SYMPOSIUM CM7

Genomic Approaches to Accelerated Materials Innovation April 18 - April 21, 2017

Symposium Organizers Sergei Kalinin, Oak Ridge National Laboratory Momoji Kubo, Tohoku University Carson Meredith, Georgia Institute of Technology Artem Oganov, Skolkovo Institute of Science and Technology

> <u>Symposium Support</u> Applied Materials, Inc. Georgia Institute of Technology

> > Proceedings Statement

All authors are invited to submit articles based on their 2017 MRS Spring Meeting presentations to the journals in the MRS portfolio (www.mrs.org/ publications-news). Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

TUTORIAL

21st Century Tools for Accelerating Scientific Research—From Combinatorial Synthesis and Text Mining to Artificial Intelligence

> Monday Morning, April 17, 2017 8:30 AM – 5:00 PM PCC North, 100 Level, Room 124 B

The tutorial will present novel computational analytic methods capable of unlocking the human knowledge that's been documented and archived in the unstructured text of hundreds of millions of scientific publications to extend scientific discovery beyond human capacity, and ways to automate experimental knowledge generation. The instructors will explore pathways for visualizing and comprehending knowledge propagation, evolution, and assessment of scientific research fronts, data based hypothesis generation, and methods for quantifying research impact within the scientific community and beyond.

Part I: Rama Vasudevan

Rama Vasudevan will introduce the arguments for the need for text analysis in the field of materials growth, and focus on a specific use case of text mining of papers on epitaxial thin films of complex oxides, for determination of growth conditions-functional property relationships. An open source annotation tool is modified for this purpose, using regular expressions on text from selected papers to automatically annotate text associated with growth conditions and functional properties. Via the use of crowd sourcing, the annotations are checked and matched with the materials of interest, to populate a database containing information on the type of material grown, the substrate, growth conditions, and functional property information. The methods shown here are general, and can be applied to a wide variety of growth methods and material types.

Part II: Chaomei Chen

Chaomei Chen will discuss the use of the freely available CiteSpace tool, in order to study the propagation and dynamics of scientific fields. Through use of specific examples, topics covered will include how to determine and visualize citation and author networks, observe collaborations geographically, and identify fields which are experiencing rapid growth. Semantic analysis allows identification specific areas and trends, and can be highly useful in determining the structure of fields for newcomers.

Part III: Ichiro Takeuchi

Ichiro Takeuchi will discuss the use of informatics techniques to effectively handle, visualize, and analyze the large amount of data which are generated from the combinatorial experiments and potential of data mining of publications to establish knowledge-driven research paradigms.

Part IV: Justin Fessler

Justin Fessler will introduce the natural language processing tools of IBM Watson. Through an exploration of specific test cases, he will show how natural language processing afforded by Watson can be utilized to determine latent connections between different data, identify trends, and suggest links between disparate domains. These tools can be useful to both existing researchers in fields as well as newcomers, to quickly explore the domain.

Instructors **Rama Vasudevan**, Oak Ridge National Laboratory **Chaomei Chen**, Drexel University **Ichiro Takeuchi**, University of Maryland, College Park **Justin Fessler**, IBM Federal Software

SESSION CM7.1: Advances in Data Mining for Materials Development I Session Chairs: Carson Meredith and Artem Oganov Tuesday Afternoon, April 18, 2017 PCC North, 100 Level, Room 124 B

1:30 PM *CM7.1.01

Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials <u>Surya R. Kalidindi</u>; Georgia Institute of Technology, United States.

2:00 PM *CM7.1.02

Multi-Way Hyperspectral Image Analysis Based on Scanning Transmission Electron Microscopy and Associated Spectroscopic Methods <u>Shunsuke</u> <u>Muto</u>; Nagoya University, Japan.

2:30 PM CM7.1.03

A Priori Knowledge vs Computation Cost—Comparison of Different Segmentation Approaches of Large X-Ray Diffraction Datasets Fang Ren; SLAC National Accelerator Center, United States.

2:45 PM CM7.1.04

Automatic Segmentation and Fingerprint Matching for Atomic Resolution TEM Images <u>Eric Schwenker^{1,2}</u>; 'Northwestern University, United States; ²Argonne National Laboratory, United States.

3:00 PM BREAK

3:30 PM CM7.1.05

Data Mining for New Two-Dimensional Materials Gowoon Cheon; Stanford University, United States.

3:45 PM CM7.1.06

Computational Design for Stimuli Responsive MOFs <u>Charles A. Manion;</u> Oregon State University, United States.

4:00 PM *CM7.1.07

Facilitating the Development of a "High Throughput Experimental Materials Science Virtual Laboratory" <u>Martin L. Green</u>; National Institute of Standards and Technology, United States.

4:30 PM CM7.1.08

Order and Disorder in Ternary and Quaternary Atomic Laminates (MAX phases) from DFT Predictions and Material Synthesis <u>Martin Dahlqvist</u>; The Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden.

4:45 PM CM7.1.09

Discovery of New Metallic Glass Former in a Ternary Composition Space through a Genomic Approach <u>Fang Ren</u>; SLAC National Accelerator Center, United States. SESSION CM7.2/CM3.3: Joint Session: Accelerating Materials Discovery and Design with Computing Session Chair: Yibin Xu Wednesday Morning, April 19, 2017 PCC North, 100 Level, Room 124 B

8:00 AM *CM7.2.01/CM3.3.01

NIST—The Materials Genome Initiative and Computation James A. Warren; National Institute of Standards and Technology, United States.

8:30 AM CM7.2.02/CM3.3.02

Intelligently Navigating Parameter Space with Machine Learning <u>Matthew</u> <u>Spellings</u>; University of Michigan, United States.

8:45 AM CM7.2.03/CM3.3.03

Materials Data Management with Signac Carl Simon Adorf; University of Michigan, United States.

9:00 AM CM7.2.04/CM3.3.04

Digital Alchemy—An Inverse Approach to Mesoscale Soft Materials Design Greg van Anders; University of Michigan, United States.

9:15 AM CM7.2.05/CM3.3.05

Pressure-Induced Phase Transitions in Shape Space Rose Cersonsky; University of Michigan, United States.

9:30 AM CM7.2.06/CM3.3.06

Determining Molecular Orientation via Physics Based Polymer Models with Polarized X-Ray Scattering <u>Adam F. Hannon^{1, 2}</u>; ¹NIST, United States; ²Georgetown University, United States.

9:45 AM BREAK

10:15 AM *CM7.2.07/CM3.3.07

Evolutionary Structure Prediction from Complex Crystals to Defects <u>Qiang</u> <u>Zhu;</u> University of Nevada, Las Vegas, United States.

10:45 AM CM7.2.08/CM3.3.08

Large-Scale Molecular Dynamics Simulation on Fracture Properties of Ni Anode for Highly Durable Solid Oxide Fuel Cell <u>Jingxiang Xu</u>; Institute for Materials Research, Tohoku University, Japan.

11:00 AM CM7.2.09/CM3.3.09

Integrated Imaging and Simulation to Investigate Lattice Deformations in Externally Stimulated Nanocrystals <u>Kiran Sasikumar</u>; Argonne National Laboratory, United States.

11:15 AM CM7.2.10/CM3.3.10

DFT Applied to Transition Metals and Binaries—Developing the V/DM-17 Test Set Elizabeth Decolvenaere; University of California, Santa Barbara, United States.

11:30 AM CM7.2.11/CM3.3.11

Development of Crystal Structure Prediction Method for Magnet Materials <u>Tomoki Yamashita^{1,2}</u>; ¹National Institute for Materials Science (NIMS), Japan; ²Osaka University, Japan.

SESSION CM7.3: Advances in Data Mining for Materials Development II Session Chairs: Shunsuke Muto and Zhe Qiang Wednesday Afternoon, April 19, 2017 PCC North, 100 Level, Room 124 B

1:30 PM CM7.3.01

Automated First-Principles Calculations for Building Dopant Property Database of Doped-ZnO <u>Kanghoon Yim</u>; Seoul National University, Korea (the Republic of).

1:45 PM CM7.3.02

Machine Learned Approximations to Density Functional Theory Hamiltonians—Towards High-Throughput Screening of Electronic Structure and Transport in Materials <u>Ganesh Hegde</u>; Samsung Semiconductor Inc, United States.

2:00 PM CM7.3.03

High-Throughput Detection and Data Mining of Coordination Environments in Oxides <u>Geoffroy Hautier</u>; Université catholique de Louvain, Belgium.

2:15 PM CM7.3.04

Making Materials Data Discoverable, Accessible, Interoperable and Reusable—A Focus on High-Throughput Experimental Materials Science Zachary T. Trautt; National Institute of Standards and Technology, United States.

2:30 PM BREAK

3:30 PM *CM7.3.05

A Data Platform for Materials Research by Information Integration <u>Yibin</u> Xu; National Institute for Materials Science, Japan.

4:00 PM *CM7.3.06

Data-Driven Routes to New Insight into Materials Properties <u>Claudia</u> <u>Draxl^{1,2}</u>; 'Humboldt University of Berlin, Germany; ²Fritz Haber Institute of the Max Planck Society, Germany.

4:30 PM CM7.3.07

Multi-Fidelity Information Fusion for Materials Informatics <u>Ghanshyam</u> <u>Pilania</u>; Los Alamos National Laboratory, United States.

4:45 PM CM7.3.08

Materials Synthesis Insights Guided by Data Mining and First-Principles Calculations Edward Kim; Massachusetts Institute of Technology, United States.

> SESSION CM7.4: Poster Session: High-Throughput Screening in Materials Design Session Chair: Sergei Kalinin Wednesday Afternoon, April 19, 2017 8:00 PM - 10:00 PM Sheraton, Third Level, Phoenix Ballroom

CM7.4.01

Data Mining in Ti-6Al-4V Alloy Design Lei Fang; National Institute for Materials Science, Japan.

CM7.4.02

Molecular Dynamics Simulations of Substitutional Diffusion Xiaowang Zhou; Sandia National Labs, United States.

CM7.4.03

Genetically Tunable M13 Phage Films Utilizing Evaporating Sessile Droplet Techniques <u>Erik Alberts</u>; Engineer Research and Development Center, United States.

CM7.4.04

Combinatorial Synthesis of New High-Dielectric Constant Film Materials for Nanoelectronics <u>Takahiro Nagata^{1,2}</u>; ¹NIMS, Japan; ²JST-PRESTO, Japan.

CM7.4.05

Graph Theoretical Representation, Analysis and Synthesis of Amorphous Metal Oxide Networks . Divya; Indian Institute of Technology, Kanpur, India.

CM7.4.06

The Predictive Semi-gSEM Models of Waterborne Acrylic Coatings under Multi-Factor Accelerated Weathering Test <u>Donghui Li</u>; Case Western Reserve University, United States.

CM7.4.07

Pycroscopy—An Open Source Approach for Analyzing and Storing Material Science Data Suhas Somnath; Oak Ridge National Laboratory, United States.

CM7.4.08

High-Throughput Study of Defect Energetics and Proton Transport in Cubic Perovskites Janakiraman Balachandran; Oak Ridge National Laboratory, United States.

CM7.4.09

Influence of Strain and Doping on Local Material Structure and Proton Transport Properties in Disordered Oxides Janakiraman Balachandran; Oak Ridge National Laboratory, United States.

CM7.4.10

Critical Current by Design through Large-Scale Simulations <u>Andreas</u> <u>Glatz</u>^{1,2}; ¹Argonne National Laboratory, United States; ²Northern Illinois University, United States.

> SESSION CM7.5: Machine Learning in Materials Discovery and Development Session Chairs: Anastassia Alexandrova, Artem Oganov and Alexander Tropsha Thursday Morning, April 20, 2017 PCC North, 100 Level, Room 124 B

8:00 AM *CM7.5.01

Machine Learning for Materials Discovery: Low-LTC Compounds, Grain Boundaries, Superlattices and RNAs <u>Koji Tsuda</u>; The University of Tokyo, Japan.

8:30 AM CM7.5.02

A Semi-Supervised Feature Learning Mechanism for Microstructure Reconstruction and Optimal Design <u>Ruijin Cang</u>; Arizona State University, United States.

8:45 AM CM7.5.03

Transforming Data into Knowledge using Machine Learning Applied to Experimental Data John D. Perkins; NREL, United States.

9:00 AM CM7.5.04

Connecting Structure and Kinetics—Using Machine Learning Representations to Model Disordered Materials <u>Ekin D. Cubuk;</u> Stanford University, United States.

9:15 AM CM7.5.05

A Computational Graph-Based Approach for Stochastic Reconstruction of Microstructures Using a Deep Learning Framework <u>Xiaolin Li</u>; Northwestern University, United States.

9:30 AM BREAK

10:00 AM *CM7.5.06

Active Learning in High-Throughput Diffraction of Combinatorial Libraries Ichiro Takeuchi; University of Maryland, United States.

10:30 AM CM7.5.07

Machine Learning Approaches for Experiment-Guided Atomistic Structure Determination <u>Maria K. Chan</u>; Argonne National Laboratory, United States.

10:45 AM CM7.5.08

Machine Learning towards Better Growth of Materials—A Test Case with Epitaxial Oxide Thin Films <u>Rama K. Vasudevan</u>; Oak Ridge National Laboratory, United States.

11:00 AM CM7.5.09

Accelerated Discovery of Solar Fuels Materials by Integrating High Throughput Characterization and Machine Learning Techniques <u>Santosh</u> <u>K. Suram</u>; California Inst of Technology, United States.

11:15 AM CM7.5.10

Statistical Learning of Kinetic Monte Carlo Models for Complex Chemistry from Molecular Dynamics Qian Yang; Stanford University, United States. SESSION CM7.6: Simulation and Experiment Applied to Materials Discovery I Session Chairs: Momoji Kubo and Koji Tsuda Thursday Afternoon, April 20, 2017 PCC North, 100 Level, Room 124 B

1:30 PM *CM7.6.01

Materials Informatics—Computer-Aided Design of Novel Materials with the Desired Electronic and Physical Properties <u>Alexander Tropsha</u>; University of North Carolina, United States.

2:00 PM *CM7.6.02

Functional 2D and 3D Borides <u>Anastassia N. Alexandrova</u>; University of California, Los Angeles, United States.

2:30 PM CM7.6.03

The Thermodynamic Scale of Inorganic Crystalline Metastability Wenhao Sun^{1, 2}; ¹Massachusetts Institute of Technology, United States; ²Lawrence Berkeley National Laboratory, United States.

2:45 PM CM7.6.04

Coarse Grained Microstructure Field Modeling From Fine Grained Features in Continuous Fiber Composite Structures <u>Jeff Simmons</u>; Air Force Research Laboratory, United States.

3:00 PM BREAK

3:30 PM *CM7.6.05

Conjugated Polymers Unraveled—A Poly(3-Hexylthiophene) Case Study Martha Grover; Georgia Tech, United States.

4:00 PM *CM7.6.06

Construction of Standardized Neural Network-Based Interatomic Models for Structure Prediction Acceleration <u>Alexey Kolmogorov</u>; Binghamton University, United States.

4:30 PM CM7.6.07

Structure Prediction for Sn₂N₂, a New Metastable Binary Nitride <u>Stephan</u> Lany; NREL, United States.

4:45 PM CM7.6.08

Automated Tools to Enable High-Throughput Calculations of Intrinsic Point-Defect Properties—Applications to Halide Perovskite Compounds Danny Broberg; University of California, Berkeley, United States.

SESSION CM7.7: Simulation and Experiment Applied to Materials Discovery II Session Chairs: Toyohiro Chikyow and Jason Hattrick-Simpers Friday Morning, April 21, 2017 PCC North, 100 Level, Room 124 B

8:00 AM *CM7.7.01

Entropy Descriptors as the Key for Synthesizability <u>Stefano Curtarolo;</u> Duke University, United States.

8:30 AM CM7.7.02

Improve the Simulation Accuracy with Abandoned Information <u>Ying</u> <u>Zhang</u>; Toyota Research Institute of North America, United States.

8:45 AM CM7.7.03

Holistic Computational Structure Screening of more than 12,000 Candidates for Solid Lithium-Ion Conductor Materials <u>Austin D. Sendek;</u> Stanford University, United States.

9:00 AM CM7.7.04

High-Throughput Design of Two-Dimensional Electron Gas Systems Based on Perovskite Oxide Heterostructures <u>Kesong Yang</u>; University of California, San Diego, United States.

9:15 AM CM7.7.05

Supercomputer Post-K Project "Challenge of Basic Science" in Japan Momoji Kubo; Tohoku University, Japan.

9:30 AM BREAK

10:00 AM *CM7.7.06

Exploration of Photo-Functional Materials Using Ab Initio Evolutionary Searching Junjie Wang^{1, 2}; ¹Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan; ²National Institute for Materials Sciences, Japan.

10:30 AM CM7.7.07

A High-Throughput Experimental Approach to Study Transition Metal Ternary Chalcogenides <u>Ankita Bhutani</u>; University of Illinois at Urbana-Champaign, United States.

10:45 AM CM7.7.08

Fabrication and Characterization of High-Coercivity L1₀-FeNi Films Using a Combinatorial Sputtering Approach <u>Andreas Kaidatzis</u>; NCSR Demokritos, Greece.

11:00 AM CM7.7.09

Assessment of Trends in the Hydrogen Evolution Reaction and CO₂ Reduction on Metal Nanoparticles <u>Dominic Alfonso</u>; National Energy Technology Laboratory, United States.

11:15 AM CM7.7.10

Cheminformatics-Inspired Materials Discovery Platform <u>Olexandr Isayev</u>; University of North Carolina at Chapel Hill, United States.

SESSION CM7.8: Simulation and Experiment Applied to Materials Discovery III Session Chairs: Momoji Kubo and Carson Meredith Friday Afternoon, April 21, 2017 PCC North, 100 Level, Room 124 B

1:30 PM *CM7.8.01

High Throughput Experimentation and Materials Informatics Toyohiro Chikyow^{1,2}; ¹MANA National Institute for Materials Science, Japan; ²MI2I National Institute for Materials Science, Japan.

2:00 PM *CM7.8.02

A Materials Genome Approach to the Discovery of Novel Multi-Principal Component Alloys Jason R. Hattrick-Simpers^{1, 2, 5}; ¹University of South Carolina, United States; ²South Carolina SmartStateTM Center for the Strategic Approaches to the Generation of Electricity Columbia, United States; ⁵Materials Measurement and Science Division, United States.

2:30 PM CM7.8.03

Controlled Growth of 2D Materials via Simulation Guided

Experiments Kasra Momeni; Louisiana Tech University, United States.

2:45 PM CM7.8.04

Materials Informatics for Magnetic Properties <u>Hitoshi Fujii</u>; National Institute for Materials Science, Japan.

3:00 PM CM7.8.05

Automating Crystallographic Analysis and Reciprocal Space Feature Extraction <u>Andrew Stevens^{1, 2}</u>; ¹Pacific Northwest National Laboratory, United States; ²Duke University, United States.