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\textsuperscript{1}, Munekazu Ohno\textsuperscript{2}, Yasushi Shibuta\textsuperscript{3}, Shinji Sakane\textsuperscript{4}, Takashi Shimokawabe\textsuperscript{4}, Takayuki Aoki\textsuperscript{4}
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\textsuperscript{1}, Emiliano Poli\textsuperscript{1}, Gilberto Teobaldi\textsuperscript{2,1}
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\textsuperscript{1,2*,} Ming Yang\textsuperscript{3}, Ting Ting Song\textsuperscript{3}, Martin Callsen\textsuperscript{1}, Shijie Wang\textsuperscript{3}
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 Bokdam¹, Tobias Sander¹, Alessandro Stroppa², Silvia Picozzi², D.D. Sarma³, Cesare Franchini¹, Georg Kresse¹
1. University of Vienna, Faculty of Physics, Computational Materials Physics
2. Consiglio Nazionale delle Ricerche - CNR-SPIN, L'Aquila, 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 Liu¹, Da Wang¹, Limin Liu¹, Woon-Ming Lau¹, Yanning Zhang²
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 AxB4-x (A, B = C, Si, Ge, x = 1, 3)
Xuming Qin¹, Yi Liu¹, Baoqian Chi¹, Xinluo Zhao¹, Xiaowu Li³
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 α-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 Ti3+ ions in the photoabsorption and photocatalytic activity of reduced rutile TiO2
Bo Wen1, Zhiqiang Wang2,4, Quanqing Hao1, Li-min Liu1, Chuanyao Zhou1, Annabella Selloni1, Xueming Yang1
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

13:30-13:50 Z-20(Invited)
Quantitative phase-field modeling and simulations of competitive growth of dendrites in alloy systems
Munekazu Ohno1*, Tomohiro Takaki2, asushi Shibuta3
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

14:50-15:20 Coffee Break

15:20-15:40 Z-24(Invited)
Irradiation-induced void evolution in iron: a phase-field approach
Yuanyuan Wang1, Jianhua Ding1, Wenbo Liu2, Jijun Zhao1, Chi Zhang3
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

15:40-16:00 Z-25(Invited)
Nanoscaled martensitic transition and its abnormal properties in shape memory alloys
Dong Wang1, Yunzhi Wang1,2
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 Niu1, Huileng Choo1, Wei Sun2, Edwin Mok3
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
16:30-18:00  Poster Session

Session Z5: Sunday Morning, Oct. 23, 2016
Chairs: Xiaoli Fan, Shiyou Chen
Room: 5601

08:30-08:50    Z-28(Invited)
Theoretical study on ternary and quaternary semiconductors: chemical stability, defects and dopants
Shiyou 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: NiRuCl6
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-Rioux¹, Lei Zhang¹,²,³, Hong Guo¹
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-In2O3-B2O3 system in B2O3-rich corner
Xing Fan, Liumei Su, Gemi 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 MS2 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@Si12 sheets
Zhifeng Liu¹, Xinqiang Wang¹, Jiangtao Cai³, Hengjiang Zhu¹
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 Ag3[Co(CN)6]  
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 Mg2Sn phases from first-principles calculations  
Zhipeng Lu1, Hui Ren1, De-Jiang Li2, Xiao-Qin Zeng3, Yong Liu1  
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

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 CeIn3: A first-principles many-body perspective
Haiyan Lu1, Li Huang2, Xi Dai
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 Zhang1,2, Haiqing Yin1,2, Xuanhui Qu1,2, Qingjun Zheng3
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 Hu1, Yang Li1, Yue Chen2, Jian-Rong Liu1, Rui Yang1
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 Liu1, Lilong Zhu2, Gemei Cai1
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 Han1, Jiapeng Sun2, Hua Zhu1, Liang Fang3
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
10:00-10:30 Coffee Break

10:30-10:50 Z-56(Invited)
Structural and mechanical heterogeneous 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 Yang¹, Yan Peng¹, Fusheng Pan², Baodong Shi¹
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 Zhao¹², Yong Du², Lijun Zhang², Jixue Zhou¹, Yuansheng Yang¹³
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
2. Central South University, State Key Laboratory of Powder Metallurgy, Changsha 410083, China
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 Gan¹, Huiqiu Deng², Shifang Xiao², Xiaofan Li², Wangyu Hu¹
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
A front-tracking solidification model for simulation of microstructure evolution during multi-component alloy solidification
Guanyu Yi, Zhongkui Zhao, Bozu Liu
1. Advanced Materials Institute of Shandong Academy of Sciences
2. Shandong Jianzhu University

Dynamics of phase separation in Fe-Cr alloys with variational coarsening mechanisms
Yongsheng Li, Haojie Mei, Zhilong Yan
Nanjing University of Science and Technology

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

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

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

Simulating the plastic deformation of amorphous and crystalline solids at experimentally relevant timescales
Yun-Jiang Wang, Junping Du, Shigenobu Ogata, Lanhong Dai
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

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

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

Degenerate seaweed to tilted dendrite transition in directional solidification: insights from phase-field simulations
Hui Xing
Northwestern Polytechnical University

Modeling the massive-diffusive transition in multi-component substitutional alloys
Wangwang Kuang, Haifeng Wang, Feng Liu
The numerical simulation of hot die forging process of Ti-6Al-4V alloy blade
Jiahao Chen¹, Jinshan Li¹, Bin Tang¹, Lihua Du², Hongchao Kou¹
1. State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi’an, 710072, China
2. AVIC Beijing Aeronautical Manufacturing Technology Research Institute, Beijing, 100024, China

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 Wang¹, Zhukun Zhou², Mo Li²,³
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

09:00-09:25 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)
Dalian University of Technology

09:05-09:20 Z-84
Simulation of hydrogen clustering behaviors on tungsten surface
Jiannan Hao1,2, Shuo Jin1,2, Xiaolin Shu1,2, Lifang Wang1,2, Guang-Hong Lu1,2
1. School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China
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 Xu1,2, Liang-Liang Niu1,2,3, Shuo Jin1,2, Xiaolin Shu1,2, Hongxian Xie4, Lifang Wang1,2, Guang-Hong Lu1,2
1. School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China
2. Beijing Key Laboratory of Advanced Nuclear Materials and Physics, Beihang University, Beijing 100191, China
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

10:00-11:00 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 Gai1, Yang Sun1, Yafan Li2
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\textsuperscript{1,2}, Zhihua Hou\textsuperscript{1,2}, Xin Wang\textsuperscript{1,2}, Mei Bi\textsuperscript{1,2}, Li Zhang\textsuperscript{1,2}, Longjiang Deng\textsuperscript{1,2}
1. National Engineering Research Center of Electromagnetic Radiation Control Materials, University of Electronic Science and Technology of China, Chengdu 610054, China
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 AlB2-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 β-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
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Investigation of precipitation kinetics in binary Fe–Cu and ternary Fe–Cu–Ni alloys via kMC method
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