Program

Harnessing the Materials Genome:

Accelerated Materials Development via Computational and Experimental Tools

September 30 - October 5, 2012
Vail, Colorado

Conference Chairs:

Prof. **J.-C. Zhao**
The Ohio State University, USA

Prof. **Mark Asta**
University of California, Berkeley, USA

Prof. Dr. **Peter Gumbsch**
Fraunhofer-Institut fuer Werkstoffmechanik IWM, Germany

Prof. **Boyun Huang**
Central South University, China

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Sunday, September 30, 2012

16:00 – 18:00	Conference Check-in (Sun Down Foyer)
18:00 – 19:00	Welcome Reception (Sun Down Foyer)
19:00 – 21:00	Buffet Dinner (Sun Down Room)

Notes

- Technical sessions will be in the Colorado Ballroom 2 and 3
- Poster Sessions will be in the Colorado Ballroom 1.
- Breakfasts will be in the First Chair Café (vouchers will be distributed to attendees).
- Lunches will be in the First Chair Café.
- Dinners on Sunday, Monday, Tuesday will be in the Sun Down Room.
- Wednesday social hour will be in the hotel's Avalanche Pub – by hotel entrance. You must wear your conference badge in order to be served beer or wine on the conference account..
- The conference banquet on Thursday will be in the First Chair Café.
- Audiotaping, videotaping and photography of presentations are prohibited.
- Speakers – Please have your presentation loaded onto the conference computer prior to the session start (preferably the day before).
- Speakers – Please leave at least 3-5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- Turn your mobile telephones to vibrate or off during technical sessions.
- Be sure to check your contact information on the Participant List in this program and make any corrections to your name/contact information online. A corrected copy will be sent to all participants after the conference.

Monday, October 1, 2012

07:00 – 08:30 Breakfast

Session I: Computational Tools and Ab Initio Approaches I

08:30 – 08:35 Session Introduction (Session Chair: **Mark Asta**)

08:35 – 09:05 **Alex Zunger**, University of Colorado at Boulder, USA
The Inverse Problem in Material Discovery: Given a Target Property, Find the Material

09:05 – 09:35 **Jörg Neugebauer**, MPI Eisenforschung, Düsseldorf, Germany
Materials Design Based on Ab Initio Thermodynamics

09:35 – 10:05 **Karsten Wedel Jacobsen**, TU Denmark, Denmark
Atomistic Materials Design Using the Computational Materials Repository

10:05 – 10:30 Coffee Break

Session II: Materials and Microstructure Design I

10:30 – 10:35 Session Introduction (Session Chair: **Peter Lee**)

10:35 – 11:05 **David Cebon** and **Michael Ashby**, Cambridge University, UK
A Software Framework for Designing Materials

11:05 – 11:35 **Dierk Raabe** and Hauke Springer, Max-Planck-Institut für Eisenforschung, Germany
Rapid Alloy Prototyping: Compositional and Thermomechanical Bulk Combinatorial Design of Structural Materials: Example of 30Mn-1.2C-xAl Triplex Steels

11:35 – 12:05 **Rui Yang,** Institute of Metal Research, China
Computation-Assisted Design and Development of a Beta-Type Titanium Alloy for Biomedical Use

12:05 – 12:30 Discussion of Morning Sessions (Discussion Leaders: **Mark Asta & Peter Lee)**

12:30 – 14:00 Lunch

14:00 – 16:00 Ad hoc Sessions/Free Time

16:00 – 16:30 Afternoon Coffee

Session III: High-Throughput Experimental Tools I

16:30 – 16:35 Session Introduction (Session Chair: **Daniel Miracle**)

16:35 – 17:05 **Gerhard Schneider** and Dagmar Goll, Aalen University, Germany
High-Throughput Synthesis and Analysis for Searching New Permanent Magnet Materials

17:05 – 17:35 **David Cahill,** University of Illinois – Urban-Champaign, USA
High Throughput Mapping of the Thermophysical Properties of Materials

17:35 – 18:05 **J.-C. Zhao,** The Ohio State University, USA
Materials Property Microscopy Tools for the Materials Genome Initiative

18:05 – 18:35 **Alfred Ludwig,** Ruhr-Universität Bochum, Germany
Development of New Materials Using High-Throughput Thin Film Experimentation and Up-Scaling

Monday, October 1, 2012 (continued)

18:35 – 19:00	Session Discussion (Discussion Leader: **Daniel Miracle**)
19:00 – 20:30	Dinner
20:30 – 22:00	Poster Session and Social Hour

Tuesday, October 2, 2012

07:00 – 08:30 Breakfast

Session IV: Computational Tools and Ab Initio Approaches II

08:30 – 08:35 Session Introduction (Session Chair: **Adam Schwartz**)

08:35 – 09:05 **Stefano Curtarolo**, Kesong Yang, Shidong Wang, Wahyu Setyawan, and Marco Nardelli, Duke University, USA
The Quest for Descriptors in High-Throughput Searches: Robustness and Fragility of Topological Insulators

09:05 – 09:35 **Giulia Galli,** University of California, Davis, USA
Materials and Processes for Energy Conversion: Ab Initio Predictions

09:35 – 10:05 **Peter Gumbsch**, Kinshuk Srivastava, Daniel Weygand, and Matous Mrovec Fraunhofer-Institut fuer Werkstoffmechanik IWM, Germany
Multiscale Modelling of the Plastic Deformation in bcc Metals at Low and Intermediate Temperatures

10:05 – 10:30 Coffee Break

Session V: Materials Informatics and Digital Data I

10:30 – 10:35 Session Introduction (Session Chair: **James Warren**)

10:35 – 11:05 **Toshio Ogata,** National Institute for Materials Science (NIMS), Japan
New Stage of MatNavi: Materials Database at NIMS

11:05 – 11:35 **Terrell Vanderah,** Vicky Karen, Peter Linstrom, and Donald Burgess, National Institute of Standards and Technology (NIST), USA
NIST Databases for Materials Research

11:35 – 12:05 **Kristin Persson**, Lawrence Berkeley National Lab, USA
The Materials Project – A Public Materials Design Platform

12:05 – 12:30 Discussion of Morning Sessions (**Adam Schwartz** & **James Warren**)

12:30 – 14:00 Lunch

14:00 – 16:00 Ad hoc Sessions/Free Time

16:00 – 16:30 Afternoon Coffee

Session VI: Materials and Microstructure Design II

16:30 – 16:35 Session Introduction (Session Chair: **Peter Gumbsch**)

16:35 – 17:05 **Dennis Dimiduk**, Air Force Research Laboratory, USA
Integrating Materials and Structures Performance Prediction via the Materials Genome Initiative

17:05 – 17:35 **John Ågren**, The Royal Institute of Technology (KTH), Sweden
Purpose-Based Modelling of Microstructure Evolution and Kinetic Processes

17:35 – 18:05 **Yunzhi Wang**, N. Zhou, H.Z. Deutchman, P.J. Phillips, S. Keshavarzhadad, S. Ghosh, and M.J. Mills, The Ohio State University, USA
Better Property Modeling through Microstructure and Micromechanisms

18:05 – 18:35 **John Rodgers**, Innovative Materials Technologies, Canada
Design of Erosion Resistant Nanocoatings – from TRL 1 to TRL 6

Tuesday, October 2, 2012 (continued)

18:35 – 19:00	Session Discussion (Discussion Leader: **Peter Gumbsch**)
19:00 – 20:30	Dinner
20:30 – 22:00	Poster Session and Social Hour

Wednesday, October 3, 2012

07:00 – 08:30 Breakfast

Session VII: Materials and Microstructure Design III

08:30 – 08:35 Session Introduction (Session Chair: **Julie Christodoulou**)

08:35 – 09:05 **Peter Lee**, Lang Yuan, and Chedtha Puncreobutr, The University of Manchester, UK
Predicting Microstructure-Property Relationships in Structural Materials via Multiscale Models Validated by In-Situ Synchrotron Observation

09:05 – 09:35 **Tresa Pollock**, Mike Titus, and Alessandro Mottura, University of California – Santa Barbara, USA
Integration of Models and Experiments: A Case Study for New Co-Base Single Crystals

09:35 – 10:05 **Greg Olson**, Northwestern University / QuesTek, USA
From Genome to Flying Cyberalloys: The First Half Century

10:05 – 10:30 Coffee Break

Session VIII: Computational Tools and ab Initio Approaches III

10:30 – 10:35 Session Introduction (Session Chair: **Erich Wimmer**)

10:35 – 11:05 **Chris Wolverton** and Bryce Meredig, Northwestern University, USA
A Hybrid Computational-Experimental Approach for Automated Crystal Structure Solution

11:05 – 11:35 **Anton Van der Ven**, John C. Thomas, and Brian Puchala, University of Michigan, USA
Thermodynamics and Kinetics from First Principles

11:35 – 12:05 **Xin-Gao Gong,** Fudan University, China
Si_3AlP: A New Promising Material for Solar Cell Absorber

12:05 – 12:30 Discussion of Morning Sessions (Leaders: **Julie Christodoulou & Erich Wimmer**)

12:30 – 14:00 Lunch

14:00 – 18:30 Free time

18:30 – 20:00 Dinner on your own. Information on Vail restaurants is available at the hotel concierge who can also make reservations.

20:00 – 22:00 Social Hour

Thursday, October 4, 2012

07:00 – 08:30 Breakfast

Session IX: High-Throughput Experimental Tools II

08:30 – 08:35 Session Introduction (Session Chair: **Gerhard Schneider**)

08:35 – 09:05 **Michael Uchic**, Air Force Research Laboratory, USA
Modern Methods to Quantify Microstructure and Local Mechanical Properties in Engineering Alloys

09:05 – 09:35 **Christopher Hutchinson**, Monash University, Australia
The Use of Diffusion Couples in Physical Metallurgy: Model Calibration and Mapping Transitions in Alloy Behavior

09:35 – 10:05 **Ichiro Takeuchi**, University of Maryland, USA
Combinatorial Discovery of Novel Multifunctional Materials at Structural Phase Boundaries through Integrating Combinatorial X-Ray Data with ICSD

10:05 – 10:30 Coffee Break

Session X: Computational Tools and Ab Initio Approaches IV

10:30 – 10:35 Session Introduction (Session Chair: **Alex Zunger**)

10:35 – 11:05 **Ralf Drautz**, Ruhr-Universität Bochum, Germany
Simplified Models of the Electronic Structure for Analyzing High-Throughput Data

11:05 – 11:35 **Yoshitaka Umeno**, Tomofumi Tada, Shotaro Hara, and Naoki Shikazono, University of Tokyo, Japan
Multiscale Modeling for Material Design of Solid Oxide Fuel Cell Electrode

11:35 – 12:05 **Nicola Marzari,** École Polytechnique Fédérale de Lausanne, Switzerland
Thermal Transport and Thermodynamical Stability in Novel Materials, and the Challenges for Materials Genome Projects

12:05 – 12:30 Discussion of Morning Sessions (Leaders: **Alex Zunger and Gerhard Schneider**)

12:30 – 14:00 Lunch

14:00 – 16:00 Ad hoc Sessions/Free Time

16:00 – 16:30 Afternoon Coffee

Session XI: Materials Informatics and Digital Data II

16:30 – 16:35 Session Introduction (Session Chair: **Dennis Dimiduk**)

16:35 – 17:05 **Surya Kalidindi**, Tony Fast, and Stephen Niezgoda, Drexel University, USA
Leveraging Data Science to Enable Multiscale Materials Modeling and Design

17:05 – 17:35 **Thomas Bligaard,** SLAC National Accelerator Laboratory, USA
Materials Informatics Tools and Computational Methods for Catalyst Design

17:35 – 18:05 **William Marsden,** Granta Design, UK
An Information Architecture for ICME

18:05 – 18:35 **James Warren**, National Institute of Standards and Technology (NIST), USA
The Materials Genome Initiative and a New Paradigm for Materials Data

18:35 – 19:00 Session Discussion (Discussion Leader: **Dennis Dimiduk**)

Thursday, October 4, 2012 (continued)

19:00 – 21:00	Conference Banquet
21:00 – 22:00	Poster Session and Social Hour

Friday, October 5, 2012

07:00 – 08:30	Breakfast & Departures

List of Posters

1. Software Platform for Virtual Material Design demonstrated for Magnetic Phase Search and Curie Temperature Calculations
   Lothar Kunz, Robert Bosch GmbH, Germany

2. Distributed Version Control Systems For Data Sharing And Collaboration: An Application In Oxide Polymorph Stability
   John Kitchin, Carnegie Mellon University, USA

3. Computational Design Of Nanosegregated Catalysts For Polymer Electrolyte Membrane Fuel Cells
   Guofeng Wang, University of Pittsburgh, USA

4. Phase-field modeling of microstructural evolution in industrial alloys
   Youhai Wen, NETL, US Dept. of Energy, USA

5. Materials Informatics for Virtual Design of Polymer Nanocomposites
   Bharath Natarajan, Rensselaer Polytechnic Institute, USA

6. An integrated approach to design CREEP-Resistant ferritic steels
   Michael Gao, National Energy Technology Lab/URS Corp, USA

7. MedeA®: An Environment for Computational Materials Engineering in the Context of the Materials Genome
   Paul Saxe, Materials Design, Inc., USA

8. Accelerating Materials Development by *in situ* Strain and Phase Mapping Synchrotron Probe
   Thomas Tsakalakos, Rutgers University, USA

9. Design of modified properties of oxides by sulfur substitution: the nature of the transition from localized to delocalized VBM
   Giancarlo Trimarchi, Northwestern University, USA