Symposium 10: Virtual Materials (Computational) Design and Ceramic Genome

Tuesday, January 29, 2013
Prediction and Modeling of Properties of Ceramics and Composites

8:00 AM-12:00 PM
Room: Oceanview
Session Chair(s): Hans Seifert, Yanwen Zhang

8:00 AM
Wai-Yim Ching*, Neng Li, University of Missouri-Kansas City, USA

8:30 AM
(ICACC-S10-002-2013) Genome Approach for Advanced Ceramics with Extremely Low Thermal Conductivity (Invited Speaker)
Jingyang Wang*, Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, China

9:00 AM
(ICACC-S10-003-2013) A numerical method for the simulation of coupled radiative/conductive heat transfer
Gerard L. Vignoles*, University Bordeaux, France

9:20 AM
(ICACC-S10-004-2013) Structure, Phonon, Bonding, and Hardness of a series of TMB4, TMB6 and TMB12 (TM = transition metal)
Peitao Liu*, Xiuyue Cheng, Haiyang Niu, Xingqiu Chen, Dianzhong Li, Yiyi Li, Institute of Metal Research, China

9:40 AM
Break

10:00 AM
(ICACC-S10-005-2013) Kinetic Monte Carlo Simulation of Cation Diffusion in Low-K Ceramics (Invited Speaker)
Brian Good*, NASA Glenn Research Center, USA

10:30 AM
(ICACC-S10-006-2013) Elastic, Electronic Structure and Optical Properties Change with Increasing Alumina Content in Mullite (Invited Speaker)
Sita Ram Aryal*, Paul Rulis, Wai-Yim Ching, University of Missouri Kansas City, USA

11:00 AM
(ICACC-S10-007-2013) First-principles calculation of temperature dependent thermal and mechanical properties of layered ternary carbides, Ti2AlC and Cr2AlC
Jiemin Wang*, Jingyang Wang, Institute of Metal Research, China; Yanchun Zhou, Aerospace Research Institute of Material & Processing Technology, China

11:20 AM
(ICACC-S10-008-2013) Theoretical investigations of the ferroelectric domain walls in LiNbO3 by first-principles calculations
Eita Tochigi*, Lawrence Berkeley National Laboratory, USA; Atsutomo Nakamura, Nagoya University, Japan; Teruyasu Mizoguchi, The University of Tokyo, Japan

11:40 AM
(ICACC-S10-009-2013) The Effective Elastic Properties of the C/C Composites calculated Using 3D Unit Cell Presentation of the Microstructure
Romana Piat*, Galyna Stasiuk, Karlsruhe Inst of Technology, Germany
Innovative Modeling and Simulation Methods

1:30 PM-5:20 PM
Room: Oceanview
Session Chair(s): Wai-Yim Ching, John Lawson

1:30 PM
(ICACC-S10-010-2013) Grain Boundary "Phase" Diagrams -- A Useful Component for "Materials Genome"? (Invited Speaker)
Naixie Zhou, Yuanyao Zhang, Jian Luo*, Clemson University, USA

2:00 PM
(ICACC-S10-011-2013) Computational ELNES Spectral Imaging Incorporating Signal Contrast
James Currie*, Paul Rulis, University of Missouri - Kansas City, USA

2:20 PM
(ICACC-S10-012-2013) Families of Superhard Crystalline Carbon Allotropes Constructed via Cold-compressed Graphite and Nanotubes
Haiyang Niu*, Xingqiu Chen, Dianzhong Li, Yiyi Li, Institute of Metal Research, China

2:40 PM
Rachel Cramm Horn*, Anthony Caruso, Michelle Paquette, Andrew Kitahara, Paul Rulis, University of Missouri - Kansas City, USA

3:00 PM
Break

3:20 PM
(ICACC-S10-014-2013) Ab initio MD simulations of the response of ceramics to extreme conditions (Invited Speaker)
Haiyan Xiao*, University of Tennessee, USA; Yanwen Zhang, Oak ridge National Lab, USA; William J Weber, University of Tennessee, USA

3:50 PM
(ICACC-S10-015-2013) A Neural Network Approach to Non Self Consistent Total Energy Calculations for Complex Materials (Invited Speaker)
Paul Rulis*, University of Missouri - Kansas City, USA

4:20 PM
(ICACC-S10-016-2013) Multiscale extraction of morphological features in woven CMCs
Cédric Chapoullié, Jean-Pierre Da Costa, Christian Germain, University Bordeaux, France; Michel Cataldi, Herakles, France; Gerard L. Vignoles*, University Bordeaux, France

4:40 PM
(ICACC-S10-017-2013) Electronic Structure and Interatomic Bonding in Cement Crystals
Chamila Chathuranga Dharmawardhana*, University Of Missouri - Kansas City, USA; Anil Misra, University of Kansas, USA; Sita R Aryal, Paul M Rulis, Wai-Yim Ching, University Of Missouri - Kansas City, USA

5:00 PM
(ICACC-S10-018-2013) Simulations of Anisotropic Grain Growth in Single Phase Materials Using Q-State Monte Carlo
Jeffrey Allen*, Charles Cornwell, Bryce Devine, Charles Welch, US Army Corps of Engineers, USA

Wednesday, January 30, 2013
Modeling of Defects and Diffusion in Ceramics

8:00 AM-12:00 PM
Room: Oceanview
Session Chair(s): Jingyang Wang, Brian Good

8:00 AM
(ICACC-S10-019-2013) Irradiation Effects in Fluorite-Structured Oxides (Invited Speaker)
Yanwen Zhang*, Oak Ridge National Laboratory, USA; Haiyan Xiao, University of Tennessee, USA; Philip Edmondson, Oak Ridge National Laboratory,
USA; Tamas Varga, Pacific Northwest National Laboratory, USA; Fereydoon Namavar, University of Nebraska Medical Center, USA; William J Weber, Oak Ridge National Laboratory, USA

**8:30 AM**
*(ICACC-S10-020-2013) Conductive path formation in insulating oxide using dislocations and interfaces (Invited Speaker)*
Atsutomo Nakamura*, Katsuyuki Matsunaga, Nagoya University, Japan; Teruyasu Mizoguchi, University of Tokyo, Japan; Eita Tochigi, Lawrence Berkeley National Laboratory, USA; Naoya Shibata, Yuichi Ikuhara, University of Tokyo, Japan

**9:00 AM**
*(ICACC-S10-021-2013) Interaction of CSL boundaries with displacement cascades in β-SiC*
Prithwish K Nandi*, Ajay V Annamareddy, Xiaojun Mei, Anant Raj, Jacob Eapen, North Carolina State University, USA

**9:20 AM**
*(ICACC-S10-022-2013) Particle Swarm Optimization for Modeling Defect Regions in Crystalline Systems*
Naseer A. Dari*, Paul M Rulis, University of Missouri-Kansas City, USA

**9:40 AM**
Break

**10:00 AM**
*(ICACC-S10-023-2013) Materials Thermodynamics and Phase Modeling in Lithium Ion Battery Systems (Invited Speaker)*
Hans J. Seifert*, Maren Lepple, Damian M Cupid, Peter Franke, Karlsruhe Institute of Technology, Germany

**10:30 AM**
*(ICACC-S10-024-2013) Lithium ion diffusion in fast ion conducting lithium lanthanum titanate ceramics (Invited Speaker)*
Jincheng Du*, University of North Texas, USA

**11:00 AM**
*(ICACC-S10-025-2013) Theoretical Prediction of Charge Induced Point Defect Behavior of Cubic Zirconia*
Bin Liu*, Yanwen Zhang, Oak Ridge National Laboratory, USA; William J Weber, The University of Tennessee, USA

**11:20 AM**
*(ICACC-S10-026-2013) Surface structure and oxygen adsorption on Cr2AlC (0001): Density functional characterization*
Neng Li*, UMKC, USA

**11:40 AM**
*(ICACC-S10-027-2013) Surface and mechanical properties of zinc titanate crystals from first principles calculations*
Wei Sun*, Jincheng Du, University of North Texas, USA

**Virtual Materials Design and Modeling**
1:30 PM-5:00 PM
Room: Oceanview
Session Chair(s): Jian Luo, Paul Rulis

**1:30 PM**
*(ICACC-S10-028-2013) Multiscale Modeling of Ablative Composites for Atmospheric Entry Applications (Invited Speaker)*
John W Lawson*, Charles W Bauschlicher, Thomas H Squire, Joshua D Monk, NASA Ames Research Center, USA

**2:00 PM**
*(ICACC-S10-029-2013) Thermomechanical simulation of C/C composites from X-ray CMT images (Invited Speaker)*
Gerard L. Vignoles*, Olivier Caty, University Bordeaux, France; Guillaume Couégnat, CNRS, France; Morgan Charron, Thomas Agulhon, University Bordeaux, France
2:30 PM  
(ICACC-S10-030-2013) Inelastic Design of MMCs with Lamellar Microstructure  
Romana Piat*, Yuriy Sinchuk, Karlsruhe Inst of Technology, Germany

3:00 PM  
Break

3:20 PM  
(ICACC-S10-031-2013) Explicit modelling of crack initiation and propagation in the microstructure of a ceramic material generated with Voronoi tessellation  
Simone Falco*, Noor A Yahya, Richard I Todd, Nik Petrinic, University of Oxford, United Kingdom

3:40 PM  
(ICACC-S10-032-2013) Multi-scale modeling of textile reinforced ceramic composites  
Michal Sejnoha*, Jan Vorel, CTU in Prague, Faculty of Civil Engineering, Czech Republic

4:00 PM  
Louiza Benazzouk*, Eric Arquis, Nathalie Bertrand, University of Bordeaux 1, France; Cédric Descamps, Snecma, France; Marc Valat, University of Bordeaux 1, France

4:20 PM  
(ICACC-S10-034-2013) Numerical estimation of the infiltrability of woven CMC preforms  
Gerard L. Vignoles*, William Ros, Christian Germain, University Bordeaux, France

4:40 PM  
(ICACC-S10-035-2013) First Principles Calculations of Boron Suboxide  
Jennifer Synowczynski Dunn*, Todd Beudet, Army Research Laboratory, USA; John R Smith, University of Michigan, USA