

**Workshop: *Materials Informatics – Accelerating Atomistic Design and Discovery of New Materials and Concepts via Big-Data Analytics***

August 3<sup>rd</sup>, 2017 Oak Ridge National Laboratory, Oak Ridge, TN

Statistical learning approaches have revolutionized how we think, approach and solve problems in a wide range of fields, giving rise to new “informatics” disciplines. Informatics involves creating, manipulating, representing, processing and eventually communicating both data and what it means. While materials informatics has been applied to engineer new materials in the macroscale in the last decade, its application to understand and design materials atomistically, i.e., at the nano- to meso-scale is still quite nascent. Materials science has a dearth of (pertinent) atomistic data, especially when compared to other fields such as biology or astronomy. Recent advances in performing multi-modal, high-throughput experiments and reliable atomistic computations have allowed us to go past this limitation, yet several challenges remain. This requires a back-and-forth dialogue between statistical learners and domain scientists.

This workshop will attempt to bring together scientists who are working towards bridging this communication barrier, but typically do not work with each other, and allow them to identify common problems of interest where they can collaborate and push this field of materials informatics to a success at a faster pace.

**Invited Speakers:**

*Janakiraman Balachandran (ORNL), Valentino Cooper (ORNL), Stephen Jesse (ORNL), Chiho Kim (University of Connecticut), Turab Lookman (Los Alamos National Laboratory), Shyue Ping Ong (University of California, San Diego), Mallikarjun (Arjun) Shankar (ORNL), David Sholl (Georgia Tech), Jason-Hattrick Simpers (University of South Carolina & National Institute of Standards and Technology), Suhas Somnath (ORNL), Chad A. Steed (ORNL), Steven Young (ORNL)*

**Organizer:** Panchapakesan Ganesh (ORNL)

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**Location: SNS building (#8600), CLO room C-152**

9:00AM	Welcome – P. Ganesh, R&D Staff member
9:15AM	David Sholl, “ <i>Developing New Nanoporous Materials for Practical Applications Using Computational Modeling – How Close Is the Dream to Reality</i> ”
9:45AM	Valentino Cooper, “ <i>Bridging High Throughput Data to Materials Properties Without Losing Sight of Accuracy</i> ”
10:15AM	Janikaraman Balachandran, “ <i>Defect Genome of Cubic Perovskites for Fuel Cell Applications</i> ”
10:30AM	Break
10:45AM	Turab Lookman, “ <i>Inference and Design for Materials Discovery</i> ”
11:15AM	Chiho Kim, “ <i>Machine Learning Assisted Design of Polymer Dielectrics</i> ”
11:45AM	Shyue Ping Ong, “ <i>Computing + Automation Software = Data; Data + Learning Software = Insights</i> ”
12:15PM	Lunch
1:15PM	Jason-Hattrick Simperts, “ <i>Machine Learning Before, During, and After High-Throughput Experiments</i> ”
1:45PM	Stephen Jesse, “ <i>Large Scale Data Analysis for Understanding Nanoscale Phase Change</i> ”
2:15PM	Steven Young, “ <i>Deep Learning for Scientific Data Analysis</i> ”
2:30PM	Break
2:45PM	Chad Steed, “ <i>Practical Applications of Visual Analytics for Enhanced Understanding of Scientific Data</i> ”
3:15PM	Mallikarjun Shankar, “ <i>Scalable Data Services at OLCF and CADES</i> ”
3:45PM	Suhas Somnath, “ <i>Community-Driven Imaging in the Information Dimension</i> ”
4:00PM	Discussions and Farewell