



Materials Informatics – Accelerating atomistic design and discovery of new materials and concepts via big-data analytics

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Organizer:

Panchapakesan Ganesh (ganeshp@ornl.gov)
Center for Nanophase Materials Sciences, ORNL

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), 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)
