

SYMPOSIUM CM1

Emergent Material Properties and Phase Transitions Under Pressure
April 18 - April 20, 2017

Symposium Organizers

Yue Chen, The University of Hong Kong
Thomas Hammerschmidt, Ruhr-Universität Bochum
Alexey Kolmogorov, Binghamton University
Kuo Li, Center for High Pressure Science and Technology
Advanced Research
Jung-Fu Lin, The University of Texas at Austin

Proceedings Statement

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* Invited Paper

SESSION CM1.1: Superconductivity Under Pressure
Session Chairs: Yue Chen and Jung-Fu Lin
Tuesday Morning, April 18, 2017
PCC North, 100 Level, Room 125 A

10:30 AM *CM1.1.01

Superconductivity in Topological Compounds Tuned via Pressure [Changqing Jin](#); Institute of Physics, Chinese Academy of Sciences, China.

11:00 AM CM1.1.02

Superconductivity and Unexpected Chemistry of Germanium Hydrides under Pressure [M. Mahdi Davari Esfahani](#)^{1,2}; ¹State University of New York, Stony Brook, United States; ²State University of New York, Stony Brook, United States.

11:15 AM CM1.1.03

Superconductivity of Intercalation-Type Filled Skutterudite $\text{La}_x\text{Rh}_4\text{P}_{12}$ Synthesized at High Pressures and High Temperatures [Motoharu Imai](#); National Institute for Materials Science, Japan.

11:30 AM CM1.1.04

Superconductivity and Hybrid Soft Modes in 1T-TiSe₂ [Frank Weber](#); Karlsruhe Institute of Technology, Germany.

11:45 AM CM1.1.05

A Combined Theoretical and Experimental Study on the High-Pressure Phases in the Sn-Se System [Yue Chen](#); The University of Hong Kong, Hong Kong.

SESSION CM1.2: Superhard Materials and Mechanical Behaviors
Session Chairs: Alexey Kolmogorov and Kuo Li
Tuesday Afternoon, April 18, 2017
PCC North, 100 Level, Room 125 A

1:30 PM *CM1.2.01

Novel Superhard Materials in Light Element B-C-N-O System [Duanwei He](#); Sichuan University, China.

2:00 PM CM1.2.02

A Computational Characterization of a Superhard Nanomaterial B4C [Sangil Hyun](#); Korea Institute of Ceramic Engineering & Technology, Korea (the Republic of).

2:15 PM CM1.2.03

Modelling 110 Creep in Ni-Based Superalloys [Maeva Cottura](#)^{1,2}; ¹CEA, France; ²LEM - CNRS/Onera, France.

2:30 PM *CM1.2.04

Superhard Semiconducting Phases of Transition-Metal Tetraborides under Pressure [Rajeev Ahuja](#); Uppsala University, Sweden.

3:00 PM BREAK

3:30 PM *CM1.2.05

A Statistical Learning Model for Elastic Moduli of Inorganic Compounds—Application to Discovery of New Superhard Materials [Mark Asta](#)^{1,2}; ¹University of California, Berkeley, United States; ²Lawrence Berkeley National Laboratory, United States.

4:00 PM CM1.2.06

Combined Experimental and First Principles Dft Study of the Equation of State and Vibrational Properties of Bcf₂ at 300k [Andrew V. Chizmeshya](#); Arizona State University, United States.

4:15 PM CM1.2.07

Densification and Shear Mechanisms in the Plastic Deformation of Silicate Glasses [Shefford P. Baker](#); Cornell University, United States.

4:30 PM *CM1.2.08

Giant Pressure Effect on Magnetism in Cubic Perovskite $\text{Sr}_{1-x}\text{Ba}_x\text{CoO}_3$ with Competing Magnetic Orders [Shintaro Ishiwata](#)^{1,2}; ¹University of Tokyo, Japan; ²JST-PRESTO, Japan.

SESSION CM1.3: Layered Materials and Method Developments

Session Chairs: Yue Chen and Jung-Fu Lin
Wednesday Morning, April 19, 2017
PCC North, 100 Level, Room 125 A

8:30 AM *CM1.3.01

Giant Tunability of Thermal Conductivity in Multilayer MoS₂ with Pressure [Yaguo Wang](#); The University of Texas at Austin, United States.

9:00 AM CM1.3.02

Pressure and Composition Tuning of Optical Band Gap in Monolayer Transition Metal Dichalcogenides [Joonseok Kim](#); The University of Texas at Austin, United States.

9:15 AM CM1.3.03

Atomistic Visualization of Layer-Tunnel Transition Pathways in MnO₂ [Yifei Yuan](#)^{1,2}; ¹University of Illinois at Chicago, United States; ²Argonne National Laboratory, United States.

9:30 AM *CM1.3.04

High Strain Coupled Opto-Electro-Mechanics in Layered Materials [Deji Akinwande](#); The University of Texas at Austin, United States.

10:00 AM BREAK

10:30 AM *CM1.3.05

Strain-Induced Electronic Phase Changes in Layered Materials [Abhishek K. Singh](#); Indian Institute of Science, India.

11:00 AM CM1.3.06

The SIESTA Code—Basis Set Construction Strategy [Federico Marchesin](#); Simune Atomistic Simulations, Spain.

11:15 AM CM1.3.07

A Transition in the Nature of the Electron Transport that Occurs within Wurtzite Zinc Oxide in Response to the Application of Stress And the Concomitant Potential for Electron Device Applications [Stephen K. O'Leary](#); The University of British Columbia, Canada.

11:30 AM CM1.3.08

Liquid-Liquid Transition in Ti [Byeongchan Lee](#); Kyung Hee University, Korea (the Republic of).

11:45 AM CM1.3.09

Quasi-Phase Transition of Single File Water Molecules [Xuedan Ma](#); Center for Nanoscale Materials, Argonne National Laboratory, United States.

SESSION CM1.4: Phase Transition Under Pressure
Session Chairs: Alexey Kolmogorov and Kuo Li
Wednesday Afternoon, April 19, 2017
PCC North, 100 Level, Room 125 A

1:30 PM *CM1.4.01

Single Crystal Structural Studies at Multimegabar Pressures and High Temperatures [Leonid Dubrovinsky](#); University of Bayreuth, Germany.

2:00 PM CM1.4.02

Strain Engineered Pyrochlore at High Pressure [Dylan Rittman](#); Stanford University, United States.

2:15 PM CM1.4.03

Jahn-Teller Phase Transition of Icosahedral Units Under Pressure [Seyed Hossein Nasrollahi](#); Imperial College London, United Kingdom.

2:30 PM BREAK

3:30 PM *CM1.4.04

Dirac Node Lines in Pure Rare Earth Metals [Xing-Qiu Chen](#); Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, China.

4:00 PM CM1.4.05

Graphenoid Carbons—Systematic Search, Properties and Perspectives [Stefano F. Leoni](#); Cardiff University, United Kingdom.

4:15 PM CM1.4.06

Aliphatic Layered System with Emergent Chain Melting: Phase Transition Induced by Material Segmentation [Zichao Ye](#); University of Illinois at Urbana-Champaign, United States.

4:30 PM *CM1.4.07

Adventures with 5d Orbitals at High Pressure [Daniel Haskel](#); Advanced Photon Source, Argonne National Laboratory, United States.

SESSION CM1.5: Poster Session

Session Chairs: Alexey Kolmogorov and Kuo Li
Wednesday Afternoon, April 19, 2017
8:00 PM - 10:00 PM
Sheraton, Third Level, Phoenix Ballroom

CM1.5.01

Micro-Strain Dominant Solid-Solid Phase Transition under High Pressure [Qiwei Hu](#); Sichuan University, China.

CM1.5.02

Spectroscopic Studies of the Effect of High Pressure on Poly[(R)-3-Hydroxybutyrate-Co-(R)-3-Hydroxy-Hexanoate] (PHBHx) Random Copolymers Using a Diamond Anvil Cell [Chinmay D. Pawar](#); University of Delaware, United States.

CM1.5.03

Orbital Ordering in Certain Vanadium Spinel Oxides—First-Principle Electronic and Phonon Based Approach [Dibyendu Dey](#); Indian Institute of Technology, Kharagpur, India.

SESSION CM1.6: Properties of Materials Under Pressure

Session Chairs: Yue Chen and Jung-Fu Lin
Thursday Morning, April 20, 2017
PCC North, 100 Level, Room 125 A

8:00 AM *CM1.6.01

Novel High-Pressure Phenomena Discovered through Crystal Structure Prediction [Artem Oganov](#)^{1,2}; ¹Skolkovo Institute of Science and Technology, Russian Federation; ²Stony Brook University, United States.

8:30 AM CM1.6.02

Magnetism of Transition Metals under High Pressure—Combined DFT and K-XMCD Study [Yaroslav O. Kvashnin](#); Uppsala University, Sweden.

8:45 AM CM1.6.03

Enhanced Properties of Organic-Inorganic Halide Perovskites via High Pressure Treatments [Xujie Lu](#); Los Alamos National Laboratory, United States.

9:00 AM CM1.6.04

Pressure Induced Polymerization and Enhanced Conductivity of Metal Acetylides [Kuo Li](#); Center for High Pressure Science and Technology Advanced Research, China.

9:15 AM CM1.6.05

High Pressure for Parameterization of the Proton-Phonon Coupling in Solid Electrolytes [Artur Braun](#); Empa-Swiss Federal Laboratories for Materials Science and Technology, Switzerland.

9:30 AM *CM1.6.06

High Pressure Synthesis of Polymorphic Phase of Boron Nitride—2D Wide Bandgap Nature and Superhard Materials [Takashi Taniguchi](#); National Institute for Materials Science, Japan.

10:00 AM BREAK

10:30 AM *CM1.6.07

Nanocrystalline Diamond—Unique Carbon Material for Ultra-High Pressure Generation and Optical Applications [Natalia Dubrovinskaia](#); University of Bayreuth, Germany.

11:00 AM CM1.6.08

Order Parameter Aided Efficient Phase Space Exploration under Extreme Conditions [Amit Samanta](#); Lawrence Livermore National Laboratory, United States.

11:15 AM CM1.6.09

Molecular Dynamics Studies of the Melting of Copper with Edge and Screw Dislocations at High Pressures [Clarence Matthai](#); Cardiff University, United Kingdom.

11:30 AM *CM1.6.10

Barochemistry to Multifunctional High Energy Density Solids [Choong-Shik Yoo](#); Washington State University, United States.