

Symposium 5: Computational materials design

Organizers: Zi-Kui Liu, Hamid Garmestani, Moe Khaleel, Mei Li

Oral Presentations

Blue: Invited talk (30 minutes)

Black: Contributed talk (20 minutes)

Green: Posters presentation

Monday Morning

Junsheng Wang, Mei Li, John Allison and **Peter Lee**, Multiscale Modeling of the Influence of Fe Content in a W319 Alloy on the Distribution of Intermetallic Phases and Micropores

Raja Mishra, Kaan Inal and Oana Cazacu, Material Design through Multi-Scale Simulations: Aluminum Sheet Forming using an Anisotropic Yield Function Coupled with Crystal Plasticity Theory

Young-Min Kim and Byeong-Joo Lee, Computational Design of Magnesium Alloys for Improved Deformability

Duc Nguyen-Manh and Sergei L. Dudarev, A model tight-binding Hamiltonian treatment of magnetic Fe-Cr alloys

Adam Kiejna and Elwira Wachowicz, Cohesion at clean and doped grain boundaries in bcc iron

Monday Afternoon

Lei Zhang, Qiang Du and **Long-Qing Chen**, Phase-field Prediction of Critical Nucleus Morphology in Solids

Teck Tan and Duane Johnson, Rapid and Accurate Estimate of High-Temperature Alloy Phase Boundaries

Liming Xiong and Youping Chen, Modeling and simulations of polycrystalline SiC thin film through a coupled atomistic continuum theory

Monday Afternoon (2)

J.-C. Zhao, Xuan Zheng and David Cahill, High-Throughput Measurements for High-Fidelity Materials Databases for Accelerated Materials Design

Brent Adams, Incorporating Grain Size Effects into Microstructure Design

Marius Stan, Bogdan Mihaila, David Korzekwa, Petrica Cristea and Juan Ramirez,
Computational Design of Advanced Nuclear Fuels

Tuesday Morning

Christopher Woodward, Michael Groeber, Mark Tschopp, Andrew Rosenberger, Dennis Dimiduk and Stephan Russ, The Virtual Turbine Blade: Multi-Length Scale Characterization of a Single-Crystal Turbine Blade

Jorg Neugebaue, Ab initio based modeling of engineering materials: From a predictive thermodynamic description to tailored mechanical properties

Sergei Tretiak, **Chao Wu**, Multiscale Modeling of Electronic Excitations in Branched Conjugated Molecules Using an Exciton Scattering Approach

Yaroslav Shtogun and Lilia Woods, Electronic Structure Effects of Deformed and Defective Single Walled Carbon Nanotubes

Zi-Kui Liu, Quantum, Statistic and Continuum Thermodynamics of Material

Tuesday Afternoon

Janina Zimmermann, Mike Finnis and Lucio Colombi Ciacchi, Vacancy segregation in the initial oxidation stages of biomaterials surfaces

Cheng Qi and **Yan Wang**, Crystal Construction based on Periodic Surfaces

Bandeep Singh and Oliver Fritz, Computational Modeling of Materials for Electrical Insulations

Dmitri Kilin, David Micha and Chris Obara, Density matrix treatment of confinement-facilitated photovoltage in thin films of silicon

Michael Anisimov, Nucleation rate surfaces for modeling of nanomaterial generation from crystals under short pulses of energy

Wednesday Morning

Michael Gao, Omer Dogan and Paul King, Computational Design of Refractory Alloys for Fossil Energy Applications: From First Principles Calculations, CALPHAD to FEM

Veera Sundararaghavan, Multi-scale sensitivity analysis for design of polycrystalline materials with tailored properties

Alireza Asgari, Chunhui Yang, Peter D. Hodgson and Bernard F. Rolfe, Multiphase Material Modelling by Multiscale Particle-In-Cell Method

David McDowell, Robust Simulation-Based Design of Materials

Greg Olson, Systems Computational Design of Hierarchically Structured Materials

Moe Khaleel, Design and Performance Modeling Tools for Solid Oxide Fuel Cells

Thursday Afternoon

Dongsheng Li and Hamid Garmestani, Computational Materials Design of Solid State Fuel Cell Electrodes

Eunseok Lee, Wei Cai and Fritz Prinz, Computing Electrochemical Impedance of Solid Electrolyte from Fluctuations

Aravind Asthagiri and Beverly Brooks Hinojosa, Computational investigation of Bi containing pyrochlores

Poster Presentations

Wednesday Afternoon

1. **Xinghua Xie**, Lithium and Zinc Composite Ceramic Powders
2. **Reza Jalili Saffar**, A numerical simulation to relate the shot peening operation to the induced residual stresses of 15-5PH steel
3. **Masahiko Katagiri**, Hidehiro Onodera and Hiroshi Ogawa, Structural Stability of Hydrogen Storage Materials
4. **Shruba Gangopadhyay**, Jaruwan Mesit, Ratan Guha, Jayanta Kapat, Nina Orlovskaya and Artem Masunov, Multiscale Simulations combined with experimental study of Barium/Strontium Ferrate/Cobaltate (BSCF) as a Promising Material for Solid Oxide Fuel Cell (SOFC)
5. Tae-Eun Kim, Young-Su Lee, Woo-Sang Jung, Soon-Hyo Chung, Jae-Hyeok Shim, Jung-Hae Choi and **Seung-Cheol Lee**, Electronic and Bonding Characteristics of (Ti,Mo)C
6. **Satyender Goel** and Artem Masunov, First Principles Study of Transition Metal Diatomics as the First Step In Multiscale Simulations of Carbon Nanotube Growth Process
7. **Ali Ebrahimi** and Sirous Jvadvpour, Modeling Boring Operation in Machining of Microalloyed and Heat-Treated Alloy Steels for Study of Machinability at Different Cutting Condition

8. **Mansoure Ilkhani**, Mohamad Reza Abolhassani and Saeid Jalali Asadabadi,
Electronic structure and EFG calculation of CeIn₃ under pressure