International Meeting on

Study of matter at extreme conditions (SMEC2019)

March 30 - April 06, 2019

Miami - East Caribbean - Miami

SCIENTIFIC PROGRAM

International meeting on

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)

International Meeting on

Study of matter at extreme conditions (SMEC2019)

March 30 - April 06, 2019

Miami - East Caribbean - Miami

Organizers:

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Study of Matter at Extreme Conditions Miami 2019

International Meeting on

Study of matter at extreme conditions (SMEC2019)

March 30 - April 06, 2019

Miami - East Caribbean - Miami

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 Symposiums 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

Cruise Itinerary

Date	Port Location	Arrive	Depart
30 MAR	MIAMI, FLORIDA		3:30 PM
31 MAR	AT SEA		
01 APR	SAN JUAN, PUERTO RICO	3:30 PM	11:00 PM
02 APR	CHARLOTTE AMALIE, ST. THOMAS	8:00 AM	5:00 PM
03 APR	PUNTA CANA, DOMINICAN REP	7:00 AM	5:00 PM
04 APR	AT SEA		
05 APR	NASSAU, BAHAMAS	9:00 AM	6:00 PM
06 APR	MIAMI, FLORIDA	7:00 AM	

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		
8:30-10:30	**Opening & Plenary Session**	
10:30-11:00	**Coffee Break**	

11:00-12:30	Symposium 6, ***Recent developments in topological and correlated materials.*** Symposium 7, ***Emerging layered superconductors and related materials.***	Symposium 2, ***Multifunctional metal hydrides for energy storage.*** Symposium 3, ***Materials for energy applications.***
12:30-14:00	**Lunch Break**	
14:00-16:00	Symposium 6, ***Recent developments in topological and correlated materials.*** Symposium 7, ***Emerging layered superconductors and related materials.***	Symposium 2, ***Multifunctional metal hydrides for energy storage.*** Symposium 3, ***Materials for energy applications.***
16:00-16:30	**Coffee Break**	
16:30-18:30	Symposium 6, ***Recent developments in topological and correlated materials.*** Symposium 7, ***Emerging layered superconductors and related materials.***	Symposium 2, ***Multifunctional metal hydrides for energy storage.*** Symposium 3, ***Materials for energy applications.***

Monday April 01, 2019		
8:30-10:30	Symposium 6, ***Recent developments in topological and correlated materials.*** Symposium 7, ***Emerging layered superconductors and related materials.***	Symposium 2, ***Multifunctional metal hydrides for energy storage.*** Symposium 3, ***Materials for energy applications.***
10:30-11:00	**Coffee Break**	
11:00-12:30	Symposium 6, ***Recent developments in topological and correlated materials.*** Symposium 7, ***Emerging layered superconductors and related materials.***	Symposium 2, ***Multifunctional metal hydrides for energy storage.*** Symposium 3, ***Materials for energy applications.***
12:30-14:00	**Lunch Break**	
14:00-16:00	Symposium 6, ***Recent developments in topological and correlated materials.*** Symposium 7, ***Emerging layered superconductors and related materials.***	Symposium 2, ***Multifunctional metal hydrides for energy storage.*** Symposium 3, ***Materials for energy applications.***

Tuesday April 02, 2019	
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	
08:30-09:30	***Graduate Students Session – I***
16:30-18:30	***Graduate Students Session – II & Posters***

Thursday April 04, 2019		
08:30-10:30	Symposium 5, ***Unconventional superconductivity in Fe-based materials under extreme conditions.***	
10:30-11:00	**Coffee Break**	
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.*** Symposium 10, ***Two-dimensional materials: graphene and beyond.***
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	
08:30-10:30	Symposium 7, ***Emerging layered superconductors and related materials.***
17:00-19:00	Symposium 10, ***Two-dimensional materials: graphene and beyond.***

18:00-19:00	**Closing & Concluding Remarks**

DETAILED SCIENTIFIC SCHEDULE

Sunday March 31, 2019

S-1

	Room 1
	Opening Plenary Session
	Chairs: S. Saxena, R. Hennig
08:30-09:30	H. K. Mao, ***Recent advances in high-pressure physics, materials, and geoscience.***
09:30-10:30	A. Bansil, ***Raising the bar toward a first-principles description of stronger correlations: Novel superconductors to topological materials.***

10:30-11:00	Coffee Break

	S-2A Room 1	S-2B Room 2
	Topological & Correlated Materials-1	Metal Hydrides & Energy Materials-1
	Chairs: A. Bansil, X. X. Xi	Chairs: H.-W. Li, J. Chen
11:00-11:30	K. Tanigaki, ***Single crystal thin films of three-dimensional topological insulators via non-catalytic vapor phase epitaxial crystal growth.***	C. J. Webb, ***The use of oxides to kinetically enhance the sorption properties of MgH_2 at high pressure.***
11:30-12:00	T. H. Choudhury, ***Controlling epitaxial growth of transition metal dichalcogenides by gas source CVD.***	C. Jensen, ***Reversible Hydrogenation of Magnesium Boride and Magnesium Boranes to Magnesium Borohydride.***
12:00-12:30	Z. Mao, ***Layered magnetic topological semimetals and their unusual interlayer quantum transport.***	T. R. Jensen, ***Hydrogen storage and battery materials - new types of materials.***

12:30-14:00	Lunch Break

S-3A **S-3B**

	Room 1	Room 2
	Topological & Correlated Materials-2	**Metal Hydrides & Energy Materials-2**
	Chairs: K. Tanigaki, B. Barbiellini	**Chairs: T.R. Jensen, C.J. Webb**
14:00–14:30	Qi Li, ***Topological Surface States and Inducing Superconductivity in Bi_2Te_3 Nanotubes.***	C. Zlotea, ***Multi-principal-element alloys as new materials for hydrogen absorption.***
14:30-15:00	L. Balicas, ***Topological Semimetals from a High Magnetic Fields Perspective.***	K. T. Møller, ***Molten metal closo-hydridoborates.***
15:00-15:30	S. Y. Matsushita, ***Quantum hall effect and thermoelectric properties of surface Dirac states in Sn-$Bi_{1.1}Sb_{0.9}Te_2S$ crystal.***	Y. Filinchuk, ***Non-equilibrium Kr adsorption in nanoporous γ-$Mg(BH_4)_2$ by in situ synchrotron powder diffraction.***
15:30-16:00	I. Dasgupta, ***Realization of Spin-Orbital Liquid State in Iridates.***	

16:00-16:30	**Coffee Break**

S-4A **S-4B**

	Room 1	Room 2
	Topological & Correlated Materials-3	**Metal Hydrides & Energy Materials-3**
	Chairs: J. Sun, J.F. He	**Chairs:Y. Filinchuk,D. Matsumara**
16:30-17:00	Y. Ding, ***Spin-Orbit Assisted Correlated Materials at High Pressure: Novel Phases and Phenomena.***	M. Polanski, ***H2 Nautic - a hydrogen storage vessel for small touristic boats.***
17:00-17:30	T. Schmitt, ***Evolution of the spin, orbital and charge excitations upon tuning the local lattice environment of Sr_2IrO_4.***	M. Heere, ***Complex metal hydrides investigated by fast neutron powder diffraction.***
17:30-18:00	W. S. Kyung, ***Electric field driven octahedral rotation in Sr_2RuO_4 and its implication.***	Y. Song, ***Structural Stability of and Enhanced CO_2 Storage in Metal-Organic Frameworks under High Pressures Probed by Vibrational Spectroscopies and X-ray Diffraction.***
18:00-18:30	O. Eriksson, ***DMFT coupled to DFT: Case of some complex oxides.***	

Monday April 01, 2019

	S-5A	S-5B
	Room 1	**Room 2**
	Topological & Correlated Materials-4	**Metal Hydrides & Energy Materials-4**
	Chairs: A. Bansil, T. Schmitt	**Chairs: Y. Filinchuk, R. Ahuja**
08:30-09:00	D. Dessau, ***High temperature and possible topological superconductivity.***	C. E. Buckley, ***Thermal Battery Development for Concentrated Solar Power Systems.***
09:00-09:30	M. Shi, ***ARPES on topological quantum materials: from topological Kondo insulator to Weyl semimetal.***	L. Stievano, ***The sodiation-desodiation mechanism of Sb-based electrode materials revealed by operando spectroscopy assisted by chemometric data analysis.***
09:30-10:00	J. -F. He, ***Angle-resolved photoemission studies on strongly correlated materials.***	M. Heere, ***Neutron diffraction for energy storage and conversion in metal hydrides.***
10:00-10:30	N. L. Saini, ***Electronic phase separation in BiS_2-based systems.***	H. Miyaoka, ***Study on catalytic activation for Mg hydrogen storage.***

10:30-11:00	**Coffee Break**

	S-6A	S-6B
	Room 1	**Room 2**
	Emerging Superconductors	**Metal Hydrides & Energy Materials-5**
	Chairs: S. Feng, M. Shi	**Chairs: C.E. Buckley, H. Miyaoka**
11:00-11:30	D. Louca, ***Nanoscale Atomic Distortions in the BiS_2 Superconductors: Ferrodistortive Sulfur Modes.***	H. Saitoh, ***High-pressure and high-temperature synthesis of novel hydrides.***
11:30-12:00	K. Kudo, ***Superconductivity in Pt-based pnictides with ordered honeycomb networks.***	H. -W. Li, ***Solvent-free Facile Synthesis of Metal Boron Hydrides for Superionic Conductivity.***
12:00-12:30	Y. Goto, ***SnPn-based layered superconductors.***	K. T. Møller, ***Thermochemical Energy Storage Utilising Metal Carbonates.***

12:30-14:00	**Lunch Break**

S-7A S-7B

	Room 1	Room 2
	Topological & Correlated Materials-5	**Metal Hydrides & Energy Materials-6**
	Chairs: Y. Ding, D. Dessau	**Chairs: T.R. Jensen, C. Zlotea**
14:00-14:30	S. Zhang, ***Dark and half excitonic insulators.***	C. Pistidda, ***A Hydride Composite Featuring Mutual Destabilisation and Reversible Boron Exchange: $Ca(BH_4)_2$-Mg_2NiH_4.***
14:30-15:00	M. R. Vega, ***Higher-order Floquet topological phases with corner and bulk bound states.***	D. Matsumura, ***X-ray absorption spectroscopy for reaction of metal hydrides.***
15:00-15:30	T. S. Dasgupta, ***Heterostructures of 3d-5d Double Perovskites: Potential Candidates for Confined Half-metallicity & High-T Quantum Anomalous Hall States.***	M. Polanski, ***What hydride can steal from stainless steel ?About the Mg_2FeH_6 formation from magnesium hydride and austenitic steel.***
15:30-16:00	X. Wan, ***Towards ideal topological materials: Comprehensive database searches using symmetry indicators.***	C. Wu, ***Hydrogen Storage Characteristics and Applications of V-based BCC Alloys***

Tuesday April 02, 2019

S-8

	Room 1
	Correlated Oxides & Energy Materials
	Chairs: I. Dasgupta, N.L. Saini
08:30-09:00	X. X. Xi, ***Nature of the metal-insulator transition in few-unit-cell-thick $LaNiO_3$ films.***
09:00-09:30	B. Barbiellini, ***Identification of ferrimagnetic orbitals preventing Jahn-Teller distortions in $Li_xMn_2O_4$ cathodes.***
09:30-10:00	S. H. Lee, ***New Materials for Next Generation Printable Solar Cells.***

16:00-16:30	Coffee Break

S-9

	Room 1
	High Pressure Superconductivity
	Chairs: R. Hennig, A. Bansil
16:30-17:30	W. Pickett, ***How Compressed Hydride Superconductors Produce Room Temperature Superconductivity.***
17:30-18:00	E. Zurek, ***Computational Discovery of Novel Superconducting Hydride Phases Under Pressure.***
18:00-18:30	T. Shibauchi, ***High-T_c superconducting phases of FeSe-based materials at high pressure.***

Wednesday April 03, 2019

S-10

	Room 1
	Graduate Students Session-I
	Chairs: M. Polanski, C. E. Buckley
08:30-08:45	M. Jørgensen, ***Weakly coordinating anions in solid state electrolytes.***
08:45-09:00	J. B. Grinderslev, ***Extreme Hydrogen Densities in Ammonium Metal Borohydrides.***
09:00-09:15	M. Pęska, ***Magnesium – Lithium alloys as hydrogen storage materials.***
09:15-09:30	J. Vodeb, ***Correlated Configurational States and a Quantum Charge Liquid in Layered Metallic Dichalcogenides.***

16:00-16:30	Coffee Break

S-11

	Room 1
	Graduate Students Session-II
	Chairs: N. L. Saini, K. Kudo
16:30-16:45	S. R. Xie, ***Machine learning of Potential-Energy Landscapes in Two-dimensional Group-III Oxides.***
16:45-17:00	P. Nautiyal, ***Graphene Foam for Engineering Ultra-Stiff, Tough and Impact-Resistant Structural Composites.***
17:00-17:15	J. T. Paul, ***Materials Informatics Search for Strongly Correlated 1D Materials.***
17:15-18:30	Poster Presentations (Pugliese, Stramaglia, Shinzato, Karczewski, T.R. Jensen)

Thursday April 04, 2019

S-12

	Room 1
	Iron-based Superconductors - 1
	Chairs: C. Meingast, B. Buechner
08:30-09:00	P. Hirschfeld, ***Pairing mechanism in iron-based superconductors: variations on the s+/- theme.***
09:00-09:30	Y. Li, ***Spin-orbit coupling and "preferred" magnetic excitations in iron-based superconductors.***
09:30-10:00	R. Hackl, ***Microscopic origin of Cooper pairing in $Ba_{1-x}K_xFe_2As_2$ and $CaKFe_4As_4$.***
10:00-10:30	F. Hardy, ***Nodal Superconductivity in FeSe single crystals from heat capacity.***

10:30-11:00	Coffee Break

S-13A **S-13B**

	Room 1	Room 2
	Iron-based Superconductors - 2	High Pressure Earth & Planetary Sci.
	Chairs: P. Hirschfeld, F. Hardy	Chairs: J. Chen, S. Saxena
11:00-11:30	B. M. Andersen, ***Multi-orbital effects and the role of spin-orbit coupling in iron-based superconductors.***	Han Hsu, ***Iron spin crossover in the Earth and planetary interiors: A perspective from computational materials physics.***
11:30-12:00	B. Buechner, ***Orbitals and Nematicity in La-1111 Single Crystals.***	M. Hou, ***Temperature-induced amorphization in $CaCO_3$ at high pressure: implication for recycled $CaCO_3$ in subduction zones.***
12:00-12:15	A. P. Dioguardi, ***^{75}As NMR under uniaxial pressure in BaFe2As.***	W. L. Mao, ***Hydrogen-bearing iron peroxide in Earth's lowermost mantle.***
12:15-12:30	M. He, ***Ubiquitous dichotomy between the in-plane uniform magnetic susceptibility and resistivity anisotropies in iron-based superconductors.***	W. L. Mao, ***Hydrogen-bearing iron peroxide in Earth's lowermost mantle.***

12:30-14:00	Lunch Break

S-14A **S-14B**

	Room 1	Room 2
	Iron-based Superconductors - 3	**High Pressure & 2D Materials**
	Chairs: B.M Andersen, R. Hackl	**Chairs: W.L. Mao, A. L. da Rosa**
14:00-14:30	T. Shibauchi, ***Novel electronic nematicity in (Ba,Rb)Fe_2As_2.***	Jin Liu, ***Mantle-Slab Interactions and Mantle Heterogeneities.***
14:30-15:00	M. S. Ikeda, ***Feeling strain – Thermal and Resistive response in iron pnictides.***	Jiuhua. Chen, ***Kinetics of dehydrogenation of FeOOH at Earth's lower mental conditions.***
15:00-15:30	M. Christensen, ***Intertwined spin-orbit coupled orders in the iron-based superconductors.***	A. Agarwal, ***Graphene Foam-Based Multifunctional Polymer Composites for Self-Healing, De-icing and Strain-sensing Applications.***
15:30-15:45	C. Meingast, ***Intertwined and vestigial electronic phases in hole-dopes $Sr_{1-x}Na_xFe_2As_2$.***	O. Kurakevych, ***Accomplishing a suite of magnesium carbides by HPHT synthesis.***
15:45-16:00	C. Meingast, ***Intertwined and vestigial electronic phases in hole-dopes $Sr_{1-x}Na_xFe_2As_2$.***	A. Soldatov, ***Nanostructured graphene: When disorder makes things better?***

16:00-16:30	**Coffee Break**

S-15A **S-15B**

	Room 1	Room 2
	Iron-based Superconductors - 4	**Topological & Quantum Materials**
	Chairs: Y. Li, T. Shibauchi	**Chairs: A, Bansil, R. Hennig**
16:30-17:00	V. Taufour, ***Pressure dependence of the superconducting upper critical field in KFe_2As_2 and related materials.***	P. Vashishta, ***Reactive molecular dynamics simulations and machine learning.***
17:00-17:30	G. Garbarino, ***Pressure temperature phase diagram of iron based superconductors.***	E. Zurek, ***Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search.***
17:30-18:00	V. Svitlyk, ***Structure-property correlations in FeSe-based superconducting materials,***	J. Sun, ***The SCAN density functional and its surprising performance in complex materials.***
18:00-18:15	N. L. Saini, ***Local structure and superconductivity in iron-based superconductors.***	A. Nevidomskyy, ***Emergent Spin Vortex Crystals in Frustrated Quantum Magnets.***
18:15-18:30		A. Nevidomskyy, ***Emergent Spin Vortex Crystals in Frustrated Quantum Magnets.***

19:30-20:30	**Get Together Party** – *Sky Lounge*

Friday April 05, 2019

S-16

	Room 1
	Correlated Materials & Superconductivity
	Chairs: D. Louca, E. Zurek
08:30-09:00	K. Tanigaki, ***Electron-phonon and electron-electron interactions in electron doped aromatic carbon materials viewed from electrical transport.***
09:00-09:30	S. Tsuchiya, ***Development of optical pump probe spectroscopy under uniaxial pressure: Application to strongly correlated superconductors.***
09:30-10:00	K. Park, ***Projected BCS theory for the unification of antiferromagnetism and strongly correlated superconductivity.***
10:00-10:30	S. Feng, ***Autocorrelation of quasiparticle spectral intensities and its connection with quasiparticle scattering interference in cuprate superconductors***.

16:30-17:00	Coffee Break

S-17

	Room 1
	2D Materials & Concluding Session
	Chairs: N. L. Saini, J. Chen
17:00-17:30	R. Hennig, ***Materials Informatics Approaches for the Discovery of Magnetic 2D Materials.***
17:30-18:00	A. L. da Rosa, ***Role of doping and defects on the electronic properties of ZnO.***
18:00-18:30	V. Drozd & S. Saxena, ***Down the memory lane.***
18:30-19:00	Organizers & Participants, ***Concluding Remarks.***

ABSTRACTS

International Meeting on

Study of matter at extreme conditions (SMEC2019)

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March 31, 2019

Sunday 31 March, 2019, 08:30

Recent advances in high-pressure physics, materials, and geoscience

H.K. Mao[1], B. Chen[1], C. Ji[1], Y. He[1], M.Q. Hou[1], Q.Y. Hu[1], F. Ke[1], D.Y. Kim[1], B. Li[1], J. Liu[1], L.X. Yang[1], W.G. Yang[1], B. Li[1], Z.D. Zeng[1]

[1]*Center for High Pressure Science and Technology Advanced Research, 10 Xibeiwang East Road, Haidian, Beijing, 100094, China*

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.

Sunday 31 March, 2019, 09:30

Raising the bar toward a first-principles description of stronger correlations: Novel superconductors to topological materials

Arun Bansil

Physics Department, Northeastern University, Boston, Massachusetts USA

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.

[1] J. Sun, A. Ruzsinszky, J. P. Perdew, Phys. Rev. Lett. 115, 036402 (2015).
[2] J. W. Furness et al., Nature Communications Physics 1, 11 (2018).
[3] C. Lane et al., Phys. Rev. B. 98, 125140 (2018).
[4] Y. Zhang et al., arXiv:1809.08457 (2018).
[5] A. Bansil, H. Lin and T. Das, Reviews of Modern Physics 88, 021004 (2016).

Sunday 31 March, 2019, 11:00, Room 1

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

K. Tanigaki[1,2], S. Y. Matsushita[2], K. Ichimura[2]

[11]*AIMR, Tohoku University, Sendai 980-8577, Japan*

[2]*Department of Physics, Graduate School of Science, Sendai 980-8578, Japan*

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^{th} (Sb,Bi)-VI^{th} (Se,Te) elements are most frequently studied for 3D-TIs. Bi_2Se_3 and Bi_2Te_3 are known to be n-type 3D-TIs, while Sb_2Te_3 is p-type one although Sb_2Se_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 $(Bi,Sb)_2Te$ (BST) or $(Bi,Sb)_2Se_3$ (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].

[1] Y. Tanabe, K. K. Huynh, H. Shimotani, and K. Tanigaki, Journal Physical Chemistry C 118, 3533−3538 (2014).

[2] N. H. Tu, Y. Tanabe, K. K. Huynh, K. Tanigaki, Applied Physics Letters 105 , 063104 (2014).

[3] N. H. Tu, Y. Tanabe, Y. Satake, K. K. Huynh, K. Tanigaki. Nature Communications, 13763, (2016).

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Sunday 31 March, 2019, 11:30, Room 1

Controlling epitaxial growth of transition metal dichalcogenides by gas source CVD

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Monolayer transition metal dichalcogenides (TMDs, MoS_2, WSe_2, 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 MoS_2, WS_2, WSe_2 and $MoSe_2$ 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 $(Mo,W)S_2$ 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 WS_2 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.

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Sunday 31 March, 2019, 12:00, Room 1

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.

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Sunday 31 March, 2019, 14:00, Room 1

Topological Surface States and Inducing Superconductivity in Bi_2Te_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_2Te_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 $NbSe_2/Bi_2Se_3$ 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.

*Work done in collaboration with Renzhong Du, Hsiu-Chuan Hsu, Ajit C. Balram, Yuewei Yin, Sining Dong, Wenqing Dai, Weiwei Zhao, DukSoo Kim, Shih-Ying Yu, Jian Wang, Xiaoguang Li, Suzanne E. Mohney, Srinivas Tadigadapa, Nitin Samarth, Moses H.W. Chan, Jainendra. K. Jain, Chao-Xing Liu.

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Sunday 31 March, 2019, 14:30, Room 1

Topological Semimetals from a High Magnetic Fields Perspective

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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 T_d-$MoTe_2$ 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.

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Sunday 31 March, 2019, 15:00, Room 1

Quantum hall effect and thermoelectric properties of surface Dirac states in Sn-$Bi_{1.1}Sb_{0.9}Te_2S$ crystal

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The electric transport properties of single crystal of three-dimensional topological insulator Sn-$Bi_{1.1}Sd_{0.9}Te_2S$ (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.

Sunday 31 March, 2019, 15:30, Room 1

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 $Ba_3MIr_2O_9$, have all the necessary ingredients to host QSL state. In $Ba_3MIr_2O_9$, 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 $Ba_3ZnIr_2O_9$ 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 Ir2O9 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 $Ba_3YIr_2O_9$ 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 Ba_2YIrO_6 .

Work done in collaboration with S. Bhowal, S.K. Panda, A. Chakraborti, A. Nag, S. Ray and A.V. Mahajan.

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Sunday 31 March, 2019, 16:30, Room 1

Spin-Orbit Assisted Correlated Materials at High Pressure: Novel Phases and Phenomena

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Pressure is an effective and clean means to tune fundamental interactions in 5*d* 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. $Sr_3Ir_2O_7$) at high pressure, which are probed with synchrotron, optical, electric transport, as well as theoretical computation methods.

Sunday 31 March, 2019, 17:00, Room 1

Evolution of the spin, orbital and charge excitations upon tuning the local lattice environment of Sr_2IrO_4

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Sr_2IrO_4 has been in the lime light during the last years due to the discovery of a novel $J_{eff} = ½$ 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_2IrO_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_2IrO_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 (π,0) direction upon tensile strain. This effect is not present along the (π, π) 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.

Sunday 31 March, 2019, 17:30, Room 1

Electric field driven octahedral rotation in Sr_2RuO_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_2RuO_4. Originally rotated octahedra in the surface layer of Sr_2RuO_4 are restored to the bulk structure upon K dosing on the surface. Our theoretical investigation shows that OR in Sr_2RuO_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.

Sunday 31 March, 2019, 18:00, Room 1

DMFT coupled to DFT: Case of some complex oxides

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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 photoelecton spectroscopy and x-ray absorbtion spectroscopy. Materials to be discussed involve complex oxides.

Sunday 31 March, 2019, 11:00, Room 2

The use of oxides to kinetically enhance the sorption properties of MgH_2 at high pressure

C.J. Webb

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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_2O_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.

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Sunday 31 March, 2019, 11:30, Room 2

Reversible Hydrogenation of Magnesium Boride and Magnesium Boranes to Magnesium Borohydride

Craig Jensen

University of Hawaii, Hawaii, USA

Sunday 31 March, 2019, 12:00, Room 2

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 has 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, $p(H_2) \sim 0.5$ - 1 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 divers, 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.

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Sunday 31 March, 2019, 14:00, Room 2

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.[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.[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[3], the potential use of these materials is largely unexplored in the clean energy field (electrochemical conversion and hydrogen storage).[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* ↔ monohydride *bct* ↔ dihydride *fcc*), the hydride absorption in these MPEAs occurs into a single step (alloy *bcc* ↔ 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.[5]

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Molten metal *closo*-hydridoborates

Kasper T. Møller,[1,2] Mark Paskevicius,[1,2] Jacob G. Andreasen,[2] Junqiao Lee,[3] Nigel Chen-Tan,[1] Jacob Overgaard,[2] SeyedHosein G. Payandeh,[2] Debbie S. Silvester,[3] Craig E. Buckley,[1] Torben R. Jensen.[1]

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Metal *closo*-hydridoborates, *e.g.* $M_2B_{12}H_{12}$, have received increased attention as ion conductors due to extraordinary ionic conductivity in their high-temperature structural polymorphs.[1–5] Recently, nanoconfinement of $Li_2B_{12}H_{12}$ was achieved *via* a solid-gas reaction inside a nanoporous SiO_2 (SBA-15) scaffold between $LiBH_4$ and gaseous B_2H_6.[6] However, the reaction yields moderate purity (94 mol%) $Li_2B_{12}H_{12}$ with 6 mol% $Li_2B_{10}H_{10}$. The ionic conductivity of the nanoconfined sample was 1.0 x 10^{-7} $S{\cdot}cm^{-1}$ at room temperature, which is similar to bulk $Li_2B_{12}H_{12}$.[6]

In this work, solvated lithium *closo*-dodecaborate, $Li_2B_{12}H_{12}{\cdot}$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 $Li_2B_{12}H_{12}$ 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 $Li_2B_{12}H_{12}$ was measured by EIS.

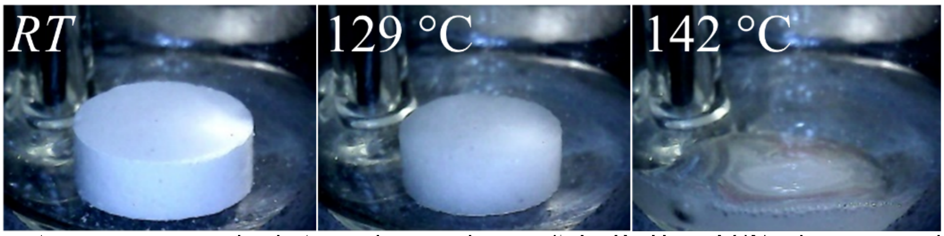

Figure 1. Temperature programmed photographic analysis of $Li_2B_{12}H_{12}{\cdot}x$ACN showing melting at low temperature.

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Sunday 31 March, 2019, 15:00, Room 2

Non-equilibrium Kr adsorption in nanoporous γ-$Mg(BH_4)_2$ by *in situ* synchrotron powder diffraction

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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 quest 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. γ-$Mg(BH_4)_2$ 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 $Mg(BH_4)_2{\cdot}0.66Kr$, 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 γ-$Mg(BH_4)_2$. 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.

Sunday 31 March, 2019, 16:30, Room 2

H_2 Nautic - a hydrogen storage vessel for small touristic boats.

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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.

Sunday 31 March, 2019, 17:00, Room 2

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 ($Mg(BH_4)_2$) 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 $Mg(BH_4)_2$ including different gases such as D_2, He, Ne, Ar, Kr & Xe at the Wide Angle Neutron Diffractometer WAND[2] 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 $Mg(^{11}BD_4)_2$ forms a new hydride phases at 25 K and 1 bar D_2 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-$Mg(BH_4)_2$. 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 H_2 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.

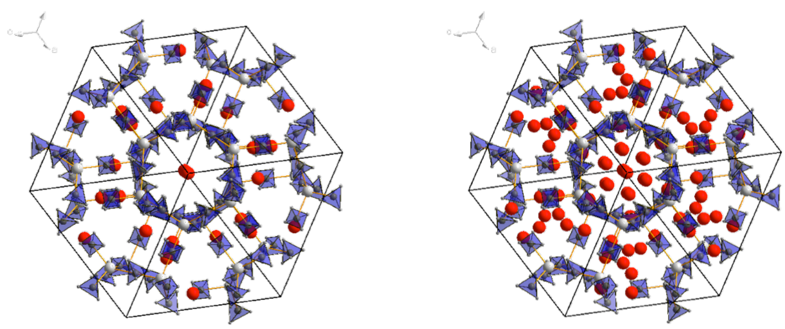

Figure 1. Crystal structure of the two D_2-loaded phases with the limiting compositions γ-$Mg(^{11}BD_4)_2\cdot 1.33D_2$ (left) and γ-$Mg(^{11}BD_4)_2\cdot 2.33D_2$ (right). Mg atoms are shown as gray spheres, BH_4 groups as blue tetrahedral, and unit cells are defined by red lines, positions of D_2 molecules (D_2-superatoms) as red spheres.

Sunday 31 March, 2019, 17:30, Room 2

Structural Stability of and Enhanced CO_2 Storage in Metal-Organic Frameworks under High Pressures Probed by Vibrational Spectroscopies and X-ray Diffraction

Y. Song[1], S. Jiang[1] and Y. Huang[1]

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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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April 01, 2019

Monday 01 April, 2019, 08:30, Room 1

High temperature and possible topological superconductivity

Dan Dessau

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I discuss two high temperature superconductors:

a) T_c=39K 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].

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Monday 01 April, 2019, 09:00, Room 1

ARPES on topological quantum materials: from topological Kondo insulator to Weyl semimetal

Ming Shi[1]

[1] *Swiss Light Source, Paul Scherrer Institut, Switzerland*

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.

Monday 01 April, 2019, 09:30, Room 1

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].

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Monday 01 April, 2019, 10:00, Room 1

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 $EuFBiS_2$ will also be discussed revealing phase separation at mesoscopic scale that is driven by peculiar lattice distortions in these materials.

Monday 01 April, 2019, 11:00, Room 1

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 $ReO_{1-x}F_xBiS_2$ (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 $ReO_{1-x}F_xBiS_2$ 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 $ReO_{1-x}F_xBiS_2$ also manifest z-motion of apical sulfur which could act as a charge transfer conduit between the electron doping layers and superconducting layers.

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Monday 01 April, 2019, 11:30, Room 1

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 $CaPt_xP_{2-x}$, 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- (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).

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Monday 01 April, 2019, 12:00, Room 1

SnPn-based layered superconductors

Y. Goto and Y. Mizuguchi

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We report SnPn-based (Pn: pnictogen) layered superconductors $NaSn_2As_2$ and $Na_{1-x}Sn_2P_2$ [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 $NaSn_2As_2$ and 2.0 K for $Na_{1-x}Sn_2P_2$. Amount of Na deficiency (x) of $Na_{1-x}Sn_2P_2$ 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 $Na_{1-x}Sn_2P_2$ 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 $NaSn_2As_2$ 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.

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Monday 01 April, 2019, 14:00, Room 1

Dark and half excitonic insulators

Shengbai Zhang

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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 ¼ 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.

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Monday 01 April, 2019, 14:30, Room 1

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.

[1] arXiv:1811.04808 (2018)

Monday 01 April, 2019, 15:00, Room 1

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_2FeReO_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 $BaTiO_3$ (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 ~100meV and an estimated FM T_c~315K. 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*d*-5*d* or 3*d*-4*d* half-metallic DPs like Sr_2FeMoO_6 and Sr_2CrWO_6.

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

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Monday 01 April, 2019, 15:30, Room 1

Towards ideal topological materials: Comprehensive database searches using symmetry indicators

Xiangang Wan

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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.

Monday 01 April, 2019, 08:30, Room 2

Thermal Battery Development for Concentrated Solar Power Systems

C.E. Buckley, M. Paskevicius, T.D. Humphries, M.V. Sofianos, K. Moller

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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].

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Monday 01 April, 2019, 09:00, Room 2

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_3Sb 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 $FeSb_2$ 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, $FeSb_2$ and SnSb with Na by operando X-ray absorption spectroscopy (XAS),[6-8] coupled to ^{57}Fe Mössbauer spectroscopy in the case of $FeSb_2$. 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.

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Monday 01 April, 2019, 09:30, Room 2

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 *in situ* and *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 *in situ/ in operando* NPD measurements is presented. Furthermore, NPD data of the recently reported solid-state Mg-ion conductor synthesized from $Mg(BH_4)_2$ and ethylenediamine are elaborated and unpublished structural details are presented as well.

MH acknowledges the project "**E**nergy **R**esearch **wi**th **N**eutrons (ErwiN)" [1], which is funded by the German Federal Ministry of Education and Research (BMBF).

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Monday 01 April, 2019, 10:00, Room 2

Study on catalytic activation for Mg hydrogen storage

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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_2O_5 are synthesized. These Nb_2O_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_2O_5 showed catalysis for the hydrogen adsorption and absorption reactions. By comparing the catalysis of Nb_2O_5 with different crystallinity and particle size, it is clarified that structural properties of initial Nb_2O_5 more affect the catalytic effects than particle size, and amorphous Nb_2O_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_2O_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.

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Monday 01 April, 2019, 11:00, Room 2

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, Li_4FeH_6 was synthesized by hydrogenation reaction of a powder mixture of LiH and pure iron above 6 GPa [1]. Li_3AlFeH_8 was obtained by introducing two H^- anions into iron-containing complex hydride [2]. Al_2CuH_x has been synthesized by hydrogenating Al_2Cu 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.

This work was supported by JSPS KAKENHI, Grant Numbers, JP18H05513 and JP18H05518, and the Inter-University Cooperative Research Program of the Institute for Materials Research, Tohoku University (Proposal Nos. 16K0079, 17K0026, and 18K0032). The neutron scattering experiment was approved by the Neutron Scattering Program Advisory Committee of IMSS, KEK (Proposal No. 2014S06).

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Monday 01 April, 2019, 11:30, Room 2

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_2, 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].

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Monday 01 April, 2019, 12:00, Room 2

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 CO_2 with low cost and high energy density [3]. However, the major challenge is the loss of CO_2 capacity, which drastically decreases over multiple cycles [4,5].

Recently, it was established that dolomite, $CaMg(CO_3)_2$, 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 $CaCO_3$ and a reactive carbonate composition of $BaCO_3$-$BaSiO_3$ 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.

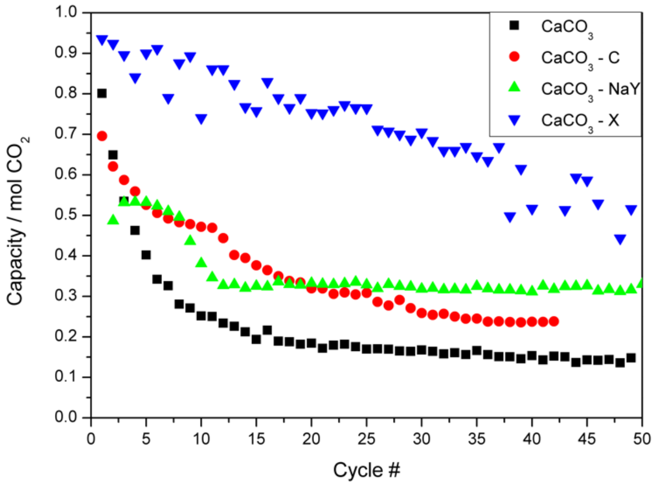

Figure 1. Showing the decreasing CO_2 capacity of $CaCO_3$ (black squares) with increasing cycling. Additives assist in maintaining the capacity over further cycles.

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Monday 01 April, 2019, 14:00, Room 2

A Hydride Composite Featuring Mutual Destabilisation and Reversible Boron Exchange: $Ca(BH_4)_2$-Mg_2NiH_4

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The system $Ca(BH_4)_2$-Mg_2NiH_4 is used as a model to prove the unique possibility to fully reverse the borohydride decomposition process even in cases where the decomposition reaction leads to undesired stable boron containing species (boron sinks). The formation of $MgNi_{2.5}B_2$ directly from $Ca(BH_4)_2$ or from $CaB_{12}H_{12}$ and amorphous boron allows an unexpectedly easy transfer of the boron atoms to reversibly form $Ca(BH_4)_2$ during rehydrogenation. In addition, to the best of our knowledge, the mutual destabilisation of the starting reactants is observed for the first time in $Ca(BH_4)_2$ 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].

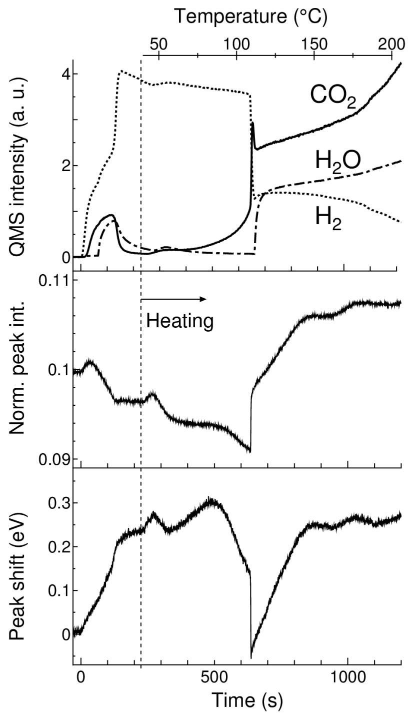

Fig. 1 Temporal variations of XAFS peak shift and intensity for Pt nanoparticles with the change of gas concentration during flow of $H_2/O_2/CO$.

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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Monday 01 April, 2019, 15:00, Room 2

What hydride can steal from stainless steel? About the Mg_2FeH_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_2FeH_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_2FeH_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.

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Monday 01 April, 2019, 15:30, Room 2

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

Tuesday 02 April, 2019, 08:30, Room 1

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.

Tuesday 02 April, 2019, 09:00, Room 1

Identification of ferrimagnetic orbitals preventing Jahn-Teller distortions in $Li_xMn_2O_4$ 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.

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Tuesday 02 April, 2019, 09:30, Room 1

New Materials for Next Generation Printable Solar Cells

Seung-Hun Lee

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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]

[1] Origin of Long Lifetime of Band-Edge Charge Carriers in Organic-Inorganic Lead Iodide Perovskites, Tianran Chen, Wei-Liang Chen, Benjamin J. Foley, Jooseop Lee, Jacob Ruff, J. Y. Peter Ko, Craig M. Brown, Leland W. Harriger, Depei Zhang, Changwon Park, Mina Yoon, Yu-Ming Chang, Joshua J. Choi, and Seung-Hun Lee, Proc. Natl. Acad. Sci. 114, 7519-7524 (2017).

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Tuesday 02 April, 2019, 16:30, Room 1

How Compressed Hydride Superconductors Produce Room Temperature Superconductivity

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The 2014-2015 prediction, discovery, and confirmation of superconductivity above 200K in SH_3, 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 XH_n 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 H_3S 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 H_3S in both the normal and superconducting states; evidence will be presented and discussed.

Tuesday 02 April, 2019, 17:00, Room 1

Computational Discovery of Novel Superconducting Hydride Phases Under Pressure

Tiange 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.

Tuesday 02 April, 2019, 17:30, Room 1

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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April 03, 2019

Wednesday 3 April, 2019, 08:30, Room 1

Weakly coordinating anions in solid state electrolytes

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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 $Na_2B_{12}H_{12}$.[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 $Na_2(CB_9H_{10})(CB_{11}H_{12})$[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.

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Wednesday 3 April, 2019, 08:45, Room 1

Extreme Hydrogen Densities in Ammonium Metal Borohydrides

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The compound ammonium borohydride, NH_4BH_4, is among the compounds known with the highest gravimetric (24.5 wt% H_2) and volumetric hydrogen content (157.3 g·H_2/L), and releases 75 % of its H_2 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, $[(NH_3)_2BH_2]BH_4$.[1,2] Furthermore, the H_2 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 NH_4BH_4 by addition reactions with stable metal borohydrides, similar to $NH_4Ca(BH_4)_3$ 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 NH_4^+. The partially positively charged $H^{\delta+}$ on NH_4^+ and partially negatively charged $H^{\delta-}$ on BH_4^- 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% H_2 and volumetric hydrogen contents of ρ_V = 88.0-158.2 kg/H_2/m^3.

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Wednesday 3 April, 2019, 09:00, Room 1

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 f.e. 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: α, α + β, β 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 (β 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.

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Wednesday 3 April, 2019, 09:15, Room 1

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 $fm=1/3, 1/4, 1/9, 1/13, 1/16$ 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 fm, 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 fm delineate the different regions of the phase diagram in accordance with observed doping and light-induced orders.

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Wednesday 3 April, 2019, 16:30, Room 1

Machine learning of Potential-Energy Landscapes in Two-dimensional Group-III Oxides

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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.

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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.

Wednesday 3 April, 2019, 17:00, Room 1

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]

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Wednesday 03 April, 2019, 17:15, Poster presentation

Local structure of $La_{1-x}Ce_xOBiSSe$ as a function of Ce substitution

G. M. Pugliese[1], F. Stramaglia[1], M. Y. Hacisalihoglu[1,2], Y. Mizuguchi[3], K. Terashima[4], T. Yokoya[4], T. Mizokawa[5], N. L. Saini[1]

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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 $La_{1-x}Ce_xOBiSSe$ 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.

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Wednesday 03 April, 2019, 17:15, Poster presentation

Study of the local structure of $CaKFe_4As_4$ as a function of temperature

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We have measured the local structure of the new superconducting Fe-based system $CaKFe_4As_4$ (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 $CaFe_2As_2$. 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 $CaFe_2As_2$ 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.

Wednesday 03 April, 2019, 17:15, Poster presentation

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 $Na_{15}Sn_4$ as follows,

Thermal reaction (decomposition): $Na_{15}Sn_4 \rightarrow 15Na + 4Sn$ (1)

Electrochemical reaction (discharge): $15Na \rightarrow 15Na^+ + 15e^-$ (2)

$15Na^+ + 4Sn + 15e^- \rightarrow Na_{15}Sn_4$ (3).

Thermal energy can be converted to electric energy by combining above reactions. Although electrochemical properties of $Na_{15}Sn_4$ 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 $Na_{15}Sn_4$ (eq. 1) is investigated under various conditions. $Na_{15}Sn_4$ 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, $Na_{15}Sn_5$ 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, $Na_{15}Sn_4$ is recognized as a potential material for thermoelectric conversion of heat energy at 150-500 °C.

[1] L. D. Ellis, et al, *Journal of The Electrochemical Society*, **159**(11), A1801 (2012).

Wednesday 3 April, 2019, 17:15, Poster presentation

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.

Wednesday 3 April, 2019, 17:15, Poster presentation

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'.

April 04, 2019

Thursday 04 April, 2019, 08:30, Room 1

Pairing mechanism in iron-based superconductors: variations on the s+/- theme

P. Hirchfeld

University of Florida, USA

I review some of the recent developments in the theory of superconductivity of iron-based systems that go beyond the s+/- 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.

Thursday 04 April, 2019, 09:00, Room 1

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 $BaFe_2As_2$ 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 $Sr_{1-x}Na_xFe_2As_2$, 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 $Sr_{1-x}Na_xFe_2As_2$, and provide a fresh view on how to make a good superconductor out of a magnetic "Hund's metal".

[1] C. Wang *et al.*, *Phys. Rev. X* **3**, 041036 (2013).
[2] M. Ma *et al.*, *Phys. Rev. X* **7**, 021025 (2017).
[3] J. Guo *et al.*, *Phys. Rev. Lett.* **122**, 017001 (2019).

Thursday 04 April, 2019, 09:30, Room 1

Microscopic origin of Cooper pairing in $Ba_{1-x}K_xFe_2As_2$ and $CaKFe_4As_4$

T. Böhm[1,2], D. Jost[1,2], N. Lazarević[3], J.-R. Scholz[1,2], F. Kretzschmar[1,2], A. Baum[1,2], M. Rehm[1,2], R. Hosseinian Ahangharnejhad[1,2], U. Zweck[1,2], R. Thomale[4], C. Platt[4,5], T. A. Maier[6], W. Hanke[4], B. Moritz[7], T. P. Devereaux[7,8], D. J. Scalapino[9], S. Maiti[10], P. J. Hirschfeld[11] W. R. Meier[12,13], A. E. Böhmer[13,14], P. C. Canfield[13,12], P. Adelmann[14], T. Wolf[14], Hai-Hu Wen[15], and R. Hackl[1]

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We present results of Raman scattering experiments on $Ba_{1-x}K_xFe_2As_2$ ($0.22 \leq x \leq 0.7$) [1] and $CaKFe_4As_4$ [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 $8k_BT_c$. Inside the large gaps narrow lines are found for $Ba_{1-x}K_xFe_2As_2$ for doping levels $0.35 \leq x \leq 0.48$. The spectra in $CaKFe_4As_4$ are similar to those of $Ba_{0.65}K_{0.35}Fe_2As_2$. Among the suggested explanations of the in-gap modes we observe Bardasis-Schrieffer excitons, resulting from anisotropic pairing interactions $V_{\mathbf{k},\mathbf{k}'}$, 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].

[1] T. Böhm et al., NPJ Quantum Mater. **3**, 48 (2018).

[2] D. Jost et al., Phys. Rev. B **98**, 020504(R) (2018).

Thursday 04 April, 2019, 10:00, Room 1

Nodal Superconductivity in FeSe single crystals from heat capacity

Frédéric Hardy [1], Minqguan He [1], Liran Wang [1], Thomas Wolf [1], Robert Eder [1], Peter Schweiss [1], Michael Merz [1], and Christoph Meingast [1]

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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.

[1] F. Hardy et al, Phys. Rev. B 99, 035157, (2019).
[2] P. O. Sprau, et al, Science 357, 75 (2017).

Thursday 04 April, 2019, 11:00, Room 1

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

B.M. Andersen

University of Copenhagen, Denmak

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.

Thursday 04 April, 2019, 11:30, Room 1

Orbitals and Nematicity in La-1111 Single Crystals

B. Buechner

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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 $BaFe_2S_3$. 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.

Thursday 04 April, 2019, 12:00, Room 1

^{75}As NMR under uniaxial pressure in $BaFe_2As_2$

A. P. Dioguardi[1], T. Schorr[1], C. W. Hicks[2], S. Aswartham[1], S. Wurmehl[1], B. Büchner[1,3], and H.-J. Grafe[1]

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We have conducted systematic ^{75}As nuclear magnetic resonance (NMR) experiments in $BaFe_2As_2$ 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.

[1] T. Kissikov, R. Sarkar, M. M. Lawson, B. T. Bush, E. I. Timmons, M. A. Tanatar, R. Prozorov, S. L. Bud'ko, P. C. Canfield, R. M. Fernandes, and N. J. Curro, Nature Communications 9, 1058 (2018).

Thursday 04 April, 2019, 12:15, Room 1

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

Mingquan He[1,2], Liran Wang[1], Felix Ahn[3], Frédéric Hardy[1], Thomas Wolf[1], Peter Adelmann[1], Jörg Schmalian[1,4], Ilya Eremin[3],Christoph Meingast[1]

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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 $Ba_{1-x}K_xFe_2As_2$ and FeSe systems using a simple method, in which a large symmetry-breaking ansiotropic 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 $Ba_{1-x}K_xFe_2As_2$ and FeSe. More interestingly, for $Ba_{1-x}K_xFe_2As_2$, a sign reversal occurs ~x=0.2 in resistivity anisotropy, whereas the sign of susceptibility anisotropy remains unaffected. However, compared to $BaKFe_2As_2$, both resistivity and susceptibility antitropies 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.

[1] Mingquan He et al, *Nat. Commun.* **8**, 504(2017,).

[2] Mingquan He et al, Phys. Rev. B **97**, 104107(2018).

Thursday 04 April, 2019, 14:00, Room 1

Novel electronic nematicity in (Ba,Rb)Fe_2As_2

T. Shibauchi

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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 $Ba_{1-x}Rb_xFe_2As_2$ 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.

[1] K. Ishida et al, arXiv:1812.05267

Thursday 04 April, 2019, 14:30, Room 1

Feeling strain – Thermal and Resistive response in iron pnictides

Matthias S. Ikeda, Alexander T. Hristov, Thanapat Worasaran, Johanna C. Palmstrom, Joshua A. W. Straquadine, Philip Walmsley, and Ian R. Fisher

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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.

This work was supported in part by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4414 and by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DEAC02-76SF00515.

Thursday 04 April, 2019, 15:00, Room 1

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 occuring 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 **Q**=(0,0,π) [3] while in compounds with no staggering (e.g. 111) these are **Q**=0 orders. While the vestigial orders are composite in spin-space, they induce simple orbital terms with measureable 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].

[1] R. M. Fernandes, P. P. Orth, and J. Schmalian, arXiv:1804.00818
[2] MHC, J. Kang, and R. M. Fernandes, arXiv 2019
[3] W. R. Meier, MHC, A. Kreyssig, and R. M. Fernandes, in progress

Thursday 04 April, 2019, 15:30, Room 1

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

C. Meingast

Karlsruhe Institute of Technology, Karlsruhe

Hole-doped $ReFe_2As_2$ (Re = Ba, Sr, Ca) exhibit much richer phase diagrams than the corresponding electron-doped systems. In particular, the phase diagram of Na-doped $BaFe_2As_2$ 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 $SrFe_2As_2$ 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 $SrFe_2As_2$ exhibits even more complexity than the K- and Na-doped $BaFe_2As_2$ counterparts.

[1] J. M. Allred et al., *Nature Physics* **12**, 493–498 (2016).
[2] L. Wang et al., Phys. Rev. B**93**, 014514 (2016).
[3] B. Keimer et al. Nature 518, 179 (2015).
[4] A. E. Boehmer et al., Nat. Commun. 6, 7911 (2015).

Thursday 04 April, 2019, 16:30, Room 1

Pressure dependence of the superconducting upper critical field in KFe_2As_2 and related materials

V. Taufour[1], U. Kaluarachchi[2], P. Wiecki[2], Y. Furukawa[2], N. Foroozani[3], J. S. Schilling[3], A. E. Bohmer, M. A. Tanatar[2], V. G. Kogan[2], R. Prozorov[2], T. A. Lograsso[2], S. L. Bud'ko[2], P. C. Canfield[2]

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Superconductivity in KFe_2As_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].

[1] F. F. Tafti, A. Juneau-Fecteau, M.-E. Delage, S. R. de Cotret, J.-P. Reid, A. F. Wang, X.-G. Luo, X. H. Chen, N. Doiron-Leyraud, and L. Taillefer, Nature Physics 9, 349 (2013).
[2] Valentin Taufour, Neda Foroozani, Makariy A. Tanatar, Jinhyuk Lim, Udhara Kaluarachchi, Stella K. Kim, Yong Liu, Thomas A. Lograsso, Vladimir G. Kogan, Ruslan Prozorov, Sergey L. Bud'ko, James S. Schilling, and Paul C. Canfield, "Upper critical field of KFe_2As_2 under pressure: A test for the change in the superconducting gap structure," Phys. Rev. B 89, 220509 (2014).
[3] Udhara S. Kaluarachchi, Valentin Taufour, Anna E. Bohmer, Makariy A. Tanatar, Sergey L. Bud'ko, Vladimir G. Kogan, Ruslan Prozorov, and Paul C. Canfield, "Nonmonotonic pressure evolution of the upper critical field in superconducting FeSe," Phys. Rev. B 93, 064503 (2016).
[4] Udhara S. Kaluarachchi, Valentin Taufour, Aashish Sapkota, Vladislav Borisov, Tai Kong, William R. Meier, Karunakar Kothapalli, Benjamin G. Ueland, Andreas Kreyssig, Roser Valenti, Robert J. McQueeney, Alan I. Goldman, Sergey L. Bud'ko, and Paul C. Canfield, "Pressure-induced half-collapsed-tetragonal phase in $CaKFe_4As_4$," Phys. Rev. B 96, 140501 (2017).
[5] P. Wiecki, V. Taufour, D. Y. Chung, M. G. Kanatzidis, S. L. Bud'ko, P. C. Canfield, and Y. Furukawa, "Pressure dependence of coherence-incoherence crossover behavior in KFe_2As_2 observed by resistivity and ^{75}As-NMR/NQR," Phys. Rev. B 97, 064509 (2018).

Thursday 04 April, 2019, 17:00, Room 1

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.

[1] G. Garbarino et al, Phys Rev B (R) 78, 100507 (2008)
[2] G.Garbarino et al, Phys Rev B 84, 024510 (2011)
[3] M. Mito, M. Pitcher, W. Crichton, G. Garbarino et al, J. Am. Chem. Soc 131, 2986 (2009)
[4] G. Garbarino et al, EPL 131, 2986 (2009)
[5] G. Garbarino, et al, EPL 96, 57002 (2011)

Thursday 04 April, 2019, 17:30, Room 1

Structure-property correlations in FeSe-based superconducting materials

V. Svitlyk[1], M. Raba[2], A. Krzton-Maziopa[3], D. Chernyshov[1], A. Bosak[1],E. Pomjakushina[4], K. Conder[4], V. Pomjakushin[4], V. Dmitriev[1], G. Garbarino[1], P. Toulemonde[2], P. Rodière[2] and M. Mezouar[1]

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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, *P*4/*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.

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Thursday 04 April, 2019, 18:00, Room 1

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 $Ca_{10}Pt_4As_8(Fe_2As_2)_5$ (Pt10418) and $Ca_{10}Ir_4As_8(Fe_2As_2)_5$ (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.

Thursday 04 April, 2019, 11:00, Room 2

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 3*d* 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 $NaMg_2(Si,Al)_6O_{12}$ [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.

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Thursday 04 April, 2019, 11:30, Room 2

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.

Thursday 04 April, 2019, 12:00, Room 2

Hydrogen-bearing iron peroxide in Earth's lowermost mantle

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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_2Hx (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.

Thursday 04 April, 2019, 14:00, Room 2

Mantle-Slab Interactions and Mantle Heterogeneities

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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 O2 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 valance states, ferric Fe3+ and ferrous Fe2+. 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 Fe2O3, through Fe5O7, Fe3O4, Fe4O5, Fe5O6 to the other end-member ferrous oxide FeO at the highly reducing core-mantle boundary. Interestingly, iron superoxides (FeO2Hx 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 FeO2Hx 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.

Thursday 04 April, 2019, 14:30, Room 2

Kinetics of dehydrogenation of FeOOH at Earth's lower mental conditions

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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.

Thursday 04 April, 2019, 15:00, Room 2

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 *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 *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.

Thursday 04 April, 2019, 15:30, Room 2

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, Mg_2C [1] and β-Mg_2C_3 [2], crystallizes in the monoclinic C2/m space group, and contains rare allene-derrived C_3^{4-} anions that are isoelectronic with CO_2. 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, C_3H_4, indicative of the presence of C_3^{4-} 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 Mg_2C_3 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 Mg_2C_3 structure predicted via USPEX was a perfect match to the experimental X-ray diffraction data. Thus, the structure of β-Mg_2C_3 was solved. Unlike α-Mg_2C_3, which contains alternating layers of C_3^{4-} chains oriented in opposite directions, all C_3^{4-} chains within β-Mg_2C_3 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 MgC_2, (2) orthorhombic α-Mg_2C_3, (3) monoclinic β-Mg_2C_3 [2], and (4) cubic Mg_2C [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.

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Thursday 04 April, 2019, 15:45, Room 2

Nanostructured graphene: When disorder makes things better?

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Since the discovery of fullerene C_{60} 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 C_{60} 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 C_{60} polymers during subsequent HPHT treatment. We show that mechanical properties of the NGP produced from C_{60} 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.

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Thursday 04 April, 2019, 16:30, Room 2

Reactive molecular dynamics simulations and machine learning

Priya Vashishta, Pankaj Rajak[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 tosincreasing 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 $MoSe_2$. 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.

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Thursday 04 April, 2019, 17:00, Room 2

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.

Thursday 04 April, 2019, 17:30, Room 2

The SCAN density functional and its surprising performance in complex materials

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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 Exc. 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 Exc, 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.

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Thursday 04 April, 2019, 18:00, Room 2

Emergent Spin Vortex Crystals in Frustrated Quantum Magnets

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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 $Sr_2F_2Fe_2OS_2$ and show how it can be understood as a spin vortex crystal.

April 05, 2019

Friday 05 April, 2019, 08:30, Room 1

Electron-phonon and electron-electron interactions in electron doped aromatic carbon materials viewed from electrical transport

K. Tanigaki[1,2], S. Heguri[2], Y. Matsuda[2]
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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 antracene, tetracene, pentacene, and expanded C_{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 Tc superconductivity. On the other hand, the highest superconductivity surpassing the cuprates recently found in H_2S under high pressure gives the discussion back to the electron-phonon (e-ph) mediated superconductivity for achieving extremely high T_c. Although, relatively high T_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_3C_{60} (A=alkali metals: K, Rb, Cs) superconductors with expanded cell ($V_{cell}(C_{60}{}^{3-})$) 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_3C_{60} and they are made only for K_3C_{60} and Rb_3C_{60} with small cell size far apart from the Mott boundary. Here, we give experimental results that accurate electrical resistivity (ρ(T,P)) can be achieved for a variety A_3C_{60} with expanded $V_{cell}(C_{60}{}^{3-})$ 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-$V_{cell}(C_{60}{}^{3-})$ 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_3C_{60} with a variety of cell volume controlled by chemical (stoichiometric composition of A_3C_{60}) and physical pressure. The new electronic phase is considered to have a common underlying physics among many materials having large freedom of entropy.

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Friday 05 April, 2019, 09:30, Room 1

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

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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.

Friday 05 April, 2019, 10:00, Room 1

Autocorrelation of quasiparticle spectral intensities and its connection with quasiparticle scattering interference in cuprate superconductors

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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.

[1] See, e.g. Xingjiang Zhou et al., Rep. Prog. Phys. **81**, 062101 (2018).
[2] See, e.g. A. Damascelli et al., Rev. Mod. Phys. **75**, 473 (2003).
[3] U. Chatterjee et al., Phys. Rev. Lett. **96**, 107006 (2006).
[4] S. H. Pan et al., Nature **413**, 282 (2001).
[5] Y. Kohsaka et al., Nature **454**, 1072 (2008).
[6] Deheng Gao et al., Phil. Mag. **99**, 752 (2019).
[7] Shiping Feng, Phys. Rev. B **68**, 184501 (2003); Shiping Feng et al., Physica C **436**, 14 (2006).
[8] Shiping Feng et al., Phys. Rev. B. **85**, 054509 (2012); Phys. Rev. B. **85**, 099902(E) (2012).
[9] See, e.g. Shiping Feng et al., Int. J. Mod. Phys. B **29**, 1530009 (2015).

Friday 05 April, 2019, 17:00, Room 1

Materials Informatics Approaches for the Discovery of Magnetic 2D Materials

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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.

[1] *Computational Methods for 2D Materials: Discovery, Property Characterization, and Application Design*. J. T. Paul, et al, J. Phys.: Condens. Matter 29, 473001 (2017), https://doi.org/10.1088/1361-648X/aa9305.

[2] *Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials*. M. Ashton, et al, Phys. Rev. Lett. 118, 106101 (2017), https://doi.org/10.1103/PhysRevLett.118.106101.

[3] *Grand Canonical Evolutionary Algorithm for the Prediction of Two-Dimensional Materials*. B. C. Revard, et al, Phys. Rev. B 93, 054117 (2016), http://doi.org/10.1103/PhysRevB.93.054117.

[4] *Genetic Algorithm Prediction of Two-Dimensional Group-IV Dioxides for Dielectrics*. A. K. Singh, et al, Phys. Rev. B 95, 155426 (2017), http://doi.org/10.1103/PhysRevB.95.155426.

[5] *Machine learning of ab-initio energy landscapes for crystal structure predictions*. S. Honrao, et al, Comp. Mater. Sci., in print (2018), https://doi.org/10.1016/j.commatsci.2018.08.041.

[6] *Two-Dimensional Half-Metals with Large Spin Gaps*. M. Ashton, et al, Nano Lett. 17, 5251 (2017), http://doi.org/10.1021/acs.nanolett.7b01367.

[7] *Stability and magnetism of strongly correlated single-layer* VS_2. H. L. Zhuang and R. G. Hennig, Phys. Rev. B 93, 054429 (2016), https://doi.org/10.1103/PhysRevB.93.054429.

[8] *Strong Anisotropy and Magnetostriction in 2D Stoner Ferromagnet* Fe_3GeTe_2. H. L. Zhuang, et al, Phys. Rev. B 93, 134407 (2016), http://dx.doi.org/10.1103/PhysRevB.93.134407.

Friday 05 April, 2019, 17:30, Room 1

Role of doping and defects on the electronic properties of ZnO

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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.

Friday 05 April, 2019, 18:00, Room 1

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	Mar 31-Sun		Apr 1-Mon		Apr 2-Tue	Apr 3-Wed	Apr 4- Thu		Apr 5-Fri	Apr 6-Sat
A R R I V E	**08:30-10:30** (Session-1) (S. Saxena, R. Hennig) 08:30 H.K. Mao 09:30 A.Bansil		**08:30-10:30** (Session-5A) (A. Bansil, T. Schmitt) D. Dessau M. Shi J.F. He N.L. Saini	(Session-5B) (Y. Filinchuk R. Ahuja) C. E. Buckley L. Stievano M. Heere H. Miyaoka	**08:30-10:00** (Session-8) (I. Dasgupta, N.L. Saini) X.X. Xi B.Barbiellini S.H.Lee	**08:30-09:30** (Session-10) (M. Polanski, C. E. Buckley) M. Jorgensen J. Grinderslev M. Peska J.Vodeb	**08:30-10:30** (Session-12) (C. Meingast, B. Buechner) P. Hirschfeld Y. Li R. Hackl F. Hardy		**08:30-10:30** (Session-16) (D. Louca, E. Zurek) K. Tanigaki S. Tsuchiya K. Park S. Feng	D E P R T
	10:30-11:00 Coffee Break		10:30-11:00 Coffee Break				10:30-11:00 Coffee Break			
	11:00-12:30 (Session-2A) (A. Bansil, X.X. Xi) K.Tanigaki T. Choudhury Z.Mao	(Session-2B) (H.-W. Li J. Chen) C. J. Webb J. Jensen T. R. Jensen	**11:00-12:30** (Session-6A) (S. Feng, M. Shi) D. Louca K. Kudo Y. Goto	(Session-6B) (C.E. Buckley H. Miyaoka) H. Saitoh H.-W. Li K.T. Moller	Discussions	Discussions	**11:00-12:30** (Session-13A) (P. Hirschfeld, F. Hardy) B. M. Andersen B. Buechner A. Dioguardi M. He	(Session-13B) (J. Chen, S.Saxena) Han Hsu M. Hou W.L. Mao	Discussions	
	12:30 - 14:00 Lunch Break		12:30 - 14:00 Lunch Break				12:30 - 14:00 Lunch Break			
15:00-17:00 **Registration**	**14:00-16:00** (Session-3A) (K. Tanigaki, B. Barbiellini) Qi Li L.Balicas S.Y. Matsushita I. Dasgupta	(Session-3B) (T.R. Jensen C.J. Webb) C. Zlotea K. T. Moller Y. Filinchuk _______	**14:00-16:00** (Session-7A) (Y. Ding, D. Dessau) S. Zhang M.R. Vega S. Dasgupta X. Wan	(Session-7B) (T.R. Jensen C. Zlotea) C. Pistidda D. Matsumura M. Polanski C. Wu	Discussions	Discussions	**14:00-16:00** (Session-14A) (B. M. Andersen R. Hackl) T. Shibauchi M. S. Ikeda M. Christensen C. Meingast	(Session-14B) (W.L Mao, A. L. da Rosa) Jin Liu J. Chen A. Agarwal O. Kurakevych A. Soldatov	Discussions	
	16:00-16:30 Coffee Break				16:00-16:30 Coffee Break		16:00-16:30 Coffee Break			
17:30 - 18:30 Welcome Party (Sky Lounge)	**16:30-18:30** (Session-4A) (J.Sun, J.F.He) Y. Ding T. Schmitt W.S. Kyung O. Eriksson	(Session-4B) Y. Filinchuk, D.Matsumara M. Polanski M. Heere Y. Song _______	Discussions		**16:30-18:30** (Session-9) (R. Hennig, A. Bansil) W.Pickett E. Zurek T. Shibauchi	**16:30-18:30** (Session -11) (N.L. Saini, K. Kudo) S.R. Xie P. Nautiyal J.T. Paul Posters: G.M. Pugliese, F. Stramaglia K. Shinzato K. Karczewski, T.R. Jensen	**16:30-18:30** (Session-15A) (Y. Li, T. Shibauchi) V. Taufour G. Garbarino V. Svitlyk N.L. Saini	(Session-15B) (A. Bansil, A. Hennig) P. Vashishta E. Zurek J. Sun A. Nevidomskyy	**17:00 -18:30** (Session-17) (N.L. Saini, J. Chen) R.Hennig A. L. da Rosa V. Drozd & S.Saxena Closing (Organizers & Participants	
							19:30 – 20:30 Party (Sky Lounge)			