



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

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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.
