

## Z. Materials Simulation, Calculation and Design

**Organizers: Jijun Zhao, Jeffrey Reimers, Chun-Hway Hsueh, Cesare Franchini, Yasushi Shibuta, Gilberto Teobaldi, Xingqiu Chen, Limin Liu, Yi Liu, Guanghong Lu**

**Session Z1: Friday Afternoon, Oct. 21, 2016**

**Chairs: Yuan Ping Feng, Tomohiro Takaki**

**Room: 5601**

**13:30-14:05 Z-01(Keynote)**

**Large-scale GPU computations of dendrite growth using phase-field method**

Tomohiro Takaki<sup>1</sup>, Munekazu Ohno<sup>2</sup>, Yasushi Shibuta<sup>3</sup>, Shinji Sakane<sup>1</sup>, Takashi Shimokawabe<sup>4</sup>, Takayuki Aoki<sup>4</sup>

1. Kyoto Institute of Technology
2. Hokkaido University
3. The University of Tokyo
4. Tokyo Institute of Technology

**14:05-14:40 Z-02(Keynote)**

**Chemically selective alternatives to photoferroelectrics for polarization-enhanced photocatalysis: the untapped potential of hybrid inorganic nanotubes**

Joshua Elliott<sup>1</sup>, Emiliano Poli<sup>1</sup>, Gilberto Teobaldi<sup>2,1</sup>

1. University of Liverpool
2. Beijing Computational Science Research Centre

**14:40-15:15 Z-03(Keynote)**

**Surface adhesion and its effect on new semiconductor technologies**

Jeffrey Reimers

Shanghai University / University of Technology Sydney

**15:15-15:45 Coffee Break**

**15:45-16:20 Z-04(Keynote)**

**Interfaces of 2D materials and oxides – first-principles studies**

Yuan Ping Feng<sup>1,2\*</sup>, Ming Yang<sup>3</sup>, Ting Ting Song<sup>4</sup>, Martin Callsen<sup>1</sup>, Shijie Wang<sup>3</sup>

1. Department of Physics, National University of

Singapore, Singapore

2. Centre for Advanced 2D Materials, National University of Singapore, Singapore

3. Institute of Materials Research and Engineering, A\*STAR, Singapore

4. Institute for Structure and Function and Department of Physics, Chongqing University, China

**16:20-16:55 Z-05(Keynote)**

**Computational discovery and design of 2D materials for energy and electronics application**

Aijun Du

Queensland University of Technology

**16:55-17:30 Z-06(Keynote)**

**Analytical modeling of steady-state interface fracture of elastic multilayered beams subjected to four-point bending**

Chun-Hway Hsueh

National Taiwan University

**Session Z2: Saturday Morning, Oct. 22, 2016**

**Chairs: Liming Liu, Xing-Qiu Chen**

**Room: 5601**

**08:30-09:05 Z-07(Keynote)**

**Grand design of new electronic materials and properties**

Xiaolin Wang

University of Wollongong, Australia

**09:05-09:40 Z-08(Keynote)**

**Topological semimetals: materials prediction by first-principles calculations**

Hongming Weng

Institute of Physics, Chinese Academy of Sciences

**09:40-10:15 Z-09(Keynote)**

**Computational materials design: from a simple**

**chemical concept to 3D topological materials**

Xing-Qiu Chen  
Shenyang National Laboratory for Materials Sciences,  
Institute of Metal Research, Chinese Academy of  
Sciences

**10:15-10:45 Coffee Break**

**10:45-11:20 Z-10(Keynote)**

**Integrated microstructure modeling during transformation and deformation**

Yunzhi Wang  
The Ohio State University / Xian Jiao Tong University

**11:20-11:55 Z-11(Keynote)**

**Stability analysis of NdFe12-based compounds as promising high performance permanent magnet materials**

Ying Chen  
Tohoku University

**Session Z3: Saturday Afternoon, Oct. 22, 2016**

**Chairs: Yi Liu, Menno Bokdam**

**Room: 5601**

**13:30-13:50 Z-12(Invited)**

**Role of polar phonons in the photo excited state of metal halide perovskites**

Menno Bokdam<sup>1\*</sup>, Tobias Sander<sup>1</sup>, Alessandro Stroppa<sup>2</sup>, Silvia Picozzi<sup>2</sup>, D.D. Sarma<sup>3</sup>, Cesare Franchini<sup>1</sup>, Georg Kresse<sup>1</sup>

1. University of Vienna, Faculty of Physics, Computational Materials Physics
2. Consiglio Nazionale delle Ricerche - CNR-SPIN, LAquila, Italy
3. Indian Institute of Science, Solid State and Structural Chemistry Unit, Bangalore, India

**13:50-14:10 Z-13(Invited)**

**Microscopic model study of strongly correlated 5d transition metal Ir oxides**

Seiji Yunoki  
RIKEN

**14:10-14:30 Z-14(Invited)**

**Origin of the metal-insulator transition of indium atom wires on Si(111)**

Jun-Hyung Cho  
Department of Physics, Hanyang University, Seoul, Korea

**14:30-14:45 Z-15**

**Jahn-Teller distortion in LiMn2O4 and its effect on the lithiation process**

Weiwei Liu<sup>1</sup>, Da Wang<sup>1</sup>, Limin Liu<sup>1</sup>, Woon-Ming Lau<sup>1</sup>, Yanning Zhang<sup>2</sup>

1. Beijing Computational Science Research Center
2. Chengdu Science and Technology Development Center of CAEP

**14:45-15:15 Coffee Break**

**15:15-15:35 Z-16(Invited)**

**Two-dimensional materials goes to binary: Dirac cone formation in  $A_xB_{4-x}$  (A, B = C, Si, Ge, x = 1, 3)**

Xuming Qin<sup>1</sup>, Yi Liu<sup>1</sup>, Baoqian Chi<sup>1</sup>, Xinluo Zhao<sup>1</sup>, Xiaowu Li<sup>3</sup>

1. Department of Physics and International Centre for Quantum and Molecular Structures, Shanghai University
2. Materials Genome Institute, Shanghai University
3. Institute of Materials Physics and Chemistry, School of Materials Science and Engineering, Northeastern University

**15:35-15:55 Z-17(Invited)**

**The role of Hubbard, dispersion and O2 overbinding corrections for  $\alpha$ -Fe2O3 surface energy, magnetic ordering and band alignment**

Bandaru Sateesh  
Beijing Computational Science Research Center

**15:55-16:15 Z-18(Invited)**

**Manipulating topological phases in honeycomb structure**

Feng-Chuan Chuang  
National Sun Yat-sen University

**16:15-16:30 Z-19**

**Localized excitation of Ti<sup>3+</sup> ions in the photoabsorption and photocatalytic activity of reduced rutile TiO<sub>2</sub>**

Bo Wen<sup>1</sup>, Zhiqiang Wang<sup>2,4</sup>, Quanqing Hao<sup>1</sup>, Li-min Liu<sup>1</sup>, Chuanyao Zhou<sup>1</sup>, Annabella Selloni<sup>3</sup>, Xueming Yang<sup>1</sup>

1. Dalian Institute of Chemical Physics, Chinese Academy of Science
2. Beijing Computational Science Research Center
3. Princeton University
4. ICQM, Peking University

**16:30-18:00 Poster Session**

**Session Z4: Saturday Afternoon, Oct. 22, 2016**

**Chairs: Yunche Wang, Munekazu Ohno**

**Room: 7109**

**13:30-13:50 Z-20(Invited)**

**Quantitative phase-field modeling and simulations of competitive growth of dendrites in alloy systems**

Munekazu Ohno<sup>1\*</sup>, Tomohiro Takaki<sup>2</sup>, asushi Shibuta<sup>3</sup>

1. Hokkaido University
2. Kyoto Institute of Technology
3. The University of Tokyo

**13:50-14:10 Z-21(Invited)**

**A quantitative and efficient phase-field model with finite interface dissipation and its application in materials science**

Lijun Zhang

State Key Lab of Powder Metallurgy, Central South University

**14:10-14:30 Z-22(Invited)**

**Prediction of the equivalent elastic modulus of mush zone during solidification process coupled with phase field simulations**

Ruijie Zhang, Pingping Ma, Xuanhui Qu

University of Science and Technology Beijing, Beijing 100083, People's Republic of China

**14:30-14:50 Z-23(Invited)**

**Irradiation-induced void evolution in iron: a phase-field approach**

Yuanyuan Wang<sup>1</sup>, Jianhua Ding<sup>1</sup>, Wenbo Liu<sup>2</sup>, Jijun Zhao<sup>1</sup>, Chi Zhang<sup>3</sup>

1. Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Ministry of Education), Dalian University of Technology, Dalian 116024, China
2. Department of Nuclear Science and Technology, Xi'an Jiaotong University, Xi'an 710049, China
3. Key Laboratory of Advanced Materials of Ministry of Education, School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

**14:50-15:20 Coffee Break**

**15:20-15:40 Z-24(Invited)**

**Design considerations of negative-stiffness composite materials for extreme viscoelastic and coupled-field properties**

Yunche Wang, Meng-Wei Shen

National Cheng Kung University

**15:40-16:00 Z-25(Invited)**

**Nanoscaled martensitic transition and its abnormal properties in shape memory alloys**

Dong Wang<sup>1</sup>, Yunzhi Wang<sup>1,2</sup>

1. Xi'an Jiaotong University
2. The Ohio State University

**16:00-16:15 Z-26**

**Finite element analysis of the tensile properties of triangular unit cell lattice structure based on selective laser melting process**

Jie Niu<sup>1</sup>, Huileng Choo<sup>1</sup>, Wei Sun<sup>2</sup>, Edwin Mok<sup>3</sup>

1. University of Nottingham, Ningbo, China
2. University of Nottingham, Nottingham, UK
3. SLM Solutions Singapore Pte Ltd

**16:15-16:30 Z-27**

**Self-healing properties of nanocrystalline materials: a first-principles analysis of the role of grain boundaries**

Jian Xu<sup>1</sup>, Jian-Bo Liu<sup>1</sup>, Shun-Ning Li<sup>1</sup>, Bai-Xin Liu<sup>1</sup>, Yong Jiang<sup>2,3</sup>

1. Key Laboratory of Advanced Materials (MOE), School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

2. Key Laboratory of Nonferrous Materials (MOE), School of Materials Science and Engineering, Central South University, Changsha, 410083, China

3. Shenzhen Research Institute of Central South University, Shenzhen 518057, China

**16:30-18:00 Poster Session**

**Session Z5: Sunday Morning, Oct. 23, 2016**

**Chairs: Xiaoli Fan, Shiyu Chen**

**Room: 5601**

**08:30-08:50 Z-28(Invited)**

**Theoretical study on ternary and quaternary semiconductors: chemical stability, defects and dopants**

Shiyu Chen

Key Laboratory of Polar Materials and Devices (MOE), East China Normal University, Shanghai 200241, China

**08:50-09:10 Z-29(Invited)**

**Two dimensional antiferromagnetic Chern insulator: NiRuCl<sub>6</sub>**

Lizhong Sun, Pan Zhou, Changqing Sun  
Xiangtan University

**09:10-09:30 Z-30(Invited)**

**Orbital-lattice design for novel electronic devices and topological quantum phases based on conventional semiconductor surface**

Miao Zhou

Chongqing University

**09:30-09:50 Z-31(Invited)**

**RESCU: An electronic structure method for large systems**

Vincent Michaud-Rioux<sup>1</sup>, Lei Zhang<sup>1,2,3</sup>, Hong Guo<sup>1</sup>

1. Department of Physics, McGill University,

Montreal, QC H3A 2T8 Canada

2. Department of Physics, The University of Hong Kong, Hong Kong

3. State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Laser Spectroscopy, Shanxi University

**09:50-10:05 Z-32**

**Phase equilibria study of BaO-In<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> system in B<sub>2</sub>O<sub>3</sub>-rich corner**

Xing Fan, Liumei Su, Gemei Cai, Huashan

Liu, Zhanpeng Jin

School of Materials Science and Engineering, Central South University, Changsha, China

**10:05-10:30 Coffee Break**

**10:30-10:50 Z-33(Invited)**

**Single-layer MS<sub>2</sub> nanoclusters: periodical structure and electronic property**

Xiaoli Fan, Yurong An

School of Materials Science and Engineering, State Key Laboratory of Solidification Processing, Northwestern Polytechnical University

**10:50-11:10 Z-34(Invited)**

**Room-temperature ordered spin structures in cluster-assembled single V@Si<sub>12</sub> sheets**

Zhifeng Liu<sup>1</sup>, Xinqiang Wang<sup>1</sup>, Jiangtao Cai<sup>3</sup>, Hengjiang Zhu<sup>4</sup>

1. School of Physical Science and Technology, Inner Mongolia University

2. College of Physics, Chongqing University

3. School of Science, Shaanxi University Science & Technology

4. College of Physics and Electronic Engineering, Xinjiang Normal University

**11:10-11:30 Z-35(Invited)**

**Thermoelectric properties of SnSe: understanding and pressure tuning**

Yongsheng Zhang

Institute of Solid State Physics, Chinese Academy of Sciences

**11:30-11:45 Z-36**

**The correlation between uniaxial negative thermal expansion and negative linear compressibility in Ag<sub>3</sub>[Co(CN)<sub>6</sub>]**

Lei Wang, Cong Wang, Ying Sun  
Beihang University

**11:45-12:00 Z-37**

**Effects of doping atom on the structural stability, mechanical and electronic structure of Mg<sub>2</sub>Sn phases from first-principles calculations**

Zhipeng Lu<sup>1</sup>, Hui Ren<sup>1</sup>, De-Jiang Li<sup>2</sup>, Xiao-Qin Zeng<sup>3</sup>, Yong Liu<sup>1</sup>

1. Key Laboratory of Near Net Forming of Jiangxi Province, Nanchang University, China
2. National Engineering research center of Light Alloys Net Forming, Shanghai Jiao Tong University, China
3. State Key Laboratory of Metal Matrix Composite, Shanghai Jiao Tong University, China

**Session Z6: Sunday Afternoon, Oct. 23, 2016**

**Chairs: Bingyun Ao, Zhimei Sun**

**Room: 5601**

**13:30-13:50 Z-38(Invited)**

**First principles investigations of two-dimensional transition metal carbides (MXenes)**

Zhimei Sun, Zhonglu Guo, Chen Si, Jian Zhou  
Beihang University

**13:50-14:10 Z-39(Invited)**

**Growth, defects, oxidization, metal intercalation, and substrate effects of silicene**

Jijun Zhao  
Dalian University of Technology

**14:10-14:30 Z-40(Invited)**

**The stability, edge reconstruction, and substrate selection of black phosphorene**

Junfeng Gao, Gang Zhang, Yong-Wei Zhang  
Institute of High Performance Computing, A\*STAR

**14:30-14:50 Z-41(Invited)**

**Two-dimensional B-C-O alloy for electronics**

Si Zhou, Jijun Zhao  
Key Laboratory of Materials Modification by Laser, Ion and Electron Beams, Dalian University of Technology

**14:50-15:10 Z-42(Invited)**

**Iron carbides across dimensionality**

Xiaodong Wen  
1. Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, PR China  
2. Synfuels China, Beijing, 100195 PR China.

**15:10-15:30 Z-43(Invited)**

**Single-spin manipulation by electric fields and adsorption of molecules**

Kun Tao  
Key Lab for Magnetism and Magnetic Materials of Ministry of Education, Lanzhou University, China

**15:30-16:00 Coffee Break**

**16:00-16:20 Z-44(Invited)**

**Application of first-principles computation on lithium-sulfur battery cathode design**

Qianfan Zhang  
Beihang University

**16:20-16:40 Z-45(Invited)**

**Regulating mechanisms of electrochemical and chemical reactions in metal-oxygen and Li-ion batteries**

Jianjun Liu  
Shanghai Institute of Ceramics, Chinese Academy of Sciences

**16:40-17:00 Z-46(Invited)**

**Electronic structure calculations on the energetics of impurity atoms in plutonium oxides**

Bingyun Ao  
Institute of Materials, China Academy of Engineering Physics

**17:00-17:15 Z-47**

**Pressure-driven 4f localized-itinerant transition in heavy fermion compound CeIn<sub>3</sub>: A first-principles many-body perspective**

Haiyan Lu<sup>1</sup>, Li Huang<sup>2</sup>, Xi Dai<sup>1</sup>

1. Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences
2. Institute of Materials, China Academy of Engineering Physics

**17:15-17:30 Z-48**

**Density-functional study of plutonium monoxide monohydride**

Ruizhi Qiu

Institute of Materials, China Academy of Engineering Science

**17:30-17:45 Z-49**

**Effects of Cr on the properties of WCoB ternary boride**

Tong Zhang<sup>1,2</sup>, Haiqing Yin<sup>1,2</sup>, Xuanhui Qu<sup>1,2</sup>, Qingjun Zheng<sup>3</sup>

1. Collaborative Innovation Center of Steel Technology, University of Science and Technology Beijing, Beijing 100083, China
2. Beijing Key Laboratory of Materials Genome Initiative, University of Science and Technology Beijing, Beijing 100083, China
3. Kennametal Inc, 1600 Technology Way, PA 15650, USA

**17:45-18:00 Z-50**

**Molecular dynamics study of the orientation effect in magnesium**

Qun Zu, Ya-Fang Guo

Beijing Jiaotong University

**Session Z7: Sunday Morning, Oct. 23, 2016**

**Chairs: Xiongjun Liu, Haiqing Yin**

**Room: 7109**

**08:30-08:50 Z-51(Invited)**

**Materials data science, a paradigm for material discovery and innovation**

Haiqing Yin, Xue Jiang, Ruijie Zhang, Guoquan Liu, Xuanhui Qu

University of Science and Technology Beijing

**08:50-09:10 Z-52(Invited)**

**Cooperative effect of silicon and other alloying elements on creep resistance of titanium alloys: insight from first-principles calculations**

Qing-Miao Hu<sup>1</sup>, Yang Li<sup>1</sup>, Yue Chen<sup>2</sup>, Jian-Rong Liu<sup>1</sup>, Rui Yang<sup>1</sup>

1. Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China
2. Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR

**09:10-09:30 Z-53(Invited)**

**The atomistic study on shape memory properties of Ni-Ti alloys**

I-Ling Chang, Wei-Chi Hung

National Cheng Kung University

**09:30-09:45 Z-54**

**Investigation of the phase equilibria and micro-performance of the Ti-Ni-Hf system using diffusion triples**

Junlei Liu<sup>1</sup>, Lilong Zhu<sup>2</sup>, Gemei Cai<sup>1</sup>

1. School of Materials Science and Engineering, Central South University, Changsha, Hunan 410083, PR China
2. State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, PR China

**09:45-10:00 Z-55**

**Orientation-dependent nanoscale abrasive wear of mono-crystalline silicon**

Jing Han<sup>1</sup>, Jiapeng Sun<sup>2</sup>, Hua Zhu<sup>1</sup>, Liang Fang<sup>3</sup>

1. School of Mechanical and Electrical Engineering, China University of Mining and Technology, Xuzhou 221116, Jiangsu Province, PR China
2. College of Mechanics and Materials, Hohai University, Nanjing 210098, PR China
3. State Key Laboratory for Mechanical Behavior of

Materials, Xi'an Jiaotong University, Xi'an 710049, Shaanxi Province, PR China

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

**10:30-10:50 Z-56(Invited)**

**Structural and mechanical heterogeneities in metallic glasses**

Xiongjun Liu, Huiyang Fan, Leqing Liu, Hui

Wang, Yuan Wu, Zhaoping Lu

State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, P. R. China

**10:50-11:10 Z-57(Invited)**

**Formation mechanism and interface strength of superhard nanocomposites**

Ruifeng Zhang

Beihang University

**11:10-11:25 Z-58**

**Strengthening effects of single particles with different mechanical property in ultra-thin Rolling of AA1235 aluminum alloys**

Chengwei Xia, Yuanzhi Zhu, Weilong Fan, Xiaohui Li  
North China University of Technology

**11:25-11:40 Z-59**

**Characterization of anisotropic mechanical behavior of AZ31 Mg alloy under non-proportional loading by means of crystal plasticity modeling**

Chong Yang<sup>1</sup>, Yan Peng<sup>1</sup>, Fusheng Pan<sup>2</sup>, Baodong Shi<sup>1</sup>

1. National Engineering Research Center for Equipment and Technology of Cold strip Rolling, College of Mechanical Engineering, Yanshan University, Qinhuangdao, Hebei, PR China

2. National Engineering Research Center for Magnesium Alloys, Chongqing University, Chongqing, PR China

**11:40-11:55 Z-60**

**Thermodynamic calculation of the liquidus surface projection of multi-component aluminum alloys**

Jingrui Zhao<sup>1,2</sup>, Yong Du<sup>2</sup>, Lijun Zhang<sup>2</sup>, Jixue

Zhou<sup>1</sup>, Yuansheng Yang<sup>1,3</sup>

1. Advanced Materials Institute, Shandong Key Laboratory for High Strength Lightweight Metallic Materials (HLM), Shandong Engineering Research Center for Lightweight Automobiles Magnesium Alloy, Shandong Academy of Sciences, Jinan 250014, China

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3. Institute of Metal Research, Chinese Academy of Sciences. Shenyang 110016, China

**Session Z8: Sunday Afternoon, Oct. 23, 2016**

**Chairs: Qing-Miao Hu, Hongxian Xie**

**Room: 7109**

**13:30-13:50 Z-61(Invited)**

**An atomic-scale study of the Fe-Li solid/liquid interface properties**

Xianglai Gan<sup>1</sup>, Huiqiu Deng<sup>2</sup>, Shifang Xiao<sup>2</sup>, Xiaofan Li<sup>2</sup>, Wangyu Hu<sup>1</sup>

1. College of Materials Science and Engineering, Hunan University, Changsha 410082, China

2. Department of Applied Physics, School of Physics and Electronics, Hunan University, Changsha 410082, China

**13:50-14:10 Z-62(Invited)**

**Effect of WC/Co coherency phase boundaries on Fracture toughness of the nanocrystalline cemented carbides**

Hongxian Xie

Hebei University of Technology (HBUT)

**14:10-14:30 Z-63(Invited)**

**Diffusion kinetics of Ni-Co-based alloys and mobility databases**

Xiao-Gang Lu

Shanghai University

**14:30-14:50 Z-64(Invited)**

**Ab initio investigation on engineering alloys**

Hualei Zhang

Center of Microstructure Science, Frontier Institute of

Science and Technology, Xi'an Jiaotong University,  
Xi'an, 710054, China

**14:50-15:05 Z-65**

**A front-tracking solidification model for simulation of microstructure evolution during multi-component alloy solidification**

Guanyu Yi<sup>1</sup>, Zhongkui Zhao<sup>2,1</sup>, Bozu Liu<sup>2,2</sup>

1. Advanced Materials Institute of Shandong Academy of Sciences
2. Shandong Jianzhu University

**15:05-15:20 Z-66**

**Dynamics of phase separation in Fe-Cr alloys with variational coarsening mechanisms**

Yongsheng Li, Haojie Mei, Zhilong Yan

Nanjing University of Science and Technology

**15:20-15:35 Z-67**

**Mapping of possible Re-substitutional elements in Ni-based superalloys**

Juan Chen, Jing Zhong, Lijun Zhang

State Key Laboratory of Powder Metallurgy, Central South University, Changsha, 410083, China

**15:35-16:00 Coffee Break**

**16:00-16:15 Z-68**

**Study of laser-induced damage resistance of PVA film using numerical stimulation and experimental measurements**

Changpeng Li, Shufan Chen, Xuan Luo, Xiaodong Jiang, Weidong Wu

Research Center of Laser Fusion, China Academy of Engineering Physics

**16:15-16:30 Z-69**

**Effects of temperature on vibration-assisted nano-scratch of monocrystalline copper via molecular dynamics simulation**

Bo Zhu, Dan Zhao, Hongwei Zhao

School of Mechanical Science and Engineering, Jilin University, 5988 Renmin Street, Changchun, Jilin 130022, China

**16:30-16:45 Z-70**

**Simulating the plastic deformation of amorphous and crystalline solids at experimentally relevant timescales**

Yun-Jiang Wang<sup>1</sup>, Junping Du<sup>2</sup>, Shigenobu Ogata<sup>2,3</sup>, Lanhong Dai<sup>1</sup>

1. State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China
2. Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Sakyo, Kyoto 606-8501, Japan
3. Graduate School of Engineering Science, Osaka University, Osaka 560-8531, Japan

**16:45-17:00 Z-71**

**A viewpoint of the yield criterion of amorphous alloy powders**

Xinxin Li, Chao Yang

National Engineering Research Center of Near-net-shape Forming for Metallic Materials, South China University of Technology, Guangzhou 510640, China

**17:00-17:15 Z-72**

**Investigation of temperature effect on nanoindentation behavior of metallic glass via molecular dynamics simulation**

Dan Zhao, Bo Zhu, Hongwei Zhao

School of Mechanical Science and Engineering, Jilin University, 5988 Renmin Street, Changchun, Jilin 130022, China

**17:15-17:30 Z-73**

**Degenerate seaweed to tilted dendrite transition in directional solidification: insights from phase-field simulations**

Hui Xing

Northwestern Polytechnical University

**17:30-17:45 Z-74**

**Modeling the massive-diffusive transition in multi-component substitutional alloys**

Wangwang Kuang, Haifeng Wang, Feng Liu



State Key Laboratory of Solidification Processing,  
Northwestern Polytechnical University

**17:45-18:00 Z-75**

**The numerical simulation of hot die forging process of Ti-6Al-4V alloy blade**

Jiahao Chen<sup>1</sup>, Jinshan Li<sup>1</sup>, Bin Tang<sup>1</sup>, Lihua Du<sup>2</sup>, Hongchao Kou<sup>1</sup>

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**Session Z9: Monday Morning, Oct. 24, 2016**

**Chair: Jijun Zhao**

**Room: 5601**

**08:30-08:50 Z-76(Invited)**

**Ab initio calculations of second-, third-, and fourth-order partial and inner elastic constants of diamond**

Hao Wang<sup>1</sup>, Zhukun Zhou<sup>2</sup>, Mo Li<sup>2,3</sup>

1. College of Mechatronics and Control Engineering, Shenzhen University

2. State Key Laboratory of Powder Metallurgy, Central South University

3. School of Materials Science and Engineering, Georgia Institute of Technology

**08:50-09:10 Z-77(Invited)**

**The design of HEDM and novel electronic phenomena under high pressures**

Xiaoli Wang, Jianfu Li

Institute of Condensed Matter Physics, Linyi University

**09:10-09:25 Z-78**

**Adsorbates induced work function change of metal and alloy surface: linking theoretical modeling to the electrochemical environment**

Quanxi Zhu, Shaoqing Wang

Shenyang National Laboratory for Materials Science,

Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, PR China

**09:25-09:40 Z-79**

**Investigation on change of NaCl properties in external electric field**

Xinyu Lv, Jun Wang, Anping Dong, Yongbing Dai, Da Shu, Baode Sun

Shanghai Jiao Tong University

**09:40-09:55 Z-80**

**The two-step growth pathway to crystallization in a supercooled NiAl alloy**

Simin An, Jiahao Li, Yang Li, Shunning Li, Qi Wang

Tsinghua University

**09:55-10:10 Z-81**

**Liquid/substrate interface in the heterogeneous nucleation during grain refinement of Al alloys**

Yanfeng Han, Jun Xu, Hanlong Zhang, Jiao Zhang, Yongbing Dai, Baode Sun

Shanghai Jiao Tong University

**10:20-11:00 Award Ceremony(Room 5601)**

**Session Z10: Monday Morning, Oct. 24, 2016**

**Chair: Junfeng Gao**

**Room: 7109**

**08:30-08:50 Z-82(Invited)**

**Rate theory model for the radiation-induced swelling in RAFM steels and implications for the radiation resistant design**

Mingjie Zheng, Jiawei Fu, Man Jiang, Wenyi Ding, Jingping Xin, Shenyang Hu, Qunying Huang

Key Laboratory of Neutronics and Radiation Safety, Institute of Nuclear Energy Safety Technology, Chinese Academy of Sciences

**08:50-09:05 Z-83**

**A description of the formation of vacancy on grain boundaries in copper by structure unit model**

Ke Tong, Fei Ye

Dalian University of Technology

**09:05-09:20 Z-84**

**Simulation of hydrogen clustering behaviors on tungsten surface**

Jiannan Hao<sup>1,2</sup>, Shuo Jin<sup>1,2</sup>, Xiaolin Shu<sup>1,2</sup>, Lifang Wang<sup>1,2</sup>, Guang-Hong Lu<sup>1,2</sup>

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2. Beijing Key Laboratory of Advanced Nuclear Materials and Physics, Beihang University, Beijing 100191, China

**09:20-09:35 Z-85**

**Atomistic simulations of screw dislocations in bcc tungsten: from core structures and static properties to interaction with vacancies**

Ke Xu<sup>1,2</sup>, Liang-Liang Niu<sup>1,2,3</sup>, Shuo Jin<sup>1,2</sup>, Xiaolin Shu<sup>1,2</sup>, Hongxian Xie<sup>4</sup>, Lifang Wang<sup>1,2</sup>, Guang-Hong Lu<sup>1,2</sup>

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3. Department of Nuclear Engineering and Radiological Science, University of Michigan, Ann Arbor, MI 48109, USA
4. School of Mechanical Engineering, Hebei University of Technology, Tianjin 300132, China

**9:35-9:50 Z-86**

**Modeling the plastic deformation behavior of polycrystalline ferritic stainless steel using CPFEM**

Chi Zhang, Liwen Zhang, Wenfei Shen, Qianhong Xu  
School of Materials Science and Engineering, Dalian University of Technology, Dalian, 116024, Liaoning, China

**9:50-10:05 Z-87**

**A high-throughput approach to establish the atomic mobility database in multicomponent alloys**

Jing Zhong, Lijun Zhang  
State Key Lab of Powder Metallurgy, Central South

University, Changsha, 410083, China

**10:20-11:00 Award Ceremony(Room 5601)**

**Poster**

**Z-P01**

**First-principles study of lead iodide perovskite tetragonal and orthorhombic phases for photovoltaics**

Wei Geng, Le Zhang, Yanning Zhang, Limin Liu, Woonming Lau

Beijing Computational Science Research Centre

**Z-P02**

**Two-dimensional thermoelectric materials from high-throughput screening**

Xi Zhao, Ruizhi Zhang

School of Physics, Northwest University

**Z-P03**

**Application of thermodynamic extremal principles to phase-field modeling of rapid solidification of multi-component alloys**

Xiao Zhang, Haifeng Wang, Jianbao

Zhang, Wangwang Kuang, Feng Liu

State Key Laboratory of Solidification Processing, Northwestern Polytechnical University

**Z-P04**

**Experiment and simulation study of temperature field of jominy test of 7055 aluminum alloy**

Dengyu Gai<sup>1</sup>, Yang Sun<sup>1</sup>, Yafan Li<sup>2</sup>

1. Material Science and Chemical Engineering College, Harbin Engineering University, Harbin 150001, China

2. Harbin Electric Equipment Company Limited, Harbin 150040, China

**Z-P05**

**Texture grain growth of a 95% alumina ceramic in surface and multiphase-field study**

Jishi Du, Binghua Tang, Yangjun Lei

Institute of Electronic Engineering, China Academy of Engineering Physics

#### **Z-P06**

##### **Micromagnetic simulation of a new L10-FePt/X exchange coupled structure with low coercivity and high remanent magnetization**

Haipeng Lu<sup>1,2</sup>, Zhihua Hou<sup>1,2</sup>, Xin Wang<sup>1,2</sup>, Mei Bi<sup>1,2</sup>, Li Zhang<sup>1,2</sup>, Longjiang Deng<sup>1,2</sup>

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2. State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, Chengdu 610054, China

#### **Z-P07**

##### **First-principles calculations on interfaces between Al and AlB<sub>2</sub>-type transition metal diborides**

Jun Xu, Yanfeng Han, Yongbing Dai, Jiao Zhang, Baode Sun

#### **Z-P08**

##### **Characterization of anisotropy of AZ31 Mg alloy based on molecular dynamics**

Chong Yang, Yan Peng, Jianliang Sun, Baodong Shi  
National Engineering Research Center for Equipment and Technology of Cold strip Rolling, College of Mechanical Engineering, Yanshan University, Qinhuangdao 066004, Hebei, PR China

#### **Z-P09**

##### **First principles study of the phase stability Pt-Ir-Y Intermetallics**

Yuanyuan Kong, Yong Sun, Yonghua Duan  
School of Material Science and Engineering, Kunming University of Science and Technology, 253 Xuefu Road, Kunming 650093, China

#### **Z-P10**

##### **Phase stability of Ti-Mo alloys with low Mo content**

Mingjia Li, Xiaohua Min, Fei Ye, Congqian Cheng, Jie Zhao

School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, Liaoning, China

#### **Z-P11**

##### **Theoretical design and computational screening of precursors for atomic layer deposition**

Guoyong Fang  
Wenzhou University

#### **Z-P12**

##### **Design of 2D organic materials for photocatalyst and magnetic storage device**

Xue Jiang, Peng Wang, Jijun Zhao  
Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Ministry of Education), Dalian University of Technology, Dalian, 116024, China

#### **Z-P13**

##### **Ab initio study of the surface energy and the point defect of $\beta$ -SiC**

Dan Sun, Jijun Zhao  
Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Ministry of Education), Dalian University of Technology, Dalian, 116024, China

#### **Z-P14**

##### **Effects of interstitial nitrogen atoms on atomic oxygen adsorption on Fe (001) surface from ab initio calculations**

Yakun Wang, Fei Ye  
Dalian University of Technology, School of Materials Science and Engineering

#### **Z-P15**

##### **Effects of uniaxial strain on the structure evolution of vacancy clusters in FCC metals**

Hongbo Xv, Fei Ye  
School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, China.

#### **Z-P16**

**Stacking sequence dominated stability and strength of ultraincompressible tungsten carbides**

Zhijie He, Zhongheng Fu, Ruifeng Zhang  
School of Materials Science and Engineering, Beihang University, Beijing 100191, P. R. China; Center for Integrated Computational Engineering, International Research Institute for Multidisciplinary Science, Beihang University, Beijing 100191, P. R. China

**Z-P17**

**Roles of surface functional group on mechanical strength of two-dimensional titanium carbide**

Zhongheng Fu, Q. F. Zhang, C. Si, Ruifeng Zhang  
School of Materials Science and Engineering, Beihang University, Beijing 100191, P. R. China; Center for Integrated Computational Engineering, International Research Institute for Multidisciplinary Science, Beihang University, Beijing 100191, P. R. China

**Z-P18**

**Investigation of precipitation kinetics in binary Fe–Cu and ternary Fe–Cu–Ni alloys via kMC method**

Yi Wang<sup>1</sup>, Huaiyu Hou<sup>1</sup>, Xiangbing Liu<sup>2</sup>, Rongshan Wang<sup>2</sup>, Jingtao Wang<sup>1</sup>

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