1-y}$Mn$_{1-z}$Sb$_2$ [1,2]. In Sr$_{1-y}$Mn$_{1-z}$Sb$_2$, Dirac fermions are found to coexist with ferromagnetism, offering a rare opportunity to investigate the interplay between relativistic fermions and spontaneous time reversal symmetry breaking and explore a possible magnetic Weyl state [1]. Then I will discuss the unusual interlayer quantum transport behavior resulting from the zeroth Landau level (LL) mode observed in type-II Weyl semimetal YbMnBi$_2$ [3]. The interlayer magnetoresistivity and Hall conductivity of this material were found to exhibit surprising angular dependences under high fields, which can be well fitted by a model which considers the interlayer quantum tunneling transport of the zeroth LL’s Weyl fermions. Our results shed light on the unusual role of zeroth LL mode in transport. Finally I will show our experimental evidences for the topological nodal line semimetal states found in ZrSiSe and ZrSiTe [4]. Since atomically thin crystals of these two materials are accessible via mechanical exfoliation, they raise the possibility of realizing the theoretically predicted 2D topological insulators.

Topological Surface States and Inducing Superconductivity in Bi$_2$Te$_3$ Nanotubes
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Topological insulators and topological superconductors have been the subject of intensive research in recent years due to their exotic behaviors as well as the possibility to host Majorana Fermions. Bi$_2$Te$_3$ nanotubes have been synthesized and studied in order to maximally increase the surface-to-volume ratio as well as near a quasi-1D system. The nanotubes have an outer diameter in the range of 70-120 nm and the wall width 9-12 nm, thicker than the critical thickness for outer-inner surface state hybridization. The bulk conduction at low temperatures is further suppressed by disorder. Nonetheless, the magnetoresistance exhibits quantum oscillations as a function of the magnetic field along the nanotubes.\(^1\) Detailed numerical simulations support that the resistance oscillations are arising from the topological surface states which have substantially longer localization length than that of other non-topological states. This result demonstrates the inherent nature of the topological surface states protected from strong disorder in the bulk. We have tested inducing superconductivity in the nanotubes with superconducting Nb contacts. We have previously studied NbSe$_2$/Bi$_2$Se$_3$ bilayer films and observed both proximity-induced bulk and two-dimensional surface superconductivity.\(^2,3\) However, contrary to the results in thin films, inducing superconductivity in the nanotubes results in an anomalous resistance increase when the Nb contact becomes superconducting. The experimental results, though still lacking explanation, will be presented and discussed.


Topological Semimetals from a High Magnetic Fields Perspective

L. Balicas¹

¹National High Magnetic Field Laboratory and Physics Department, Florida State University

Topological semimetals such as Weyl and Dirac systems are three-dimensional phases of matter characterized by topology and symmetry protected gapless electronic excitations. In the past few years, we have studied a few of these compounds [1-8] under high magnetic fields, with the goal of

i) extracting their electronic structure at the Fermi level in order to

ii) compare it with theoretical predictions, and of

iii) exposing their transport properties which are expected to be unconventional due to their “topological” character. Quantum oscillatory phenomena, such as the de Haas van Alphen-effect (dHvA), provide information about their electronic structure and have a higher energy resolution when compared to angle resolved photoemission spectroscopy (ARPES), which insofar has been the technique of choice for studying these compounds. Here, we will provide a (very) brief introduction to associated concepts and discuss the specific case of Ta₂MoTe₂ which is a candidate for the so-called Weyl type-II semimetallic state [5]. Although a number of ARPES based publications claim an excellent agreement with the theoretical predictions, dHvA reveals a Fermi surface which is rather distinct from the predicted one. Time permitting, we will also discuss the observation of planar Hall and anomalous planar Hall effects in TaAs [9] and the physics of nodal line systems, such as ZrSiSe [10], previously claimed to display non-trivial topology although the calculations yield trivial topological invariants.

Quantum hall effect and thermoelectric properties of surface Dirac states in Sn-Bi\textsubscript{1.1}Sb\textsubscript{0.9}Te\textsubscript{2}S crystal

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The electric transport properties of single crystal of three-dimensional topological insulator Sn-Bi\textsubscript{1.1}Sd\textsubscript{0.9}Te\textsubscript{2}S (Sn-BSTS) has been studied. A series of transport measurements including resistivity, Hall coefficient, Shubnikov-de-Haas (SdH) quantum oscillations, and Seebeck coefficient have been carried out with several samples in different thicknesses from 110 µm to 3 µm. The thickness dependence of the resistivity and Seebeck coefficient clearly shows the suppression of bulk carries, where the surface transport becomes dominant at around 200 K for 3 µm-sample. At low temperature, a clear SdH oscillations of surface Dirac states are observed for each sample. Moreover, a quantized Hall plateau appears for 3 µm-sample, which shows an integer quantized value indicating the contribution of both top and bottom Dirac surfaces.
Realization of Spin-Orbital Liquid State in Iridates
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The search for quantum spin (orbital) liquids (QSL) -materials where local moments are well formed but continue to fluctuate quantum mechanically down to zero temperature still remains a fundamental challenge in condensed matter physics. In this talk, we shall show that the electronic structure of 6H perovskite type quaternary iridates \( \text{Ba}_3\text{MIr}_2\text{O}_9 \), have all the necessary ingredients to host QSL state. In \( \text{Ba}_3\text{MIr}_2\text{O}_9 \), Ir ions form structural dimers and non-magnetic M provides a knob to tailor the valence of Ir leading to emergent quantum phases. As a first example [1], we shall consider the pentavalent (d\(^4\)) 6H perovskite iridate \( \text{Ba}_3\text{ZnIr}_2\text{O}_9 \) and argue that the ground state of this system is a realization of novel spin-orbital liquid state. Our results reveal that such a system provides a very close realization of the elusive J=0 state where Ir local moments are spontaneously generated due to the comparable energy scales of the singlet-triplet splitting driven by spin-orbit coupling (SOC) and the super-exchange interaction mediated by strong intra-dimer hopping. While the Ir ions within the structural \( \text{Ir}_2\text{O}_9 \) dimer prefers to form a spin-orbit singlet states(SOS) with no resultant moment, however substantial frustrated inter-dimer exchange interactions induce quantum fluctuations in the SOS states favoring spin-orbital liquid phase at low enough temperature. As a second example [2] we shall consider the d\(^{4.5}\) insulator \( \text{Ba}_3\text{YIr}_2\text{O}_9 \) and explain the origin of the pressure induced magnetic transition to a spin-orbital liquid state in this system. We shall also discuss the importance of Kitaev interactions in the realization QSL phases for the d\(^5\) members of the same family[3]. Finally we shall compare our results with d\(^3\) [4] and d\(^4\) [5] Ir based double perovskites, particularly explain the origin of moments and presence of spin-orbital singlets in \( \text{Ba}_2\text{YIrO}_6 \).


Pressure is an effective and clean means to tune fundamental interactions in 5d based materials, where electron-electron (Coulomb) correlations and spin-orbit coupling (SOC) are of comparable magnitude, to induce new phases and give insight into their novel properties. In this presentation, we will show some interesting novel magnetic and structural transitions emergent from some iridates (i.e. Sr$_3$Ir$_2$O$_7$) at high pressure, which are probed with synchrotron, optical, electric transport, as well as theoretical computation methods.
Evolution of the spin, orbital and charge excitations upon tuning the local lattice environment of Sr$_2$IrO$_4$

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Sr$_2$IrO$_4$ has been in the lime light during the last years due to the discovery of a novel $J_{\text{eff}} = \frac{1}{2}$ Mott state in the large spin-orbit regime. The sensitivity of this quantum state to local coordination and structural distortions suggests strain and confinement as ideal routes for studying and manipulating its properties. In particular, the entanglement of spin, orbital, lattice and charge degrees of freedom entail that modification of the local lattice distortions should be an ideal knob to tune the ground state of Sr$_2$IrO$_4$. In momentum-dependent Resonant Inelastic X-ray Scattering (RIXS) experiments at the O K- and Ir L$_3$-edges on thin films of Sr$_2$IrO$_4$ grown on different substrates we observe the evolution of the low energy elementary excitations upon strain. We report a clear softening of the spin wave dispersion along the ($\pi$,0) direction upon tensile strain. This effect is not present along the ($\pi$, $\pi$) direction, underlining the complex modification characteristics of the exchange interactions. By comparison with simulations based on band structure calculations, we assign a dispersive mode at 400 meV to electron-hole pair excitations. We find both energy and bandwidth of this mode to be highly affected by strain, connecting its development to the evolution of the band structure and the Mott insulating gap upon lattice distortions.
Electric field driven octahedral rotation in Sr$_2$RuO$_4$ and its implication

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One of the key goals in the research of perovskite transition metal oxides (TMOs) is to design and control their physical properties, for which MO$_6$ (M=transition metal) octahedron rotation (OR) is considered to be one of the key control parameters. We show that OR can be induced and thus be tuned with an electric field in Sr$_2$RuO$_4$. Originally rotated octahedra in the surface layer of Sr$_2$RuO$_4$ are restored to the bulk structure upon K dosing on the surface. Our theoretical investigation shows that OR in Sr$_2$RuO$_4$ originates from surface electric field which can be controlled via the screening effect of the overlaid K layer and that the variation of Sr-Sr vertical distance is responsible for the coupling between OR and electric field. Our finding raises a possibility for electric field control of physical properties through the variation of the OR angle even for non-piezoelectric materials.
DMFT coupled to DFT: Case of some complex oxides
Olle Eriksson
Uppsala University, Uppsala, Sweden

In this presentation I will describe how correlated electronic structures can be treated with dynamical mean field theory (DMFT) coupled to density functional theory (DFT). Applications of the method will be presented, that cover the pressure dependence of spectroscopic data, such as photoelectron spectroscopy and x-ray absorption spectroscopy. Materials to be discussed involve complex oxides.
The use of oxides to kinetically enhance the sorption properties of MgH$_2$ at high pressure
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Magnesium Hydride MgH$_2$ remains a potential solid state hydrogen storage material, despite its high thermodynamically stability (approx. 75 kJ/mol.H$_2$) and poor absorption/desorption kinetics resulting in a high dissociation temperature which currently limits practical applications [1]. This is due to a high reversible capacity – both gravimetric (7.6 wt.%) and volumetric (~0.1 g/cm$^3$) [2]. Its abundance in the earth’s crust and oceans ensures sufficient supply for use in large-scale energy technologies [3]. While methods to improve the thermodynamics by destabilizing MgH$_2$ are mostly limited to alloying and nano-sizing/confinement, the use of small amounts of additives or catalysts, as well as mechanical ball has led to a significant enhancement in the kinetics of the metal hydrogen reaction.

The benchmark additive, niobium oxide (Nb$_2$O$_5$) substantially enhances the kinetics of absorption and desorption, while reducing the reagglomeration of grains during cycling, even in small quantities (0.5 mol%). Recently, the organic liquid titanium isopropoxide (TTIP), has been shown to deliver similar improvements [4]. Following this work, a range of titanium-based liquid and non-liquid organic oxides, as well as a non-oxide, were compared to determine which additives were effective and whether differences between the additives might shed light on the role of the additive in the metal-hydrogen reaction. While the role of additives is not yet clear, there are important differences in the results of using different additives, suggesting the use of additive combinations for effective kinetic enhancement.

Reversible Hydrogenation of Magnesium Boride and Magnesium Boranes to Magnesium Borohydride

Craig Jensen

University of Hawaii, Hawaii, USA
Hydrogen storage and battery materials - new types of materials

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Hydrogen is recognized as a potential and extremely interesting energy carrier, which can facilitate efficient utilization of unevenly distributed renewable energy. Furthermore, hydrogen has an extremely interesting chemistry and form compounds with most elements in the periodic table and with a variety of different types of bonds. Metal hydrides have recently become very interesting as new classes of energy materials for batteries and hydrogen storage [1]. Here we report an overview of new synthetic strategies and structural, physical and chemical properties for metal borohydrides, revealing a number of new trends correlating composition, structure, bonding and thermal properties towards the rational design of novel functional materials [1,2]. Hydrogen uptake at moderate temperatures and high pressures, \( p(H_2) \sim 0.5 \text{ - } 1 \text{ kbar} \), is also investigated [3]. Some new hydrides also show extremely high ion conductivity. We discuss that structural dynamics in the solid state of hydrides, i.e. entropy effects, are of extreme importance for ionic conductivity [4,5]. This presentation demonstrates that there is still room for discovering new hydrides with extreme flexibility in composition, structure and properties [6]. We conclude that the chemistry of hydrides is very diverse, towards rational design of multi-functional materials, including new ion-conductors for batteries, hydrogen storage materials, and possibly materials with new types of optical properties.

Multi-principal-element alloys as new materials for hydrogen absorption  
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Hydrogen is currently considered as a renewable and sustainable solution for reducing worldwide fossil fuel consumption and subsequent pollution. However, the main drawback for the development of hydrogen as clean energy carrier is its safe and efficient storage. Among various materials for hydrogen storage such as, alloys forming hydrides, none fulfil the requirements for a competitive storage media. Consequently, innovative materials are stringently required.\textsuperscript{[1]}  
Recently, a new paradigm of alloying strategy has emerged based on the original concept of multi-principal-element alloys (MPEAs), initially proposed to develop materials with enhanced properties.\textsuperscript{[2]} The principle is laid on the mixing of elements close to the equimolar proportion for systems up to five and more containing elements. This mixing may lead to the formation of simple single-phased solid solutions (bcc, fcc...). Among all multi-principal-element effects, the development of large lattice strain distortions due to the atomic size mismatch among different component elements is particularly interesting for hydrogen storage. The creation of large interstitial sites is considered beneficial for the insertion of large amount of hydrogen. However, despite promising hydrogen storage capacity reported for some MPEAs\textsuperscript{[3]}, the potential use of these materials is largely unexplored in the clean energy field (electrochemical conversion and hydrogen storage).\textsuperscript{[4]}  
We report here the hydrogen absorption properties of novel MPEAs that are based on refractory elements (Ti, V, Zr, Nb...) and light-weighted metals (Mg, Al...) to increase the gravimetric storage capacity. These materials have been prepared by mecanochemical synthesis (ball-milling under inert or hydrogen gas). The ball milling under inert gas produces single-phased bcc materials. In contrast to conventional bcc alloys that show two phase transformation (alloy bcc $\leftrightarrow$ monohydride bct $\leftrightarrow$ dihydride fcc), the hydride absorption in these MPEAs occurs into a single step (alloy bcc $\leftrightarrow$ dihydride bct). Hydrogen atoms occupy the tetrahedral sites of the bct structure, as evidenced by neutron diffraction. The lattice distortion introduced by the atomic size mismatch seems to be responsible for this new reaction pathway: the classical bcc alloys with small lattice distortion possess two phase transformation, whereas MPEAs with relative large lattice distortion have one step transition.\textsuperscript{[5]}  

Molten metal closo-hydridoborates
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Metal closo-hydridoborates, e.g. M₂B₁₂H₁₂, have received increased attention as ion conductors due to extraordinary ionic conductivity in their high-temperature structural polymorphs.1–5 Recently, nanoconfinement of Li₂B₁₂H₁₂ was achieved via a solid-gas reaction inside a nanoporous SiO₂ (SBA-15) scaffold between LiBH₄ and gaseous B₂H₆.6 However, the reaction yields moderate purity (94 mol%) Li₂B₁₂H₁₂ with 6 mol% Li₂B₁₀H₁₀. The ionic conductivity of the nanoconfined sample was 1.0 x 10⁻⁷ S·cm⁻¹ at room temperature, which is similar to bulk Li₂B₁₂H₁₂.6

In this work, solvated lithium closo-dodecaborate, Li₂B₁₂H₁₂·Solv. (Solv. = tetrahydrofuran, acetonitrile), show unexpected melting at low temperature (T < 145 °C, Figure 1) and subsequent recrystallisation of the parent compound at higher temperature. This feature has been explored to melt infiltrate Li₂B₁₂H₁₂ into a nanoporous scaffold (SBA-15), which ensures a 100% purity. Small-angle X-ray scattering confirms that melt infiltration occurred, while the ionic conductivity of the nanoconfined and molten Li₂B₁₂H₁₂ was measured by EIS.

Figure 1. Temperature programmedphotographic analysis of Li₂B₁₂H₁₂·xACN showing melting at low temperature.

Non-equilibrium Kr adsorption in nanoporous $\gamma$-Mg(BH$_4$)$_2$ by \textit{in situ} synchrotron powder diffraction

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$^1$Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, 1348 Louvain-la-Neuve, Belgium

$^2$Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, 38000 Grenoble, France

Gas adsorption by porous frameworks can result in structure “breathing”, “pores gate opening/closing”, negative pressure adsorption, and other fascinating phenomena. The time-dependent diffraction probes kinetics of the guest uptake and structural response of the host framework; time evolution of the crystal structure carries information on the mechanisms and kinetic barriers of guest adsorption.

Crystalline materials with pore sizes comparable to the kinetic diameters of the guest molecules were proposed for efficient adsorption and separation of Kr and Xe. $\gamma$-Mg(BH$_4$)$_2$ features 1D channels matching this criterion. Kr adsorption has been probed using synchrotron powder diffraction at various pressures and temperatures. It results in two co-existing crystalline phases with the limiting composition Mg(BH$_4$)$_2$·0.66Kr, 50.7 wt\% of Kr in the crystalline phase, the highest reported for porous materials. Quasi-equilibrium isobars built from Rietveld refinement of Kr site occupancies were rationalized with a non-cooperative lattice gas model yielding the values of the thermodynamic parameters for Kr adsorption. The latter were independently confirmed from Kr fluorescence. We have parameterized the pronounced kinetic hysteresis with a modified mean-field model adopted for the Arrhenius kinetics.

We also report on sub-second diffraction experiment to the Kr absorption by $\gamma$-Mg(BH$_4$)$_2$. We resolve the contributions of two kinetic barriers: most likely, the first is via Kr diffusion along the pore 1-D channels of the crystal structure and the second mechanism is through the interchannel aperture window.
H₂ Nautic - a hydrogen storage vessel for small touristic boats.

M. Polanski

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The concept of new type of energy storage container for small touristic boats is presented. Heat exchange between powder bed and cooling medium is improved by introducing the movement of the powder in the vessel. Due to this specific design, a number of factors have to be considered and investigated including wear problems, materials compatibility, particles’ filtration and cyclic stability of structural materials. Several new functionalities of the vessel were proposed and will be presented.

The storage tank is being built within the “Hydrogen storage” program funded by The National Center of Research and Development of Poland which is based on competition between several teams working in parallel on their projects and trying to reach goal set by funding institution.
Complex metal hydrides investigated by fast neutron powder diffraction

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The European Spallation Source (ESS) is presently under construction in Lund, Sweden, and the neutron community aims to develop in situ/in operando capacities and expertise in order to take advantage of the new opportunities ESS will present. In that respect, efforts have been made to investigate a series of complex metal hydrides by fast neutron powder diffraction measurements not only to find and solve new structures but to look in detail into the kinetics of various processes. One example is magnesium borohydride (Mg(BH₄)₂) which is a promising material for solid state hydrogen storage. However, the predicted reversible hydrogen sorption properties at moderate temperatures have not been reached due to sluggish hydrogen sorption kinetics. Recently, we investigated Mg(BH₄)₂ including different gases such as D₂, He, Ne, Ar, Kr & Xe at the Wide Angle Neutron Diffractometer WAND² at Oak Ridge National Lab, Oak Ridge, TN, USA and at the dedicated hydrogen storage beamline NOVA at J-Parc, Tokai, Japan. It was shown that Mg(¹¹BD₄)₂ forms a new hydride phases at 25 K and 1 bar D₂ pressure. This first hydride with functional porosity pores was recently discovered by Filinchuk et al. (Angew. Chem. Int. Ed. 2011). It has a 3D net of interpenetrating channels of ~8 Å diameter giving ~33% empty void space. Small molecules such as dichloromethane, nitrogen or hydrogen can be absorbed inside γ-Mg(BH₄)₂. Recent unpublished volumetric and neutron powder diffraction (NPD) experiments show that this framework forms two hydride phases, reaching the composition of up to 2.33 H₂ molecules per Mg atom, which was now confirmed also by fast neutron powder diffraction. The hydrogen density in the pores exceeds the one in the liquid hydrogen by the factor of 2 and has no analogues among porous solids.

Figure 1. Crystal structure of the two D₂-loaded phases with the limiting compositions γ-Mg(¹¹BD₄)₂·1.33D₂ (left) and γ-Mg(¹¹BD₄)₂·2.33D₂ (right). Mg atoms are shown as gray spheres, BH₄ groups as blue tetrahedral, and unit cells are defined by red lines, positions of D₂ molecules (D₂-superatoms) as red spheres.
Structural Stability of and Enhanced CO$_2$ Storage in Metal-Organic Frameworks under High Pressures Probed by Vibrational Spectroscopies and X-ray Diffraction

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Metal-organic frameworks (MOFs) are an emerging class of porous materials that have attracted much attention due to their enormous surface areas, high thermal stabilities, and high tunabilities. One of the most promising applications of MOFs is gas storage, especially CO$_2$ storage. It is known that high external pressure can provide an effective driving force to achieve structural modifications. Subsequently, these pressure-induced changes will affect the sorption selectivity, capacity and access to the binding sites of the porous materials, and likely the CO$_2$ storage capacity. Using in situ Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy and synchrotron X-ray diffraction measurements, we investigated the high pressure effects on the framework structures, carbon dioxide adsorption capacity as well as guest-host interactions on selected MOFs, including Pb(Cd)SDB, SIFSIX-3-Zn and ZIF-8. These MOFs possess different pore sizes, topologies, as well as accessible binding sites. Our results show highly structural dependent stabilities and pressure-induced modifications as well as pressure-regulated guest-host interactions. These findings demonstrated great potentials for the MOFs with specific structural characteristics for CO$_2$ storage applications that require extreme loading pressures.

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**High temperature and possible topological superconductivity**

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I discuss two high temperature superconductors:

a) $T_c=39\text{K}$ MgB$_2$, in which we experimentally show the presence of Dirac nodal lines connected by a topological “waterslide” surface state existing on the (010) edges of the crystal [1]. This topological surface state is expected to go superconducting via the proximity effect – if it does it would be a novel type of high temperature topological superconductor.

b) High temperature d-wave cuprate superconductors. In these we access the fully causal electronic self-energy utilizing a brand new 2-dimensional method of ARPES analysis [2], which removes the critical limitations of the previous one-dimensional MDC (Momentum Distribution Curve) and EDC (Energy Distribution Curve) methods. This new method, which utilizes orders-of-magnitude fewer parameters than the MDC and EDC methods, brings in the energy, momentum, and temperature -dependence of the self-energies and is fully consistent with the already-successful studies showing the gap filling-in behavior [3, 4]. The full set of parameters we access allows us to make the first direct measurements of the shape and size of the pairs, which are 4-armed starfish with ultrashort length scales in the antinodal direction - of order 4.5 Angstroms independent of doping level [5].


ARPES on topological quantum materials: from topological Kondo insulator to Weyl semimetal
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Recently, significant advances in topological theory extend the topological classifications from non-interacting insulators to strongly correlated insulators, and further to semimetals. In this presentation, I will present our recent works on direct visualizations of topological quantum states in topological Kondo insulators and Weyl semimetals by using angle-resolved photoemission spectroscopy (ARPES) and its spin-resolved variant (SARPES). Furthermore, using MoTe$_2$ as an example, we will discuss the importance of on-site Coulomb interaction which leads to a Lifshitz transition and results in the formation of a hybrid Weyl semimetal state with a pair of energy bands touching at both type-I and type-II Weyl nodes.
Angle-resolved photoemission studies on strongly correlated materials

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In quantum materials, many emergent phenomena appear when correlation is at play. A key issue in strongly correlated materials is to understand the relationship between multiple orders and interactions. Using angle-resolved photoemission spectroscopy (ARPES), we have performed systematic studies on cuprate superconductors. In hole-doped cuprates, we have quantitatively examined electron-boson coupling as a function of momentum and doping [1]. We further demonstrate that electron-phonon coupling and pseudogap related electronic correlation reinforce each other in a positive-feedback loop upon entering the strange-metal regime, which in turn drives a stronger superconductivity [2]. In electron-doped cuprates, we have revealed an intrinsic Fermi surface reconstruction in a doping regime where the antiferromagnetic (AFM) long-range order is absent. This observation suggests the existence of a mysterious order in this system. A cooperation between AFM short-range order and topological order provides an ansatz for its origin [3].

Electronic phase separation in BiS$_2$-based systems

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Here, I will review some of our recent studies using space resolved photoemission on BiS$_2$-based systems. Using space resolved ARPES we have found metallic phase embedded in the morphological defects and at the sample edges of stoichiometric CeOBiS$_2$. While bulk of the sample is semiconducting, the embedded metallic phase is characterized by the Fermi surface similar to the one of doped BiS$_2$-based superconductors. Typical size of the observed metallic domains is larger than the superconducting correlation length of the system suggesting that the observed superconductivity in undoped CeOBiS$_2$ is likely to be due to this embedded metallic phase at the defects. Space resolved ARPES of self-doped EuFBI$_2$ will also be discussed revealing phase separation at mesoscopic scale that is driven by peculiar lattice distortions in these materials.
Nanoscale Atomic Distortions in the BiS$_2$ Superconductors: Ferrodistortive Sulfur Modes

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The discovery of phonon-mediated superconductivity in the BiS$_2$ class led to a renewed interest in compounds that exhibit a strong structure-property relationship due to its intrinsic disorder. The ReO$_{1-x}$F$_x$BiS$_2$ (Re = La, Nd, and Pr) systems were investigated using neutron and synchrotron X-ray diffraction to reveal the nature of electron–phonon coupling that leads to unconventional states with intricate microstructures and physical properties. In ReO$_{1-x}$F$_x$BiS$_2$ the distortions are manifested in the form of in-plane sulfur distortions which split the in-plane Bi–S bonds while the splitting gives rise to different bond lengths around Bi atoms. The proposed distortion modes create an unequal charge distribution around the Bi atom giving rise to charge fluctuations. The superconducting phases of ReO$_{1-x}$F$_x$BiS$_2$ also manifest z-motion of apical sulfur which could act as a charge transfer conduit between the electron doping layers and superconducting layers.

Superconductivity in Pt-based pnictides with ordered honeycomb networks
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Alkaline-earth platinum pnictides exhibit a variety of hexagonal structures that are characterized by honeycomb networks, such as CaPt$_x$P$_{2-x}$, SrPtAs, and BaPtSb with an AlB$_2$- ($P6/mmm$, $D_{6h}^1$, No. 191), a KZnAs- ($P6_3/mmc$, $D_{6h}^4$, No. 194), and a SrPtSb-type ($P-6m2$, $D_{3h}^1$, No. 187) structures, respectively. SrPtAs exhibits superconductivity at the transition temperature $T_c$ of 2.4 K, as we reported [1]. Superconductors with honeycomb networks have attracted interest since the theoretical predictions of exotic superconductivity in SrPtAs, such as a singlet-triplet mixed state [2], a chiral $d$-wave state [3], and an $f$-wave state [4]. In order to explore the exotic superconducting states, we have developed novel compounds with honeycomb networks.

We will report on the discovery of superconductivity in BaPtAs and BaPtSb with ordered honeycomb networks. BaPtSb exhibited superconductivity at 1.64 K [5]. The muon spin rotation/relaxation measurements showed a slight increase in the relaxation rate of muon spins below $T_c$. The result suggested the occurrence of the spontaneous magnetic field below $T_c$ and thus the chiral $d$-wave state as a possible superconducting state [6]. BaPtAs was known as a cubic LaIrSi-type compound. We have discovered the hexagonal structures of BaPtAs, namely, SrPtSb-type ($P-6m2$, $D_{3h}^1$, No. 187) and YPtAs-type ($P6_3/mmc$, $D_{6h}^4$, No. 194) structures [7]. Both structural phases exhibited superconductivity at 2.8 and 2.1-3.0 K, respectively [7]. Inversion symmetry is broken in the SrPtSb-type, whereas it is preserved in the YPtAs-type. Our discovery provides opportunities not only for the experimental examination of the predicted superconductivity but also for further studies on exotic states that result from the strong spin-orbit interaction of Pt under broken inversion symmetry.

This work was conducted in collaboration with M. Nohara, Y. Saito, T. Takeuchi, H. Ota (Okayama University), and T. Adachi (Sophia University).

SnPn-based layered superconductors
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We report SnPn-based (Pn: pnictogen) layered superconductors NaSn$_2$As$_2$ and Na$_{1-x}$Sn$_2$P$_2$ [1,2]. The crystal structure of these compounds is characterized by two layers of a buckled honeycomb network of SnPn, bound by the van der Waals (vdW) forces and separated by Na ions. Measurements of electrical resistivity and specific heat indicate the bulk nature of superconductivity with transition temperature ($T_c$) of 1.3 K for NaSn$_2$As$_2$ and 2.0 K for Na$_{1-x}$Sn$_2$P$_2$. Amount of Na deficiency ($x$) of Na$_{1-x}$Sn$_2$P$_2$ was estimated to be 0.07(2) using synchrotron X-ray diffraction. First-principles calculation using density functional theory shows that these compounds have comparable electronic structure, suggesting higher $T_c$ of Na$_{1-x}$Sn$_2$P$_2$ is a result of increased density of states at the Fermi level due to Na deficiency. Recent studies on temperature-dependent magnetic penetration depth [3] and thermal conductivity [4] show that superconductivity of NaSn$_2$As$_2$ is fully gapped s-wave state in the dirty limit. Because there are various structural analogues containing SnPn conducting layers, our results indicate that SnPn-based layered compounds can be categorized into a novel family of vdW-type superconductors. In the conference, recent experimental results including doping effect to increase $T_c$ of these compounds will also be presented.

Dark and half excitonic insulators
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Excitonic insulator (EI) with a many-body ground state is a new state of matter. It forms when the exciton binding energy of a semiconductor exceeds the bandgap, leading to a spontaneous formation of excitons. Because an exciton is made of two fermions, it obeys bosonic statistics on scale larger than the exciton radius, allowing for a Bose condensation. As a naturally-formed electron-hole condensate, EI behaves as a perfect insulator for both charge and heat transport.

The search for EI can be traced half century back but compelling experimental evidence is still lacking. In early days, much attention was on materials with interacting electron-hole pockets located at different regions of the Brillouin zone for semiconductors with a small band gap or semimetals with a small band overlap to minimize the effect of screening. Unfortunately, the perceived formation of indirect-gap EIs is always accompanied by a strong structural distortion such as a charge density wave, which makes it difficult to determine whether the observed instability is originated from an excitonic effect or purely a band-type Jahn-Teller distortion. The situation is not any better for direct-gap materials, as they suffer from the divergence of polarizability when the band gap approaches zero, leading to a diminishing exciton binding energy. For example, the exciton binding energy in two-dimensional (2D) materials is roughly $\frac{1}{4}$ of the band gap [1].

By extensive first-principles calculations, here we present theoretical evidences for direct-gap EI in 2D materials where exciton binding energy is decoupled from the band gap as a result of optical selection rules, e.g., when the band-edge states have the same parity [2]. These dark EI include 2D GaAs [3] and single-layer TiS$_3$. The latter can be experimentally exfoliated from its layered bulk form [4]. More intriguing is the prediction of half EIs in monolayer 1T-MX$_2$ where M = Co, Ni and X = Cl, Br; all of them exist in layered bulk form [5]. In these half EIs, one spin channel has a many-body EI ground state, while the other spin channel remains to be a conventional band insulator, which potentially results in a spin superfluid. Also counterintuitive is the fact that these strongly-correlated monolayer 1T-MX$_2$ have sizable single-particle band gaps, as large as $> 3$ eV, implying gigantic exciton binding energies due to strong real-space wavefunction localizations.

Work was in collaboration with Zeyu Jiang, Yuanchang Li, and Wenhui Duan.

Higher-order Floquet topological phases with corner and bulk bound states
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In recent years, the notion of bulk-boundary correspondence has been generalized to higher-order topological phases in equilibrium. Such higher-order phases have been already engineered and observed in a variety of systems. In this talk, we will discuss the characterization of higher-order Floquet topological phases dynamically generated in a periodically driven system with mirror symmetries. We will show that these phases support lower-dimensional Floquet bound states protected by the non-equilibrium higher-order topology induced by the drive. Finally, we will show that bulk vortex structures can be dynamically generated by a drive that is spatially inhomogeneous.

Heterostructures of 3d-5d Double Perovskites: Potential Candidates for Confined Half-metallicity & High-T Quantum Anomalous Hall States

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Considering the specific case of double perovskite (DP) compound Ba\textsubscript{2}FeReO\textsubscript{6} (BFRO) made out of 3d transition metal (TM) ion Fe and 5d transition metal ion Re, we show that by embedding the BFRO in the band insulator BaTiO\textsubscript{3} (BTO) in a heterostructure quantum well geometry, the electrons of the DP can be confined to two dimensions due to potential energy mismatch created between the TM ions in the DP and in the insulating oxide. The 2D confinement achieved in the BTO/BFRO/BTO quantum well structures provides significant improvement over that in polar catastrophe-driven LAO/STO in terms of (i) 2D confinement length is an order of magnitude smaller, (ii) complete spin polarization of the 2D electron gas (2DEG), (iii) polarity control of the 2DEG, suggestive of magnetoelectric coupling, and (iv) realization of ultrathin half metals with topological bands.

Extending on the idea of driving topologically non-trivial features, we further find that BFRO/BTO geometry with termination at Fe layer, leads to formation of a C=1 quantum anomalous hall insulator (QAHI) state with a large topological gap \(\sim 100\text{meV}\) and an estimated FM \(T_c \sim 315\text{K}\). The large gap and high \(T_c\) should enable practical use of our proposal. Our study identifies three key ingredients for the formation of this QAHI, which should be broadly applicable to other \(t_{2g}\) physics dominated 3\textit{d}-5\textit{d} or 3\textit{d}-4\textit{d} half-metallic DPs like Sr\textsubscript{2}FeMoO\textsubscript{6} and Sr\textsubscript{2}CrWO\textsubscript{6}.

Work done in collaboration with Santu Baidya, Arun Paramekanti and Umesh Waghmare.

Towards ideal topological materials: Comprehensive database searches using symmetry indicators

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Topological materials (TMs) showcase intriguing physical properties defying expectations based on conventional materials, and hold promise for the development of devices with new functionalities. While several theoretically proposed TMs have been experimentally confirmed, extensive experimental exploration of topological properties as well as applications in realistic devices have been held back due to the lack of excellent TMs in which interference from trivial Fermi surface states is minimized. We tackle this problem in the present work by applying our recently developed method of symmetry indicators to all non-magnetic compounds in the 230 space groups. An exhaustive database search reveals thousands of TM candidates. Of these, we highlight the excellent TMs, the 258 topological insulators and 165 topological crystalline insulators which have either noticeable full band gap or a considerable direct gap together with small trivial Fermi pockets. We also give a list of 489 topological semimetals with the band crossing points located near the Fermi level. All predictions obtained through standard generalized gradient approximation (GGA) calculations were cross-checked with the modified Becke-Johnson (MBJ) potential calculations, appropriate for narrow gap materials. With the electronic and optical behavior around the Fermi level dominated by the topologically non-trivial bands, these newly found TMs candidates open wide possibilities for realizing the promise of TMs in next-generation electronic devices.
Thermal Battery Development for Concentrated Solar Power Systems
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Solar energy is the most abundant renewable energy resource and therefore logically represents the most important renewable energy resource for the future. The IEA roadmap for solar energy set a target of ca. 22% of global electricity production from solar energy by 2050, with 50% being produced from concentrating solar thermal (CST) power systems. Achieving this target will be possible only if the costs of producing electricity from solar energy are significantly reduced and cost effective energy storage technologies can be developed.

A major challenge is to achieve continuous, low-variability power generation from renewable energy sources, for stand-alone applications or for integration with domestic power grids. Solar mirror collection fields can collect thermal energy during the day and run a heat engine to convert it into electricity, but cannot provide power at night. However, if some of the heat is used to remove hydrogen from a metal hydride, the reverse reaction where hydrogen absorbs back into the metal hydride can then occur at night, releasing heat for power generation. This allows solar energy to provide 24 hour power generation. By combining a high temperature metal hydride with a low temperature metal hydride, a coupled pair reversible metal hydride thermochemical solar energy storage system is created [1]. Concentrated solar thermal coupled to a high and low temperature metal hydride has the potential to provide a continuous supply of electricity to remote areas in Australia and around the World. I will discuss the use of CST worldwide and will present some results on the properties of materials that are suitable for CST applications, focussing on high temperature hydrides [2 – 8].

The sodiation-desodiation mechanism of Sb-based electrode materials revealed by operando spectroscopy assisted by chemometric data analysis

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In the exciting search for efficient electrode materials for Na-ion batteries, p-block elements were found to be viable alternatives to hard carbon, showing interesting performance with reversible capacities exceeding 400 mAh/g.[1] In particular, Sb showed a specific affinity for Na, exhibiting excellent cycling stability even in the simplest form of bulk Sb.[2] Yet, the reason of this affinity is not thoroughly understood. Indeed, while the electrochemical signature suggests the formation of several possible intermediates, only Na\textsubscript{3}Sb formed at the end of sodiation is detected by X-ray diffraction (XRD), all intermediates being amorphous. Only a recent study of the mechanism by Pair Distribution Function (PDF) analysis revealed possible short-range structures for the intermediates formed while cycling pure Sb.[3] The same is observed for other Sb-based materials such as FeSb\textsubscript{2} and SnSb.[4,5]

With the goal of better understanding this specific affinity of Na for Sb, we undertook a thorough study of the electrochemical reaction of Sb, FeSb\textsubscript{2} and SnSb with Na by operando X-ray absorption spectroscopy (XAS),[6-8] coupled to \textsuperscript{57}Fe Mössbauer spectroscopy in the case of FeSb\textsubscript{2}. The whole sets of spectra were analysed using multivariate chemometric tools (Principal Component Analysis and Multivariate Curve Resolution), in order to extract all information on the mechanisms of three compounds. The results of this analysis show that, while it allows gathering important information for the reconstruction of their reaction paths, it is intrinsically impossible to prove by XAS the existence of some of the intermediates proposed in the case of Sb. On the contrary, in the case of SnSb, the possibility of studying simultaneously the absorption edges of Sn and Sb was essential to clarify the sodiation mechanism, which goes through a two-step process clearly distinct from the lithiation of SnSb.

Neutron diffraction for energy storage and conversion in metal hydrides
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Neutrons are a unique probe for non-destructive structural studies of energy materials and with the European Spallation Source presently under construction in Lund, Sweden, the neutron community aims to develop \textit{in situ} and \textit{operando} capacities, and expertise in order to take advantage of the new opportunities ESS will present. Especially energy storage and energy conversion devices mostly consists of materials with light elements such as hydrogen, lithium, carbon and oxygen, which neutrons have a high sensitivity for and are therefore very important for characterization. Diffraction itself offers the most comprehensive information about the crystal and microstructures of materials. The good neutron penetration depth allows access to the inner section for instance in a prototype energy storage/conversion device with full functionality or even commercially available products. Therefore, an overview of recent instrumentational advances such as fast neutron powder diffraction (NPD) measurements and \textit{in situ} / \textit{in operando} NPD measurements is presented. Furthermore, NPD data of the recently reported solid-state Mg-ion conductor synthesized from Mg(BH\textsubscript{4})\textsubscript{2} and ethylenediamine are elaborated and unpublished structural details are presented as well.
MH acknowledges the project “\textbf{E}nergy \textbf{R}esearch with \textbf{N}eutrons (ErwiN)” \cite{1}, which is funded by the German Federal Ministry of Education and Research (BMBF).

\cite{1} Heere, M., M.J. Mühlbauer, A. Schökel, M. Knapp, H. Ehrenberg, and A. Senyshyn, Energy research with neutrons (ErwiN) and installation of a fast neutron powder diffraction option at the MLZ, Germany. Journal of Applied Crystallography, 2018. 51(3).
Magnesium (Mg) is one of attractive media for hydrogen storage and transportation because of its high gravimetric hydrogenation density 7.6 wt%. However, the hydrogen absorption reaction is kinetically slow and requires higher temperature than 300 °C as thermal activation. To improve the kinetic properties of Mg, various catalysts such as transition metals, oxides, chlorides, and fluorides are studied so far. Among them, niobium oxide (NbO$_x$) is an excellent catalyst to drastically improve the reaction kinetics of Mg [1, 2] although the detailed catalytic mechanism is not clarified yet.

In this work, to understand the important factors for catalysis of niobium oxide, various types of Nb$_2$O$_5$ are synthesized. These Nb$_2$O$_5$ are dispersed on MgH$_2$ by ball-milling. The hydrogen desorption and absorption properties are evaluated by thermogravimetry-differential thermal analysis under Ar and H$_2$ flow conditions, respectively. The morphology and chemical state of catalysts are characterized by electron microscopes and X-ray photoelectron spectroscopy (XPS). All the synthesized Nb$_2$O$_5$ showed catalysis for the hydrogen adsorption and absorption reactions. By comparing the catalysis of Nb$_2$O$_5$ with different crystallinity and particle size, it is clarified that structural properties of initial Nb$_2$O$_5$ more affect the catalytic effects than particle size, and amorphous Nb$_2$O$_5$ revealed higher catalytic effects. The distribution of Nb species on MgH$_2$ was investigated by electron microscopes. There was no clear difference for the dispersion states of crystalline and amorphous Nb oxides, suggesting that the initial structure would not be related to the dispersion process. From the XPS spectra, it was found that the amorphous Nb$_2$O$_5$ was more reduced than the crystalline ones. It is reported that the catalytic active Nb oxides is reduced during the milling process[3]. Therefore, the amorphous structure affects the reduction process, resulting in the higher catalytic activity for the hydrogen absorption and desorption reactions of Mg.

High-pressure and high-temperature synthesis of novel hydrides

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Chemical potential of hydrogen steeply increases at high pressures above 1 GPa. Such reactive hydrogen enables us to realize novel hydrogenation reactions of metals and alloys to form novel hydrides. We are trying to synthesize iron-containing complex hydrides [1,2] and aluminum-based hydrides under high pressure. The hydrogenation reaction conditions were searched with the aid of in-situ synchrotron radiation x-ray diffraction measurement. Iron-containing complex hydride, Li₄FeH₆ was synthesized by hydrogenation reaction of a powder mixture of LiH and pure iron above 6 GPa [1]. Li₃AlFeH₈ was obtained by introducing two H⁻ anions into iron-containing complex hydride [2]. Al₂CuHₓ has been synthesized by hydrogenating Al₂Cu alloy at 10 GPa, and 800°C [3] which is the first aluminum-based interstitial hydride. We have synthesized other aluminum-based hydrides consisting of aluminum and transition metals using the same technique.

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Solvent-free Facile Synthesis of Metal Boron Hydrides for Superionic Conductivity
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Metal boron hydrides, expressed as $M(B_xH_y)_n$, are potential candidates for multiple energy applications [1-4], including high capacity hydrogen storage, superionic conductivity, high density thermal energy storage, etc. For example, metal dodecaborate $M_2(B_{12}H_{12})_n$ with stable icosahedral cage structure, regarded as the major obstacle for rehydrogenation to metal borohydrides $M(BH_4)_n$ [5], have been drawing increasing attention as promising solid-state electrolyte for all-solid-state batteries [6,7]. $M_2(B_{12}H_{12})_n$ can be synthesized by a solvent-based wet chemistry process [8], however, the very careful dehydration step limits its application mostly to $M_2(B_{12}H_{12})_n$ comprised of alkali-metals like Li, Na, K, Cs, etc. A facile non-solvent synthesis process, therefore, is in great need to overcome such limitation of wet process, such as the synthesis of anhydrous $MgB_{12}H_{12}$ [9]. Inspired by the synthesis method of metal alanates $M(AlH_4)_n$ or metal amides $M(NH_2)_2$ from the reaction between $MH_n$ and $AlH_3$ or $MH_n$ and $NH_3$, we successfully developed a new solvent-free process based on the reaction between $MH_n$ or $M(BH_4)_n$ and decaborane $B_{10}H_{14}$ [10]. A large variety of anhydrous $M_2(B_{12}H_{12})_n$ comprised of alkali metal (Li, Na, K), alkaline earth metal (Mg, Ca) and bi-metal (LiNa, LiK) have been successfully synthesized based on the new solvent-free process [7,10-13]. Moreover, this process was found recently to be feasible for the synthesis of metal boron hydrides comprised of multiple anions like $Na_3NH_2B_{12}H_{12}$, which will help to develop novel compounds with superionic conductivity [13].

Thermochemical Energy Storage Utilising Metal Carbonates
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Concentrated solar thermal power is a quickly emerging technology [1,2]. However, the search for a more efficient and cost effective energy storage media as a successor for molten salts is highly relevant. Metal carbonates have great potential as thermochemical energy storage materials through the endo- and exothermic release and uptake of CO₂ with low cost and high energy density [3]. However, the major challenge is the loss of CO₂ capacity, which drastically decreases over multiple cycles [4,5].

Recently, it was established that dolomite, CaMg(CO₃)₂, dug straight out of the ground, is a candidate for thermochemical energy storage – even better than laboratory synthesized dolomite due to the positive effect of chemically inert impurities present in the sample [3]. However, its relatively low 550 °C operational temperature leaves room for improvement. Thus, both CaCO₃ and a reactive carbonate composition of BaCO₃-BaSiO₃ have been investigated, which have operational temperatures at 900 and 850 °C, respectively. Preliminary results suggest that a suitable additive enhances the cyclic stability and reaction kinetics, see Figure 1. This presentation will give an overview of present research and an outline of future perspectives.

Figure 1. Showing the decreasing CO₂ capacity of CaCO₃ (black squares) with increasing cycling. Additives assist in maintaining the capacity over further cycles.

A Hydride Composite Featuring Mutual Destabilisation and Reversible Boron Exchange: Ca(BH₄)₂-Mg₂NiH₄

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The system Ca(BH₄)₂-Mg₂NiH₄ is used as a model to prove the unique possibility to fully reverse the borohydrde decomposition process even in cases where the decomposition reaction leads to undesired stable boron containing species (boron sinks). The formation of MgNi₂.₅B₂ directly from Ca(BH₄)₂ or from CaB₁₂H₁₂ and amorphous boron allows an unexpectedly easy transfer of the boron atoms to reversibly form Ca(BH₄)₂ during rehydrogenation. In addition, to the best of our knowledge, the mutual destabilisation of the starting reactants is observed for the first time in Ca(BH₄)₂ based Reactive Hydride Composite (RHC) systems. A detailed account of dehydrogenation and rehydrogenation reaction mechanisms as the function of applied experimental conditions is given.
X-ray absorption spectroscopy for reaction of metal hydrides

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Time-resolved X-ray absorption fine structure (XAFS) system has been developed in order to reveal the relation between structure and property during reaction. XAFS technique is an element specific photon-in photon-out probe and sensitive for local structure. These features allow us to observe only structure change of the target element under in situ condition.

I will present some time-resolved XAFS results. All XAFS spectra were taken at BL14B1 and BL28B2 of SPring-8, Japan. Time-resolved measurement was achieved by using dispersive optics.

Pd metal nanoparticles show different hydrogen adsorption and desorption properties from bulk materials. The hydrogen absorption and desorption processes were observed by time-resolved XAFS at a rate of 200 Hz. It was succeeded to observe the change of Pd-Pd interatomic distance under 5 ms exposure time and determine the reaction time below 10 ms [1].

Local structure of TiCl$_3$ additive in Mg(BH$_4$)$_2$ was studied to understand correlation between the structure of the additive and dehydrogenation property of Mg(BH$_4$)$_2$. Simultaneous measurement of the dehydrogenation curve and XAFS spectra revealed that a part of TiCl$_3$ additive is converted to Ti$_x$(BH$_4$)$_y$ right after ball milling mixture and then promptly resolved to TiB$_2$ at 100-150 °C with the first dehydrogenation peak [2].

Hydrogen elimination by water formation reaction is one of the candidates for creating hydrogen safe system. We observed structure change of Pt metal nanoparticle catalyst during the reaction with poisoning gas of CO. Figure 1 shows that the creation of oxidized layer (increase of peak intensity), desorption of CO (decrease of peak shift), and water formation reaction on Pt metal nanoparticles occur at the same time [3].

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What hydride can steal from stainless steel?

About the Mg$_2$FeH$_6$ formation from magnesium hydride and austenitic steel.

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Magnesium iron hydride is one of the most effective materials for solid state hydrogen and heat storage at elevated temperatures [1]. There are many ways of its synthesis with the use of pure elements but also hydrides and other precursors [2-6]. Mechanical synthesis, reactive mechanical synthesis or just sintering under hydrogen pressure are commonly used. The mechanisms of formation of this compound were already described in details [7-9]. Here we present the attempt of synthesis of magnesium iron hydride using austenitic stainless steel as a reaction substrate. This kind of steel is commonly used as structural material in harsh environments but also in many cases in hydrogen industry due to very low diffusivity of hydrogen up to 450 °C, no susceptibility to hydrogen embrittlement combined with high temperature corrosion resistance and acceptable mechanical properties. It is also paramagnetic and characterized by A1 type crystal lattice. In this study we investigate the ability of Mg$_2$FeH$_6$ formation when austenitic steel is used for the synthesis instead of pure iron. It is shown that the reaction does not occur by sintering under static conditions (high hydrogen pressure and high temperature) even after mechanoactivation[10], but the ternary hydride is formed by reactive milling very effectively. The influence of the synthesis reaction time on its yield and properties of the product is shown and compared to the synthesis of Mg$_2$FeH$_6$ from pure iron. It is likely that the product of the meachnosynthesis posses not only iron atoms in the lattice but likely other alloying elements that can be found in the steel.

Hydrogen Storage Characteristics and Applications of V-based BCC Alloys

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V-based hydrogen storage alloy is regarded as a promising candidate material for small-scale to large-scale hydrogen storage. In this work, the microstructures, defects, phase-transformation characteristics and hydrogen uptake-release properties of quarternary V-Ti-Cr-Fe alloys are introduced. The main factors to affect the cycle life of the alloy are also summarized. The possible applications of V-Ti-Cr-Fe alloys including on-board vehicles are discussed from the hydrogen storage capacity, cost, and operation condition points of view.


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April 02, 2019
Nature of the metal-insulator transition in few-unit-cell-thick LaNiO$_3$ films

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The nature of the metal insulator transition in thin films and superlattices of LaNiO$_3$ with only few unit cells in thickness remains elusive despite tremendous effort. Quantum confinement and epitaxial strain have been evoked as the mechanisms, although other factors such as growth-induced disorder, cation non-stoichiometry, oxygen vacancies, and substrate-film interface quality may also affect the observable properties in the ultrathin films. Here we report results obtained for near-ideal LaNiO$_3$ films with different thicknesses and terminations grown by atomic layer-by-layer laser molecular beam epitaxy on LaAlO$_3$ substrates. We find that the room-temperature metallic behavior persists until the film thickness is reduced to an unprecedentedly small 1.5 unit cells (NiO$_2$ termination). Electronic structure measurements using x-ray absorption spectroscopy and first-principles calculation suggest that oxygen vacancies existing in the films also contribute to the metal insulator transition.
Identification of ferrimagnetic orbitals preventing Jahn-Teller distortions in Li$_x$Mn$_2$O$_4$ cathodes

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The Lithium manganese oxide (LMO) spinel is a very important cathode material for commercial Li-ion batteries. Unfavorably, its Verwey’s transition near the room temperature perturbs the cathode functioning. X-ray Compton investigations have already provided an incisive spectroscopic technique for directly probing cathode redox orbitals [1-3]. Here, we show that magnetic properties studies based on first-principles modeling combined with parallel x-ray magnetic Compton scattering experiments reveals how the antiferromagnetic charge-ordered Verwey phase can be avoided by taking advantage of a robust ferrimagnetic phase, which is stable for slightly non-stoichiometric LMO samples. In this surprising magnetic state, charge-ordering and Jahn-Teller distortions are found to be strongly suppressed. Moreover, by examining the magnetic Compton profiles, we identify the ferrimagnetic orbitals that can avoid the undesired charge ordering. Thus, our method opens up a new spectroscopic pathway for improving the performance of battery materials.

The realization of economical renewable energy technologies is critical for securing long term prosperity of mankind and mitigating the threat of climate change. Power from the Sun is the most abundant source of renewable energy. In just one hour, more solar energy hits the Earth’s surface than humanity uses in an entire year. Therefore, development of solar cells that can produce electrical power at a cheaper rate than fossil fuel based electricity is highly desirable. However, only about 1 percent of the world’s energy production currently comes from solar cells. This is because the conventional technologies, mostly based on silicon solar cells, are too expensive to be competitive with energy generated by burning fossil fuels. What is needed is research on new solar cell materials that can be fabricated into solar cells with high-efficiency and low-cost simultaneously.

Hybrid Organic-Inorganic perovskites (HOIPs) have recently been discovered as one of the most promising next generation solar cell materials. Solar cells based on HOIPs have achieved high efficiency that rivals that of the conventional silicon solar cells. At the same time, HOIPs can be deposited on surfaces from ink solutions which enable low-cost and high-throughput manufacturing of solar cells as if printing out newspapers. In this talk, I will present our recent research that revealed microscopic mechanism of the photovoltaic properties of HOIPs. [1-3]

How Compressed Hydride Superconductors Produce Room Temperature Superconductivity

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The 2014-2015 prediction, discovery, and confirmation of superconductivity above 200K in SH₃, followed by the 2018-2019 extension to record high temperature superconductivity (HTS) in the 250-280K range in lanthanum hydride -- room temperature of cold laboratories -- marks a new era in the longstanding quest for room temperature superconductivity: quest achieved, at the cost of requiring extreme pressure (150-200 GPa). Predictions of HTS in numerous other metal hydrides at high pressure have appeared.

Though the mechanism of pairing is convincingly electron-phonon coupling (EPC), nothing has been decided about the relative importance of the few underlying characteristics that determine T_c. We have applied a novel atomic decomposition of metal (X) and H atom contributions to T_c. This simple technique has been applied to five XHₙ hydrides, n = 3, 6, 10, that have very high predicted T_c. This method enables us to separate, pinpoint, and quantify the role of hydrogen. Among other results, we establish that while the metal X atom contributes significantly (~15-20%) to the EPC strength λ, it is practically useless in increasing T_c and (contrary to accepted wisdom) can be detrimental. Based on these results, we construct a phase diagram illustrating the position of these five compounds with respect to each other, and show that the maximum Tc of each (versus pressure) borders a region of lattice instability. Time allowing, the electron self-energy of H₃S will be presented and discussed, emphasizing the surprising effect it has on the spectral density in the region of the van Hove singularities at the Fermi level and the renormalization of the band structure. The vHs results in strong particle-hole symmetry breaking in H₃S in both the normal and superconducting states; evidence will be presented and discussed.
Computational Discovery of Novel Superconducting Hydride Phases Under Pressure

Tiangen Bi, Niloofar Zarifi, Eva Zurek

The pressure variable opens the door towards the synthesis of materials with unique properties, e.g. superconductivity, hydrogen storage media, high-energy density and superhard materials. Under pressure elements that would not normally combine may form stable compounds or they may mix in novel proportions. As a result, we cannot use our chemical intuition developed at 1 atm to predict phases that become stable when compressed. To enable our search for novel hydride phases that can by synthesized under pressure we have developed XtalOpt, an open-source evolutionary algorithm for crystal structure prediction. XtalOpt has been employed to find the most stable structures of hydrides with unique stoichiometries. Some of these are superconducting at high temperatures. Herein, we describe our predictions of the binary hydrides of scandium, phosphorus, calcium, and iron. The electronic structure and bonding of the predicted phases is analyzed by detailed first-principles calculations.
High-$T_c$ superconducting phases of FeSe-based materials at high pressure

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A fundamental issue concerning iron-based superconductivity is the roles of electronic nematicity and magnetism in realizing high transition temperature ($T_c$). To address this issue, FeSe is a key material, as it exhibits a unique pressure phase diagram involving non-magnetic nematic and pressure-induced antiferromagnetic ordered phases [1-3]. However, as these two phases in FeSe have considerable overlap, how each order affects superconductivity remains perplexing. Here we construct the three-dimensional electronic phase diagram, temperature ($T$) against pressure ($P$) and isovalent S-substitution ($x$), for FeSe$_{1-x}$S$_x$ [4]. By simultaneously tuning chemical and physical pressures, against which the chalcogen height shows a contrasting variation, we achieve a complete separation of nematic and antiferromagnetic phases. In between, an extended non-magnetic tetragonal phase emerges, where $T_c$ shows a striking enhancement. The completed phase diagram uncovers that high-$T_c$ superconductivity lies near both ends of the dome-shaped antiferromagnetic phase, whereas $T_c$ remains low near the nematic critical point.

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Weakly coordinating anions in the carborate family have been studied as liquid-like scaffolds for Li$^+$ and Na$^+$ to promote cation mobility in the solid state. Closo-borates and their derivatives, such as carborates, generally show impressive ionic conductivities above an order-disorder phase transition, as first shown for Na$_2$B$_{12}$H$_{12}$.[1] In just a few years the transition temperature in this family of materials was lowered from ~260 °C to below RT, in the mixed phase material Na$_2$(CB$_9$H$_{10}$)(CB$_{11}$H$_{12}$).[2] This compound showed a remarkable ionic conductivity surpassing that of liquid electrolytes. However, the relation between structure, anion-cation interaction, etc. and the transition temperature is still not fully understood. In this study we investigated the influence of the interaction strength between the anion and cation looking at some of the most weakly coordinating anions known. The thermal behavior was investigated and structures were solved based on in-situ synchrotron powder X-ray diffraction data. Further insight into the thermal behavior was gathered from cyclic differential scanning calorimetry, showing that the order-disorder transition, also present in these materials, is reversible. Electrochemical impedance spectroscopy revealed that above the phase transition temperature the ionic conductivity rivals that of liquid electrolytes.

Extreme Hydrogen Densities in Ammonium Metal Borohydrides

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The compound ammonium borohydride, NH₄BH₄, is among the compounds known with the highest gravimetric (24.5 wt% H₂) and volumetric hydrogen content (157.3 g·H₂/L), and releases 75 % of its H₂ in three distinct exothermic reactions below 130 °C. However, it is metastable at room temperature with a half-life time of ~6 h and decomposes into diammoniate of diborane, [(NH₃)₂BH₂]BH₄.¹,² Furthermore, the H₂ release is accompanied by a release of toxic gasses such as ammonia and borazine, which should be suppressed for practical applications.

We present new strategies to stabilize the unstable NH₄BH₄ by addition reactions with stable metal borohydrides, similar to NH₄Ca(BH₄)₃ reported by Schouwink et al.³ Extensive systematic synthetic work has resulted in twenty new compounds, of which the crystal structures have been solved and investigated in detail by a combination of synchrotron powder X-ray diffraction and density functional theory. This reveals a variety of compositions and structures ranging from crystalline, solid solutions to polymeric and amorphous compounds. Trends in crystal structures, dihydrogen bonding, and thermal properties are presented. Several of the crystal structures show resemblance to known potassium or rubidium based bimetallic metal borohydrides, due to the similarity in ionic radii to that of NH₄⁺. The partially positively charged Hδ⁺ on NH₄⁺ and partially negatively charged Hδ⁻ on BH₄⁻ facilitate the release of hydrogen at low temperatures, hence making these materials interesting candidates for solid state hydrogen storage. The compounds exhibit extreme hydrogen densities with gravimetric hydrogen contents in the range ρ_{m} = 7.47-24.5 wt% H₂ and volumetric hydrogen contents of ρ_{V} = 88.0-158.2 kg/H₂/m³.

Magnesium – Lithium alloys as hydrogen storage materials

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The development of efficient hydrogen storage methods is crucial for its use as a fuel. One of the most comprehensively examined candidates for hydrogen storage is magnesium hydride. Magnesium has a high ability to hydrogen absorption (up to 7.65% by weight), it is widely available, not expensive and is characterized by a full reversibility of the absorption and desorption process. There are many methods of changing its kinetic and thermodynamic properties e.g. by alloying or doping with elements [1-4]. Not much research has been devoted to the modification of magnesium by elements from alkali metal groups since most of them like Na and K do not form both solid and liquid solutions with magnesium [5,6]. Lithium belonging to the group mentioned above, behaves differently. According to the phase diagram, only 11 wt.% of Li addition to hexagonal magnesium leads to the stabilization of lithium based BCC solid solution [7].

In current study the hydrogen storage properties of magnesium lithium alloys were investigated. AZ31 Alloy with the addition of different amounts of lithium (4, 7.5, 15 wt.%) was used. This modification resulted in obtaining different phase composition: \( \alpha \), \( \alpha + \beta \), \( \beta \) respectively. The abilities of hydrogen absorption of obtained alloys were tested and compared. X-ray phase analysis for both as synthesized and hydrogenated samples was performed. Tetragonal (\( \beta \) phase) magnesium hydride was found to be the main constituent of the post hydrogenation powders despite the different phase compositions before the absorption. The decomposition properties and hydrogen content of samples were examined by DSC/TGA and MS.

The presence of a large amount of other (than Mg) elements in the AZ31 alloy makes impossible to determine the unequivocal effect of the lithium content on the hydrogen absorption mechanisms in alloys. By that reason similar to abovementioned tests were carried out for “model” samples of pure magnesium-lithium alloys with three different lithium contents.

The results of this experiment are also presented and discussed.

Correlated Configurational States and a Quantum Charge Liquid in Layered Metallic Dichalcogenides

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Two-dimensional metallic dichalcogenides display diverse charge ordering phenomena, but the mechanisms for the formation of low-temperature commensurate order have proven surprisingly controversial [1,2]. Fermi surface instabilities [3], the electron-phonon interaction [4], exciton condensation [5] and strong correlations [6] are commonly discussed, but each mechanism is typically applied individually, and is usually applicable only in a certain range of temperature or doping. In the term doping we include applied pressure, high intensity laser pulses as well as actual doping. In this paper we propose a new and universally applicable viewpoint on charge ordering in triangular lattices based on the sparse ordering of polarons subject to (only) screened Coulomb interactions. Using a charged lattice gas model, our parallel tempering Monte Carlo simulations find stable regularly ordered polaronic crystals at certain magic filling fractions $f_m=1/3, 1/4, 1/9, 1/13, 1/16$ which are observed as commensurate charge density waves in different materials. Upon doping, a multitude of near-degenerate domain wall configurations appear which accommodate the doped charges. In large regions of doping between $f_m$, an apparently infinite number of configurationally near-degenerate states result in an amorphous state, which is stable down to very low temperatures. The effective degeneracy of configurational states subject to quantum fluctuations may lead to a quantum charge liquid at low temperatures, analogous to the canonical quantum spin liquid. Critical points, possibly quantum, at $f_m$ delineate the different regions of the phase diagram in accordance with observed doping and light-induced orders.

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We present a machine learning approach to predict the formation energies of compounds in two-dimensional group-III oxide systems with chemical accuracy at a fraction of the cost of first-principles calculations. Using support vector regression and artificial neural networks, we generate interatomic potentials and achieve small root-mean square prediction errors across the Ga2O3 and In2O3 phase spaces. To investigate the transferability and generalizability of these potentials, we use the Genetic Algorithm for Structure Prediction to obtain structurally-diverse materials, which are relaxed using density functional theory, and perform cross validation [1,2]. Furthermore, we explore different methods of encoding relevant physical information into machine-readable data, called descriptors, including radial and angular distribution functions [2]. The choice of descriptor is known to affect the speed and accuracy of a machine learning potential [3]. Finally, we discuss methods to improve model performance with fewer training samples by augmenting the training data using atom-centered local descriptors and local atomic energies, decomposed from DFT total energies. The overarching goal is to accelerate crystal structure prediction in multicomponent systems using these machine-learning models.

Graphene Foam for Engineering Ultra-Stiff, Tough and Impact-Resistant Structural Composites
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Graphene foam, with 3D macroporous architecture, has excellent load bearing capability. As opposed to 2D graphene flakes, incorporation of 3D foam in the material matrix does not require complex dispersion techniques and is not marred with agglomeration challenges. Metallic, polymeric and ceramic composites with graphene foam filler are fabricated and their mechanical properties investigated at multiple length scales. Polymer composites based on graphene foam are synthesized by facile dip-coating and mold-casting techniques. Graphene foam addition results in ~300% improvement in the loss tangent of polyimide structures, indicating excellent energy-dissipation and impact-resistance. The epoxy composite exhibits improved tensile and flexural strength by adding as low as 0.1 – 0.6 wt.% graphene foam. Digital image correlation analysis of the tensile videos shows graphene foam cells restrict the deformation of epoxy, and the graphene branches are responsible for crack-deflection. An ultra-low density metallic metamaterial based on graphene foam and aluminum is fabricated by electron beam evaporation technique. The composite metamaterial is highly stiff, with spring constant value (~1.13 N/m) comparable to 2D graphene membranes. In-situ indentation inside the electron microscope shows long distance stress-transfer in the metamaterial, making it highly flexible and resistant to localized failure. When subjected to 50 indentation loading-unloading-reloading cycles, the metamaterial exhibits impressive ~98% displacement recovery at the end of each cycle, indicating good fatigue-resistance. A ceramic composite was also fabricated by incorporating 3D foam inside a low temperature ceramic by spark plasma sintering approach. Indentation response of the composite showed a four-fold improvement in load-bearing capacity. Additionally, sub-surface examination by focused ion beam machining and electron microscopy shows extensive crack deflection because of 3D graphene reinforcement. Superior toughness in materials is vital for application in extreme conditions. These findings demonstrate the immense promise of utilizing 3D graphene foam material for engineering high-performance nanocomposites for advanced structural applications.
Materials Informatics Search for Strongly Correlated 1D Materials
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Two-dimensional (2D) materials have been of great interest since the discovery of free-standing graphene in 2004.\(^1\) One-dimensional (1D) materials present a complementary class of low-dimensional materials, which has not received much attention. Using our recently developed algorithm that identifies the dimensionality of materials,\(^2\) we search the MaterialsProject database to identify 437 compounds with 1D structural motif. Since electronic correlations and magnetism strongly depend on the dimensionality of a material, we focus on the 293 1D compounds that contain elements with \(d\) or \(f\) valence electrons and calculate their thermodynamic stability. Next, we identify their magnetic behavior and test for antiferromagnetism, followed by calculating the band structure of the most stable configuration. We follow by calculating the electronic structure for the chains that are more stable than single chain tellurium, identifying over several metallic chains and chains whose band gap is larger than 3 eV. Afterward, we test the 1D materials that display half-metallicity for potential Peierls distortions. Finally, we calculate the magnetic anisotropy energy for selected magnetic chains to identify materials that, following the Mermin-Wanger theorem, can exhibit long-range magnetic order.\(^3\)

Local structure of La$_{1-x}$Ce$_x$OBiSSe as a function of Ce substitution
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In the BiCh$_2$-based (Ch: S, Se) superconductors, the electronic and superconducting properties are linked with the structural configuration of these materials. The La$_{1-x}$Ce$_x$OBiSSe system, recently discovered by Sogabe et al. [1], was studied by Extended X-ray Absorption Spectroscopy to reveal the evolution of the local structural properties by La substitution for Ce. The two in plane Bi-Se distances, revealing a distorted phase for LaOBiSSe, merge in one single distance as the Ce content increases, showing a reduction of the in plane distortion that should be linked with the emergence of superconductivity. Furthermore, the distance between the bismuth and the sulfur out of plane increases, affecting the electronic interaction between the Ce ions in the spacer layer and the superconducting layer.

Study of the local structure of CaKFe$_4$As$_4$ as a function of temperature
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We have measured the local structure of the new superconducting Fe-based system CaKFe$_4$As$_4$ (T$_c$~35K) by temperature dependent in-plane polarized extended x-ray absorption fine structure (EXAFS) at the Fe and As K-edges. We found that the system has local structure parameters similar to the ones found in its parent compound CaFe$_2$As$_2$. Fe-As and Fe-Fe distances are found to be equal to the distances measured by diffraction, while the corresponding mean-square relative displacements (MSRD) reveal no anomalies in correspondence to the superconducting transition, although the system is a bulk superconductor. The local force constant for Fe-As bondlenght (k ~ 5.9 eV/Å$^2$) is similar to the one found in the 122 parent compound while that for the Fe-Fe bondlenght (k ~ 2.83 eV/Å$^2$) appears higher (in CaFe$_2$As$_2$ was found k = 2.57 eV/Å$^2$). The results reveal a small anomaly around 100 K, seen in both Fe-As and Fe-Fe MSRD. The results are discussed in compare to the local structure of other iron-based superconductors.
Thermal Decomposition of Na-based Alloy for Thermoelectric conversion

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We propose a new type of thermoelectric conversion system by using thermal decomposition and electrochemical alloying of Na₁₅Sn₄ as follows,

Thermal reaction (decomposition): \( \text{Na}_{15}\text{Sn}_4 \rightarrow 15\text{Na} + 4\text{Sn} \) (1)

Electrochemical reaction (discharge): \( 15\text{Na} \rightarrow 15\text{Na}^+ + 15\text{e}^- \) (2)
\( 15\text{Na}^+ + 4\text{Sn} + 15\text{e}^- \rightarrow \text{Na}_{15}\text{Sn}_4 \) (3).

Thermal energy can be converted to electric energy by combining above reactions. Although electrochemical properties of Na₁₅Sn₄ is reported as electrode material of sodium ion battery [1], the thermochemical properties is not investigated before. In this work, the thermal decomposition properties of Na₁₅Sn₄ (eq. 1) is investigated under various conditions. Na₁₅Sn₄ single phase is synthesized by mechanical alloying used planetary ball-milling. The thermal decomposition is carried out in a closed system, open system, and dynamic vacuum condition. In the closed system, the decomposition reaction does not proceed below 500 °C. On the other hand, Na₁₅Sn₅ decomposed at 300-500 °C in the open system. The decomposition temperature is decreased down to 150 °C in the dynamic vacuum condition. From the above results, it is suggested that the partial pressure of Na around alloy particles is an important factor to reduce the reaction temperature. Therefore, Na₁₅Sn₄ is recognized as a potential material for thermoelectric conversion of heat energy at 150-500 °C.

Investigation of light metal hydrides by Scanning Electron Microscopy – methodology and challenges
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Due to popularity and easy access, SEM equipped with EDS (and rarely WDS) is used for investigation of chemical composition of light metal hydrides – ball milled or processed in any different way. Not considering the obvious limitations (impossibility of lithium and hydrogen detection) the quality of the quantitative data obtained during measurement is influenced by many factors such as: the resolution of the methods, sample preparation, shape of the sample, the combination of the elements in the sample as well as calibrations used in the hardware. This work was done to show the potential errors in such investigations and to show that in most cases only qualitative measurements should be presented. Different mixtures or light metal hydrides with heavy metals were prepared and given to SEM operator to perform “blind test” of the chemical composition measurements. Two methods were used for this analysis, namely the energy-dispersive X-ray spectrometry (EDS) and wavelength-dispersive spectrometry (WDS). Energy dispersive and wave length dispersive X-ray spectroscopy are complementary techniques where the EDS is quite fast and enables the observation of elements from which the hydride is composed but with a lower precision, whereas WDS is slower method but has a significantly greater precision. Presented results shows the potential errors and give suggestions as to the measurement resolution to which we can trust the obtained data in reality. It is clearly presented that 0.01% accuracy given in most cases in scientific publication is far from what we can trust even using the best available equipment and experienced staff.
FunHy - Neutrons for multi-functional hydrides

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The synthesis and discovery of useful new materials strongly depends on a detailed understanding of material structure and property relationships. The ambition of this project, FunHy, is to conduct cutting-edge international research on the design and preparation of novel functional hydride materials and to exploit neutron scattering methods for conclusive characterization of structural and dynamic properties. Hydrides form large varieties of different types of materials and we target: i) light element hydrides relevant for hydrogen storage and ii) metal hydrides which are new fast ion conductors for batteries and iii) hydrides with novel magnetic properties. We aim at integrating a range of neutron scattering techniques for advanced materials characterization: i) Elastic neutron scattering, including in situ powder neutron diffraction (PND) at varying temperature and pressures, high resolution PND, ii) total neutron scattering and PDF analysis for probing structural properties, iii) inelastic neutron scattering (INS) and quasielastic neutron scattering (QENS) for probing dynamic properties. Neutron scattering combined with other techniques will then provide new fundamental scientific insights into material structure-property relationships. Our goal is to develop novel useful functional hydride materials based on new understanding of structure-property correlations through rational materials design. This project is conducted within a strong Nordic and international research network and offers the highest level of energy materials science education for 3 PhDs directly funded, and a large number of Bachelor, Master and associated PhD students. An open Nordic research meeting will be organised with the aim to gather Nordic experts, start new collaborations and share our knowledge. This project will establish new broad long-lasting research networks and collaboration within ‘neutrons for materials science’.
Pairing mechanism in iron-based superconductors: variations on the $s^\pm$- theme

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I review some of the recent developments in the theory of superconductivity of iron-based systems that go beyond the $s^\pm$- paradigm established in the early days of the field. These include: a) prediction of and evidence for T-breaking mixed symmetry pair states; b) influence of orbital selective correlations on pairing; c) new pair states possibly stabilized by spin-orbit coupling, d) recent predictions for states with "Bogoliubov Fermi surfaces", surfaces of zero energy excitations in the superconducting states. The latter may explain recent puzzling experiments on doped FeSe.
Spin-orbit coupling and “preferred” magnetic excitations in iron-based superconductors

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In this talk, I will present our inelastic neutron scattering efforts to determine low-energy spin excitations in a variety of iron-based superconductors, in which spin-orbit coupling leads to anisotropic response in spin space. In BaFe$_2$As$_2$ and FeSe$_{1-x}$S$_x$ regardless of whether long-range magnetic order is present, we show that the magnetic excitations at low temperatures are preferentially polarized along the $c$-axis [1,2]. In the tetragonal and $c$-axis oriented magnetic phase of Sr$_{1-x}$Na$_x$Fe$_2$As$_2$, we find the first spectroscopic evidence that the itinerant charge carriers actually “prefer” to be assisted by $c$-axis polarized magnetic excitations in their formation of superconducting Cooper pairs [3], namely, only the weak $c$-axis response exhibits a spin resonant mode in the superconducting state. Our results naturally explains why the superconductivity competes strongly with the tetragonal magnetic phase in Sr$_{1-x}$Na$_x$Fe$_2$As$_2$, and provide a fresh view on how to make a good superconductor out of a magnetic "Hund's metal".

We present results of Raman scattering experiments on Ba$_{1-x}$K$_x$Fe$_2$As$_2$ (0.22 ≤ x ≤ 0.7) [1] and CaKFe$_4$As$_4$ [2] focusing on electronic excitations in the superconducting state below $T_c$. The redistribution of spectral weight from low to high energies upon crossing $T_c$ allows us to derive the gap energies. The gaps on the individual bands are almost isotropic and vary between 1 and 8$k_B T_c$. Inside the large gaps narrow lines are found for Ba$_{1-x}$K$_x$Fe$_2$As$_2$ for doping levels 0.35 ≤ x ≤ 0.48. The spectra in CaKFe$_4$As$_4$ are similar to those of Ba$_{0.65}$K$_{0.35}$Fe$_2$As$_2$. Among the suggested explanations of the in-gap modes we observe Bardasis-Schrieffer excitons, resulting from anisotropic pairing interactions $V_{k,k'}$, to be in full agreement with the theoretical predictions. In addition, we study the relative pairing strength in different channels using functional renormalization group and spin fluctuation theory and find the same ground state and hierarchy of pairing channels suggesting that spin fluctuations are an important if not the leading interaction in the pnictides [1].

Nodal Superconductivity in FeSe single crystals from heat capacity
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The superconducting gap in vapor-grown single-crystalline FeSe is studied via heat-capacity measurements down to 0.4 K and up to 14 Tesla. In our best crystals, i.e. with the highest $T_C$ and RRR values, we consistently find a linear $C/T$ term at low temperatures indicative of a nodal superconducting gap [1]. This is supported by the magnetic field dependence of $C/T$. The electronic specific-heat curve up to $T_C$ is shown to be consistent with a recent gap determination using quasi particle interference [2] only if one forces the gap to change sign at the minimum of one of the Fermi surface pockets. Finally, the specific heat of FeSe crystals grown under different conditions are compared to various $C/T$ data taken from the literature.

Multi-orbital effects and the role of spin-orbit coupling in iron-based superconductors

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Iron-based superconductors continue to fascinate the research community by its unusual electronic properties. This includes both the normal states transport properties, the fascinating variability of the magnetic structures found in these materials, and the unusual gap structure present in the superconducting order parameter. In this talk I will present our recent theoretical developments to understand the interplay between electronic interactions, spin-orbit coupling, and superconductivity in iron-based systems. I will highlight the role of self-energy effects from the itinerant electron perspective, and show how recent experimental developments point to interesting orbital selective effects in e.g. the magnetic susceptibility and the superconducting properties.
Orbitals and Nematicity in La-1111 Single Crystals

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While there is broad consensus that superconductivity in Fe based superconductors is due to an unconventional, most likely electronic pairing, many important aspects of the normal and superconducting state are still unexplored. In particular, the role of orbital degrees of freedom for the normal state electronic properties, nematicity, and pairing is discussed very controversial. In my talk I will present results on a series of large high quality La-1111 single crystals which have been grown for the first time using a method based on anomalous solid state reaction. We have reexamined the phase diagram and studied magnetism and nematic order by means of NMR and strain dependent transport measurements. The possible formation of polaron-like structures will be discussed and evidence for an unusual state with suppressed long range order and soft nematic fluctuations will be presented. In addition I will present our recent studies of a pressure-induced transition from a Mott insulating state to superconductivity present in BaFe$_2$S$_3$. It will be shown that lattice degrees of freedom are indispensable for the understanding of this transition again pointing to the crucial role of orbital degrees of freedom in Fe based superconductors.
We have conducted systematic $^{75}$As nuclear magnetic resonance (NMR) experiments in BaFe$_2$As$_2$ under controlled conditions of uniaxial pressure. We find that the electric field gradient (EFG), spin-lattice relaxation rate $T_1^{-1}$, and Knight shift $K$ at the As site are sensitive to applied uniaxial pressure. We find that uniaxial pressure increases, broadens, and separates the Néel temperature $T_N$ and the tetragonal-to-orthorhombic structural transition $T_S$. Our spectral measurements in the magnetic state exhibit no evidence for a predicted spin reorientation [1] for both positive and negative applied uniaxial pressure up to the point of sample failure.

Ubiquitous dichotomy between the in-plane uniform magnetic susceptibility and resistivity anisotropies in iron-based superconductors

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Despite a decade of intensive research, the interplay between magnetism, electronic nematicity (spontaneous rotational symmetry broken state) and superconductivity remains elusive for iron-based superconductors. Here we present direct measurements of the in-plane uniform magnetic susceptibility anisotropies of Ba\textsubscript{1-x}K\textsubscript{x}Fe\textsubscript{2}As\textsubscript{2} and FeSe systems using a simple method, in which a large symmetry-breaking anisotropic strain is applied. Instead of probing the nematic susceptibility in the zero-strain limit, we are able to study the response of both resistivity and magnetic susceptibility anisotropies under extremely strained conditions. Simple linear scaling between in-plane susceptibility and resistivity anisotropies, as expected theoretically, is not found both in Ba\textsubscript{1-x}K\textsubscript{x}Fe\textsubscript{2}As\textsubscript{2} and FeSe. More interestingly, for Ba\textsubscript{1-x}K\textsubscript{x}Fe\textsubscript{2}As\textsubscript{2}, a sign reversal occurs \~x=0.2 in resistivity anisotropy, whereas the sign of susceptibility anisotropy remains unaffected. However, compared to BaKFe\textsubscript{2}As\textsubscript{2}, both resistivity and susceptibility anisotropies switch their signs in FeSe. Our results suggest that dichotomy between the in-plane uniform magnetic susceptibility and resistivity anisotropies is ubiquitous in these iron-based superconducting materials. Further theoretical considerations are desired to explore the exact relation between these two anisotropies.

Novel electronic nematicity in (Ba,Rb)Fe$_2$As$_2$

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Electronic nematicity, a correlated state that spontaneously breaks rotational symmetry, is observed in several layered quantum materials. In contrast to their liquid-crystal counterparts, the nematic director cannot usually point in an arbitrary direction (XY nematics), but is locked by the crystal to discrete directions (Ising nematics), resulting in strongly anisotropic fluctuations above the transition. Here, we report on the observation of isotropic XY-nematic fluctuations, via elastoresistance measurements, in hole-doped Ba$_{1-x}$Rb$_x$Fe$_2$As$_2$ iron-based superconductors. While for $x=0$ the nematic director points along the in-plane diagonals of the tetragonal lattice, for $x=1$ it points along the horizontal and vertical axes. Remarkably, for intermediate doping, the susceptibilities of these two symmetry-irreducible nematic channels display comparable Curie-Weiss behavior, thus revealing a nearly XY-nematic state [1]. This opens a new route to assess this elusive electronic quantum liquid-crystalline state, which is a candidate to host unique phenomena not present in the Ising-nematic case.

Feeling strain – Thermal and Resistive response in iron pnictides
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The response of materials to non thermal control parameters such, as pressure or magnetic field, are of fundamental interest since these tuning knobs open up a large additional space of states that have to be understood within the established paradigms. In this talk, I will focus on the effects of strain on Fe-pnictides. Being a possible common thread for unconventional superconductivity, the role of nematic fluctuations for superconductivity needs to be assessed. This calls for new techniques that allow for tuning nematicity continuously towards quantum criticality.

In the first part of this talk I will discuss how to disentangle the response of nematicity to strain components of different symmetry, and will show that both symmetric (A1g) and antisymmetric (B1g) strain are suitable means to tune the critical temperature of the nematic phase transition in Fe based superconductors. The second part of this talk focuses on our recent experimental advances exploring the thermoelastic properties of these materials. In particular, the response of electronic nematicity to strain causes anomalies in the elastocaloric effect as well as in the elastoresistivity which can be measured via an ac technique. These anomalies are proportional to the corresponding heat capacity anomalies and are understood to be a direct consequence of the strain dependence of the nematic and the antiferromagnetic transition temperatures. A similar mechanism should more generally be expected for any phase transition tunable by strain.

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Intertwined spin-orbit coupled orders in the iron-based superconductors

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The phase diagram of the underdoped iron-based superconductors exemplify the complexity associated with correlated systems. Multiple ordered phases breaking distinct symmetries but displaying comparable transition temperatures appear. I will argue that such complexity can be understood within the framework of vestigial order [1]. For instance, the prevalent nematic order can be viewed as a vestigial phase of stripe magnetism. I will discuss a similar phenomenon occurring for the tetragonal magnetic orders, the spin-vortex crystal and the charge-spin density-wave phases. These vestigial phases break the glide-plane symmetry and render respectively the As/Se or Fe sites inequivalent [2]. In materials with staggered FeAs/Se layers (e.g. 122), these have ordering vector \( \mathbf{Q} = (0,0,\pi) \) [3] while in compounds with no staggering (e.g. 111) these are \( \mathbf{Q} = 0 \) orders. While the vestigial orders are composite in spin-space, they induce simple orbital terms with measurable consequences for the band structure. This includes a breaking of the two-fold spin degeneracy of the electron- and hole-bands along with Rashba- and Dresselhaus-like spin-orbit couplings [2]. Furthermore, the vestigial phases give rise to unusual effects under the application of external fields. An example of this is the ferro-Néel effect, where an external magnetic field induces Néel order [2].

Intertwined and vestigial electronic phases in hole-dopes Sr1-xNaxFe2As2

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Hole-doped ReFe$_2$As$_2$ (Re = Ba, Sr, Ca) exhibit much richer phase diagrams than the corresponding electron-doped systems. In particular, the phase diagram of Na-doped BaFe$_2$As$_2$ exhibits a small pocket of a double-Q reentrant C4 magnetic phase [1], as well as another yet unidentified magnetic phase [2]. In strong analogy with the charge order observed in underdoped cuprates [3], these additional phases compete strongly with the emerging superconducting order [2,4].

Here we present a detailed phase diagram of the Na-doped SrFe$_2$As$_2$ system using thermodynamic probes (heat capacity, thermal expansion and magnetization). The double-Q C4 reentrant phase is much more stable in this system, and our data demonstrates that the phase diagram of Na-doped SrFe$_2$As$_2$ exhibits even more complexity than the K- and Na-doped BaFe$_2$As$_2$ counterparts.

Pressure dependence of the superconducting upper critical field in KFe$_2$As$_2$ and related materials


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Superconductivity in KFe$_2$As$_2$ is observed below Tc=3.4 K. Despite this rather low transition temperature among Fe-based superconductors, the superconducting properties remain unconventional. There is no observed electron pocket in this compound, and the superconducting state is believed to be of a different symmetry than in the other 122 iron based superconductors. By means of resistivity, magnetization, AC susceptibility, and NMR under pressure, we investigate the properties of this material. The pressure dependence of Tc has a change of slope around 2 GPa possibly consistent with a transition to a superconducting state of a different symmetry [1]. Our study of the pressure evolution of the upper critical field seem to rule out most of the proposed superconducting states [2]. We will compare our results to the pressure effects in other superconducting materials, such as other compounds in the 122 family, and FeSe [3,4], and discuss the evolution of the electronic correlations with applied pressure [5].

Pressure temperature phase diagram of iron based superconductors
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Since the discovery of unconventional high $T_c$ superconductivity in layered compounds based on iron in tetrahedral coordination, an extensive work has been performed to understand their superconductivity mechanism, with the ultimate goal to raise $T_c$ of these pnictides and chalcogenides even further. The study of the pressure effects on the crystal and electronic structure is a powerful tool that helps to find clues to analyze the superconducting state. The new iron based superconductors is an excellent example, where there are still plenty of opened questions to be answered. In this presentation, we will discuss the effect of structural parameters under pressure on the superconducting properties on compounds belonging to various Fe based family. In particular, we have analyzed the correlation of the crystal structure parameters on the $T_C$ $^{[1,2,3,4,5]}$ and the pressure dependence of the antiferromagnetic transition, its correlation with the tetragonal to orthorhombic structural transition and its effect on $T_c$.

Structure-property correlations in FeSe-based superconducting materials

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While at ambient conditions the binary superconducting FeSe phase ($T_c = 8$ K [1]) features rather simple structural arrangement (2D PbO-type structure, $P4/nmm$), its structural behavior as a function of pressure ($P$) is quite complex. Notably, transition above 6 GPa to a topologically different arrangement (3D MnP-type structure, $Pnma$) results in a complex phase diagram with a broad $P$-$T$ region of phase coexistence. Interestingly, $T_c$ of FeSe as a function of pressure increases (globally) and then decreases with an onset of the structural transition at 6 GPa, which indicates that the 2D atomic arrangement is essential for the observed superconductivity in this system. Intercalation of FeSe with alkali metals increases the $T_c$ and stabilizes the 2D structural topology as a function of pressure [3,4]. However, structural properties of the corresponding Fe-deficient superconducting intercalates are more complex than the ones of the parent FeSe phase. Specifically, the Fe-vacancies are ordered at ambient conditions and the samples, even in a monocrystalline state, are intrinsically phase separated with the secondary minor phase being responsible for the observed superconductivity [5-7]. The phase separation can be suppressed with $T$ and $P$ where the minor phase becomes the main phase and this state can be quenched at low pressures [8]. The new compound is expected to exhibit superior superconducting properties than the parent FeSe or intercalated phases.

Local structure and superconductivity in iron-based superconductors

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Here, some recent studies using x-ray absorption based techniques on iron-based superconducting materials will be discussed. In particular, the local structure of skutterudite-type Ca$_{10}$Pt$_4$As$_8$(Fe$_2$As$_2$)$_5$ (Pt10418) and Ca$_{10}$Ir$_4$As$_8$(Fe$_2$As$_2$)$_5$ (Ir10418) iron-based arsenides, showing different transition temperatures ($T_c = 38$ K and 16 K respectively), will be discussed. Despite of having similar average crystal structures, the local structures of the FeAs$_4$ tetrahedra in the two compounds are found to be very different. The FeAs$_4$ in Pt10418 is close to a regular tetrahedron while it deviates largely in Ir10418. The Fe-Fe correlations in the two compounds are characterized by similar bond-length characteristics, however, the static disorder in Pt10418 is significantly lower than that in Ir10418. The results suggest that the optimized local structure and reduced disorder are the reasons for higher $T_c$ and well defined electronic states in Pt10418 unlike Ir10418 showing coexistence of glassy and normal electrons at the Fermi surface and hence provide a direct evidence of the local structure driven optimization of the electronic structure and superconductivity in iron arsenides.
Iron spin crossover in the Earth and planetary interiors: A perspective from computational materials physics

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Iron, the most abundant transition metal in the Earth, is incorporated into nearly all major constituent minerals of the Earth’s interior. With its incomplete 3d shell, iron in minerals can adopt various valence (Fe$^{2+}$ and Fe$^{3+}$) and spin states (defined by the total electron spin $S$). Remarkably, iron spin state can vary with many factors, including temperature, pressure, and chemical environments. This phenomenon, known as spin crossover or spin transition, directly affects the structural, electronic, optical, elastic, and thermal properties of the constituent minerals of the Earth’s deep interior, and also affects iron diffusion and partitioning. To investigate iron spin crossover and its geophysical and geochemical effects, tremendous efforts have been made. A major advance in theory is the development of the local density approximation + self-consistent Hubbard $U$ (LDA+$U_{sc}$) method, with the Hubbard $U$ parameters computed from the first-principles self-consistently. So far, the LDA+$U_{sc}$ method has accurately determined the spin-transition pressure and accompanying volume/elastic anomalies in several mantle minerals, including bridgmanite (Fe-bearing MgSiO$_3$ perovskite) [1,2], ferropericlase (Mg,Fe)O [3], ferromagnesite (Mg,Fe)CO$_3$ [4], and the new hexagonal aluminous (NAL) phase NaMg$_2$(Si,Al)$_6$O$_{12}$ [5]. Success of the LDA+$U_{sc}$ method is also seen in other types of transition-metal compounds, e.g. perovskite SrCoO$_3$ under compression [6]. In this presentation, I will review several LDA+$U_{sc}$ calculations of mantle minerals [1-5] and discuss the potential of this method to accurately predict iron spin crossover and accompanying anomalies in exoplanet interiors.

Temperature-induced amorphization in CaCO$_3$ at high pressure: implication for recycled CaCO$_3$ in subduction zones

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Calcium carbonate (CaCO$_3$) significantly affects the properties of upper mantle and plays a key role in deep carbon recycling. However, its phase relations above 3 GPa and 1000 K are controversial. Here we report a reversible temperature-induced aragonite-amorphization transition in CaCO$_3$ at 3.9-7.5 GPa and temperature above 1000 K. Amorphous CaCO$_3$ shares a similar structure as liquid CaCO$_3$ but with much larger C-O and Ca-Ca bond lengths, indicating a lower density and a mechanism of lattice collapse for the temperature-induced amorphous phase. The less dense amorphous phase compared with the liquid provides an explanation for the observed CaCO$_3$ melting curve overturn at about 6 GPa. Amorphous CaCO$_3$ is stable at subduction zone conditions and could aid the recycling of carbon to the surface.
Hydrogen-bearing iron peroxide in Earth's lowermost mantle

W. L. Mao\textsuperscript{1}, J. Liu\textsuperscript{1,2}, Q. Y. Hu\textsuperscript{1,2}, H. K. Mao\textsuperscript{2}

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How water cycles through the Earth's interior, is of fundamental importance for understanding the evolution of our planet. The presence of even trace amounts of water (or hydrogen) can dramatically affect many physical and chemical properties of Earth materials, such as phase stability conditions, viscosity, thermal conductivity, etc. Here, we report that the reaction between water and iron to form a pyrite-structured hydrogen-bearing iron peroxide, FeO\textsubscript{2}H\textsubscript{x} (with x = 0 to 1), under the pressure-temperature conditions relevant to the Earth’s deep lower mantle. Combined with theoretical calculations and high-pressure experiments using laser-heated diamond anvil cells coupled with a suite of in-situ characterization techniques (e.g. nuclear resonant inelastic X-ray scattering spectroscopy, X-ray absorption spectroscopy, and X-ray diffraction), we find that this extremely oxygen-rich form of iron peroxide has properties consistent with the ultralow velocity zones that are seismically observed at the core-mantle boundary. This phase may also have implications for deep volatile cycling and mantle redox.
Mantle-Slab Interactions and Mantle Heterogeneities

Jin Liu\textsuperscript{1,2}, Qingyang Hou\textsuperscript{1}, Mingqiang Hou\textsuperscript{1}, Ho-Kwang Mao\textsuperscript{1} & Wendy L. Mao\textsuperscript{2}

\textsuperscript{1}Center for High Pressure Science and Technology Advanced Research, Beijing 100094, China.
\textsuperscript{2}Department of Geological Sciences, Stanford University, Stanford, CA 94305, USA.

Knowledge of water in the Earth's interior, presumably at least several times the size of the world’s oceans, is fundamental importance to understanding the dynamics, structure, and evolution of Earth. Meanwhile, oxygen and iron are Earth’s most abundant elements by number of atoms and by mass, respectively. They form compounds dictating major chemistry of our planet. The generally accepted view believed that O\textsubscript{2} dimer only existed on Earth’s highly oxidized surface, and that oxygen anion existed in the invariable 2- valence state in minerals throughout the deep interior, where the redox states were controlled by the 3d transition element Fe which could vary between two valence states, ferric Fe\textsuperscript{3+} and ferrous Fe\textsuperscript{2+}. The oxygen fugacity decreases with increasing depth as defined by a series of iron oxides with O/Fe stoichiometry from the end-member ferric oxide Fe\textsubscript{2}O\textsubscript{3}, through Fe\textsubscript{5}O\textsubscript{7}, Fe\textsubscript{3}O\textsubscript{4}, Fe\textsubscript{4}O\textsubscript{5}, Fe\textsubscript{5}O\textsubscript{6} to the other end-member ferrous oxide FeO at the highly reducing core-mantle boundary. Interestingly, iron superoxides (FeO\textsubscript{2}H\textsubscript{x} with x = 0 to 1) with an O/Fe ratio of 2.0 form in the presence of water (hydrous materials) under deep lower mantle conditions. Here we studied pressure-induced changes on O, Fe, and H in pyrite-type FeO\textsubscript{2}H\textsubscript{x} and its physical and chemical properties at high pressures. We found many unexpected chemical behaviors. Iron remains in the reduced, spin-paired ferrous state in spite of its unprecedentedly high O/Fe ratio. The valence state of oxygen is not constant at 2- as commonly known in other oxides, but varying around 1-. It forms interactive dimer with an O–O bond length ~30% longer than commonly considered as interactive dimer, but still shorter than non-interactive dimer. Hydrogen becomes weakly bonded in the structure, and its amount does not affect the valence of iron. Their altered behaviors in the middle Earth certain have major impacts to our planet, suggesting a broad chemical paradigm change in the middle Earth.
Kinetics of dehydrogenation of FeOOH at Earth’s lower mantle conditions
Ruilian Tang1, Jiuhua Chen2,1, Ho-kwang Mao3,1, Jin Liu1, Vitali Prakapenka4, Yue Meng5, Jinyuan Yan6

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2Center for the Study of Matter at Extreme Conditions, Department of Mechanical and Materials Engineering, Florida International University, Miami, FL 33199, USA
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4Center for Advanced Radiation Sources, University of Chicago, 5640 South Ellis Avenue, Chicago, IL 60637, USA
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Time resolved in situ x-ray diffraction of FeOOH at 100 GPa and 2200 K has been conducted at Beamline 13-ID-D and 16-ID-B of Advanced Photon Source and Beamline 12.2.2 of Advanced Light Source. Sample pressure is increased to 100 GPa and then temperature is raised through laser heating. The phase transitions from α-FeOOH to pyrite-type FeOOHx and hexagonal phase are observed. After the formation of the pyrite-type FeOOHx phase, the sample is kept at 2200 K and x-ray diffraction is collected as a function of time. The sample is cooled down to room temperature periodically during the heating to stabilize the system and to measure the lattice parameter of the sample at room temperature. Total period of laser heating is about 12 hours. We observed that the volume of pyrite-type FeOOHx reduces during the heating and approaches x=0.75 while the LiF lattice remains constant. The x value decreases slightly when the pressure increases by 10 GPa. This result demonstrates that dehydrogenation happens when FeOOH transforms its high-pressure form with pyrite-type structure and a hexagonal phase may coexist with FeOOHx at the bottom of the lower mantle.
Graphene Foam-Based Multifunctional Polymer Composites for Self-Healing, De-icing and Strain-sensing Applications

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Free-standing graphene foam, with 3D cellular architecture, is characterized by excellent electrical, thermal and mechanical properties. Graphene foam-reinforced PDMS and epoxy composites are fabricated by facile dip-coating and mold-casting techniques. The porous structure of graphene foam allowed easy infiltration with polymers to fabricate composites with homogeneous microstructure. Graphene foam addition improves the electrical and thermal conductivities of epoxy and PDMS. The enhanced conductivity is exploited for de-icing application in airplane wings using PDMS-graphene foam composite. The deicing efficiency of ~477% is accomplished, with very low required power densities (~0.2 W cm\(^2\)). In addition, graphene foam addition improves the tensile strength and elastic modulus of polymer composites. Simultaneous improvement in electrical and mechanical properties is exploited for developing strain sensors. The epoxy-graphene foam composite is characterized by gauge factor as high as 4.1, twice the value for typical strain-sensor metals, attesting the promise of these polymer composites for motion-sensing. Smart nanocomposites are fabricated by adding graphene foam to a ‘shape-memory’ epoxy. The shape recovery is improved due to heat-transfer pathways provided by graphene foam. Because of shape memory effect, cracks in the material are observed to heal near transition temperature of the polymer. This self-healing behavior is examined at microstructural level by \( \text{in-situ} \) nanoindentation of the composite inside the electron microscope at elevated temperatures (up to ~70°C). The indents made at room temperature gradually vanish upon sample heating. Self-healing capability is vital for application in \( \text{extreme conditions} \). These observations demonstrate that graphene foam is a promising material for engineering multifunctional composites with remarkable properties and performance for a multitude of applications.
Accomplishing a suite of magnesium carbides by HPHT synthesis

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Magnesium and carbon, both of which form numerous compounds with other elements, have remarkably low affinity for one another. At ambient pressure, only the reaction of Mg or MgO with hydrocarbons leads to the formation of metastable carbides with reasonable yields, and pure Mg and carbon do not react to form stable compounds at any temperature. With experimental data obtained at ID06, we have demonstrated that under high-pressure conditions (above 5 GPa and 1300 K) thermodynamically stable Mg-C compounds are indeed possible. The new compounds synthesized, Mg2C [1] and β-Mg2C3 [2], crystallizes in the monoclinic C2/m space group, and contains rare allene-derived C34- anions that are isoelectronic with CO2. Bright golden-yellow powder of this new Mg-C compound was recovered from high-pressure, high-temperature experiments. Mass spectrometry analysis of the hydrolysis products showed allene, C3H4, indicative of the presence of C34- anions within the structure. In addition, 13C NMR analysis confirmed the presence of two structurally distinct carbon atoms in an approximate 1:2 ratio, and Raman spectra indicated carbon stretching modes from [C=C=C]. The crystal structure –clearly distinct from previously reported compounds– was, however, impossible to solve using available powder X-ray diffraction data. In order to resolve the structure of this new magnesium carbide, two important steps were taken. First, potential Mg2C3 structures were predicted using USPEX, an ab initio structural evolution algorithm. Second, in situ high-pressure synthesis was performed at the ESRF (ID06) using the recently-commissioned large-volume press. The in situ synthesis allowed for the phase-pure synthesis of the new compound, and high-resolution X-ray diffraction patterns obtained allowed for conclusive comparison with theoretical models. Remarkably, the high-pressure Mg2C3 structure predicted via USPEX was a perfect match to the experimental X-ray diffraction data. Thus, the structure of β-Mg2C3 was solved. Unlike α-Mg2C3, which contains alternating layers of C34- chains oriented in opposite directions, all C34- chains within β-Mg2C3 are nearly aligned along the crystallographic c-axis. After exploring pressure as additional dimension for chemistry of the Mg–C system, four magnesium carbides are now known: (1) tetragonal MgC2, (2) orthorhombic α-Mg2C3, (3) monoclinic β-Mg2C3 [2], and (4) cubic Mg2C [1]. Taking into account that at ambient pressure and at pressures up to ~5 GPa the elements do not interact at any temperature, it is quite astonishing to observe such rich chemistry. Finally, these results indicate that the Mg-C system should be completely revised under high pressure [3]. With these new results, we now have a much deeper understanding of Mg-C thermodynamics under extreme conditions.

Nanostructured graphene: When disorder makes things better?

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Since the discovery of fullerene C₆₀ in 1985 followed by synthesis of other molecular forms of carbon – e.g., nanotubes and graphene - these intrinsically nanostructured systems have been constantly attracting attention of the scientific community. This is due to rich assortment of outstanding chemical, optical, electrical and mechanical properties these materials exhibit: ultra-hardness and stiffness, very high current density limits and charge carrier mobility, exceptional light emitting characteristics, to name just a few.

At high pressure/high temperature (HPHT) fullerenes collapse is followed by formation of a nanoclustered graphene phase (NGP) which exhibits a remarkable combination of mechanical properties: high hardness, high elastic recovery and low friction coefficient [1]. Residual C₆₀ polymers jeopardize mechanical properties of the NGP therefore a special effort is needed for synthesis of “polymer-free” graphene phase. Ball milling of the source fullerene material results in loss of crystallinity and, most importantly, inhibits formation of the C₆₀ polymers during subsequent HPHT treatment. We show that mechanical properties of the NGP produced from C₆₀ can be significantly enhanced by controlling the disorder level and/or graphene clusters size in the system [2]. In this talk we present our recent study of fullerene-NGP transformation by employing multi-excitation Raman spectroscopy, SEM, High-resolution scanning TEM/EELS and mechanical testing and discus structural model of the fullerene-NGP transformation.

Reactive molecular dynamics simulations and machine learning

Priya Vashishta, Pankaj Rajak\textsuperscript{1,2}, Lindsay Bassman, Sungwook Hong, Aravind Krishnamoorthy, Kuang Liu, Ankit Mishra, Ken-ichi Nomura, Rajiv K. Kalia, and Aiichiro Nakano

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Machine learning (ML) is revolutionizing scientific and engineering disciplines owing to its ability to capture hidden patterns in large amounts of data. The recent success of ML can be attributed to an increasing amount of data, simulation resources, and improving understanding of statistical inference. For these reasons computational materials science is undergoing a paradigm shift. The main reason is that trial-and-error approach to materials design is inefficient: laboratory trials require a lot of time, and the results of previous trials are not utilized in a systematic fashion. A data-driven approach, which draws upon all relevant data from experiments, and reactive and quantum molecular dynamics simulations, can address these issues. The MAGICS (Materials Genome Innovation for Computational Software) Center develops to aid the synthesis of stacked layered materials by chemical vapor deposition, exfoliation, and intercalation. The identification of different phases can be formulated as a classification problem and can be solved using ML techniques. We have used feed-forward neural network with three hidden layers to identify the different phases present during computational synthesis of MoSe\textsubscript{2}. Work reported here was carried out in collaboration with Rajiv K. Kalia, Aiichiro Nakano, Lindsay Bassman, Sungwook Hong, Aravind Krishnamoorthy, Kuang Liu, Ankit Mishra, Ken-ichi Nomura, and Pankaj Rajak.

This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.

Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search

Patrick Avery, Xiaoyu Wang, Corey Oses, Eric Gossett, Davide Proserpio, Cormac Toher, Stefano Curtarolo, Eva Zurek

Good agreement was found between the experimental Vickers hardnesses, $H_v$, of a wide range of materials and those calculated by three macroscopic hardness models that employ the shear and/or bulk moduli obtained from: (i) first principles via the AFLOW Automatic Elastic Library, and (ii) a machine learning (ML) model trained on materials within the AFLOW repository. Because $H_v$ can be quickly estimated using ML, these values can be used in conjunction with an evolutionary algorithm to predict stable, superhard materials. This method is implemented in the XtalOpt evolutionary algorithm. Both the energy/enthalpy and the ML-based $H_v$ are employed to determine a structure’s fitness. The implementation is applied towards carbon, and 43 novel superhard phases are predicted.
The SCAN density functional and its surprising performance in complex materials

Jianwei Sun

1Department of Physics and Engineering Physics, Tulane University

The accuracy and computational efficiency of the widely used Kohn-Sham density functional theory (DFT) are limited by the approximation to its exchange-correlation energy $E_{xc}$. The earliest local density approximation (LDA) overestimates the strengths of all bonds near equilibrium (even the vdW bonds). By adding the electron density gradient to model $E_{xc}$, generalized gradient approximations (GGAs) generally soften the bonds to give robust and overall more accurate descriptions, except for the vdW interaction which is largely lost. Further improvement for covalent, ionic, and hydrogen bonds can be obtained by the computationally more expensive hybrid GGAs, which mix GGAs with the nonlocal exact exchange. Meta-GGAs are still semilocal in computation and thus efficient. Compared to GGAs, they add the kinetic energy density that enables them to recognize and accordingly treat different bonds, which no LDA or GGA can [2]. In this talk, I will present an advance in DFT, the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-GGA [1]. SCAN predicts accurate geometries and energies of diversely-bonded molecules and materials (including covalent, metallic, ionic, hydrogen, and van der Waals bonds), significantly improving over its predecessors, the GGAs that dominate materials computation, at comparable efficiency [2]. SCAN’s excellent performance on oxides and cuprates, traditionally regarded as strongly-correlated systems out of reach of DFT, will be highlighted [3]. I will further explain how SCAN was constructed [1], why it can improve over GGAs [2], and where it should fail [4]. At the end, efforts to improve SCAN via nonlocal corrections will be discussed.

Emergent Spin Vortex Crystals in Frustrated Quantum Magnets
Andriy Nevidomskyy

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Houston, TX 77005-1892

In the past several decades, the focus of condensed matter physics and materials research has been on the so-called strongly correlated electron materials. One of the most striking consequences of strong electron correlations is the emergence of exotic quantum phases of matter. In this talk, I will illustrate the phenomenon of quantum emergence on two examples of appearance of non-trivial spin textures in frustrated quantum magnets – here the term “frustration” refers to the presence of competing interactions that cannot be simultaneously satisfied. This results in complex magnetic states, for instance a three-dimensional "vortex crystal" which we predicted theoretically to form on frustrated cubic lattices, and which has recently found an experimental confirmation. We also study the details of non-collinear magnetic order observed in a quasi-2D material Sr$_2$F$_2$Fe$_2$OS$_2$ and show how it can be understood as a spin vortex crystal.
April 05, 2019
Electron-phonon and electron-electron interactions in electron doped aromatic carbon materials viewed from electrical transport

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A Mott physics on unconventional superconductors, such as cuprates, Fe pnictides, and organic conductors is now claimed for electron-doped aromatic hydrocarbon such as anthracene, tetracene, pentacene, and expanded C\textsubscript{60} [1-4] as well as even in graphene [5]. Electron-electron (e-e) correlations are thought to be the very important origin of its high T\textsubscript{c} superconductivity. On the other hand, the highest superconductivity surpassing the cuprates recently found in H\textsubscript{2}S under high pressure gives the discussion back to the electron-phonon (e-ph) mediated superconductivity for achieving extremely high T\textsubscript{c}. Although, relatively high T\textsubscript{c} in superconductivity was once claimed for simple aromatic hydrocarbons with electron carrier filling into their bands by alkali-metal insertion, the real electronics states have not yet been understood so far. This is partly because important scientific discussions have been made based on only limited magnetic and optical probes. The Fermi surface of A\textsubscript{3}C\textsubscript{60} (A=alkali metals: K, Rb, Cs) superconductors with expanded V\textsubscript{cell}(C\textsubscript{60}\textsuperscript{3-}) provides an intriguing research platform for both e-e and e-ph interactions. However, being different from other unconventional superconductors, electrical transport measurements had been very difficult in expanded A\textsubscript{3}C\textsubscript{60} and they are made only for K\textsubscript{3}C\textsubscript{60} and Rb\textsubscript{3}C\textsubscript{60} with small cell size far apart from the Mott boundary. Here, we give experimental results that accurate electrical resistivity (\(\rho(T,P)\)) can be achieved for a variety A\textsubscript{3}C\textsubscript{60} with expanded V\textsubscript{cell}(C\textsubscript{60}\textsuperscript{3-}) near the Mott boundary under various temperature (T) and pressure (P). Electrical transport was carefully measured as a function of T and P, straddling the phase boundary between the Mott insulator and the metallic/superconducting phase. A new phase diagram is proposed, which unambiguously shows an unprecedented new metallic state existing in the universal T-V\textsubscript{cell}(C\textsubscript{60}\textsuperscript{3-}) phase diagram. The new phase is interpreted to be generated by interplay between e-ph interactions via dynamic Jahn-Teller phonons and relatively large e-e correlations, showing a strong T-evolution of \(\rho(T)\). This intriguing relation can systematically be observed for A\textsubscript{3}C\textsubscript{60} with a variety of cell volume controlled by chemical (stoichiometric composition of A\textsubscript{3}C\textsubscript{60}) and physical pressure. The new electronic phase is considered to have a common underlying physics among many materials having large freedom of entropy.

Projected BCS theory for the unification of antiferromagnetism and strongly correlated superconductivity

Kwon Park

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At the core of the high-temperature superconductivity problem lies the relationship between strong correlation and superconductivity. One of the most exciting prospects on their relationship is that strong correlation is the very source of high-temperature superconductivity. To investigate the validity of this prospect, we perform an analysis of the BCS model Hamiltonian projected onto the constrained Hilbert space with infinitely strong correlation imposing the condition of no double occupancy also known as the Gutzwiller projection. Let us call such an analysis the projected BCS theory.

Specifically, we compute the overlap between the exact ground states of the projected BCS theory and the $t$-$J$ model via exact diagonalization. As a result, we show that the projected BCS theory provides excellent variational states for the exact ground states of the $t$-$J$ model in a wide range of hole concentration including both half filling and finite doping. It is emphasized that the resonating valence bond (RVB) state, i.e., the projected BCS wave function is closely related to the ground state of the projected BCS theory, while quite different at low doping. What makes the difference is whether the projection is applied to the ground state of the Hamiltonian or the Hamiltonian itself.
Autocorrelation of quasiparticle spectral intensities and its connection with quasiparticle scattering interference in cuprate superconductors

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²Department of Physics and Optoelectronic Engineering, Weifang University, Weifang 261061, China

The quasiparticle excitation is one of the most fundamental and ubiquitous physical observables in cuprate superconductors, carrying information about the bosonic glue forming electron pairs [1-5]. Here the autocorrelation of the quasiparticle excitation spectral intensities in cuprate superconductors [3] and its connection with the quasiparticle scattering interference [4,5] are investigated [6] based on the framework of the kinetic-energy driven superconducting mechanism by taking into account the pseudogap effect [7-9]. It is shown that the octet scattering model of the quasiparticle scattering processes with the scattering wave vectors \( \mathbf{q}_i \) connecting the hot spots on the constant energy contours is intrinsically related to the emergence of the highly anisotropic momentum-dependence of the pseudogap. Concomitantly, the sharp peaks in the autocorrelation of the quasiparticle excitation spectral intensities with the wave vectors \( \mathbf{q}_i \) are directly correlated to the regions of the highest joint density of states. Moreover, the momentum-space structure of the autocorrelation patterns of the quasiparticle excitation spectral intensities is well consistent with the momentum-space structure of the quasiparticle scattering interference patterns observed from Fourier-transform scanning tunneling spectroscopy experiments. The theory [6] therefore confirms an intimate connection between the angle-resolved photoemission spectroscopy autocorrelation and quasiparticle scattering interference in cuprate superconductors.

Materials Informatics Approaches for the Discovery of Magnetic 2D Materials
Richard G. Hennig\textsuperscript{1}, Janet Lu\textsuperscript{1}, Sohum Sha\textsuperscript{1}, Halee Lester\textsuperscript{1}, Nina Jovic\textsuperscript{1}, Dorde Gluhovic\textsuperscript{1}, B. E. Antonio\textsuperscript{2}, R. Ramanathan\textsuperscript{2}, Joshua Paul\textsuperscript{1}, Shreyas Honrao\textsuperscript{1}, Joshua J. Gabriel\textsuperscript{1}, Stephen Xie\textsuperscript{1}, Kiran Mathew\textsuperscript{2}, Benjamin C. Revard\textsuperscript{2}, Michael Ashton\textsuperscript{1}, Anne Marie Tan\textsuperscript{1}, Arunima K. Singh\textsuperscript{2}, and Houlong L. Zhuang\textsuperscript{2}

\textsuperscript{1} Materials Science and Engineering, University of Florida, Gainesville, Florida, United States.
\textsuperscript{2} Cornell University, Ithaca, New York, United States.

The rapid rise of novel 2D materials presents the exciting opportunity for materials science to explore an entirely new class of materials. This comes at the time when sophisticated materials informatics approaches provide the predictive capability to enable the computational discovery, characterization, and design of 2D materials and provide the needed input and guidance to experimental studies [1]. I will present our data-mining [2], evolutionary algorithm [3, 4], and machine-learning approaches [5] to identify novel 2D materials with low formation energies and show how unexpected structures emerge when a material is reduced to sub-nanometers in thickness. These materials informatics approaches identify low-dimensional materials that can be exfoliated from bulk crystal structures or by CVD and MBE synthesis. Among the low-dimensional materials, we predict a variety of magnetically ordered structures from ferromagnetic and antiferromagnetic order, to Berezinsky-Kosterlitz-Thouless phases, and half-metals [5]. These new low-dimensional materials provide the opportunity to investigate the interplay of magnetic order and reduced dimensionality and may provide materials suitable for optoelectronic and spintronic applications. The structures and calculated properties for all 2D materials are available in the MaterialsWeb database at https://materialsweb.org.

Role of doping and defects on the electronic properties of ZnO
Andreia Luisa da Rosa
Federal University of Goias, Institute of Physics
Av. Esperanca, s/n Campus Samambaia, Goiania, Goias, Brazil

Doping has been widely used to tailor the electronic, magnetic, and optical properties of semiconductors. Wide band-gap semiconductors such as ZnO are attractive for ultraviolet light-emitting diodes, lasers and high-power photonic applications. In ZnO, rare-earth elements can be incorporated in the material and the long lifetimes of the excited states allow for an easy realization of population inversion with promising applications in optoelectronics. The main challenge here is the correct description of both ZnO band edges and defect states. It is common understanding that the use of local exchange-correlation functionals wrongly described the ZnO band gap, which could lead to misleading conclusions on the location of the impurity rare-earth f states. Besides, intrinsic defects may also play an important role. In this work, the formation energies and electronic structure of rare-earth complexes in zinc oxide have been determined using density-functional theory and the many-body GW technique. In this talk we will discuss our results on complexes containing intrinsic defects and rare-earth elements in doped ZnO and the main challenges encountered to explain experimental spectra.
Down the Memory Lane
V. Drozd and S. Saxena

Florida International University, Florida
### International Meeting on Study of Matter at extreme conditions (SMEC2019)

**March 30 - April 06, 2019**  
**Miami - East Caribbean - Miami**

#### Mar 30-Sat

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#### Apr 3-Wed

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#### Apr 4-Thu

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#### Apr 5-Fri

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#### Apr 6-Sat

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#### Schedule Details

- **Coffee Breaks:** 10:30-11:00, 12:30-1:40, 15:00-16:00, 16:00-17:00
- **Lunch Break:** 12:30-14:00
- **Party (Sky Lounge):** 17:30-18:30
- **Welcome Party (Sky Lounge):** 18:30-20:30

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All times are in UTC+0.