THE UNIVERSITY OF CHICAGO

Computational and Applied Mathematics
&
Statistics Student Seminar

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Implementing and Leveraging Fast Algorithms for High-throughput Materials Characterizations

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Jones Laboratory,
Room 303

ABSTRACT

Our current (in)ability to inverse-design materials computationally with target properties (for example, batteries that won't explode on airplanes, efficient photovoltaics for solar panels, or room temperature superconductors) is limited not by our understanding of fundamental physical processes but by our ability to calculate physical properties accurately and efficiently. To realize the inverse-design of materials, we first perform high-throughput calculations of target properties on an exponential number of candidate materials, and then we confirm target properties by performing high-throughput experimental characterization of novel materials. In this talk, I will discuss recent progress on both ends of this high-throughput pipeline. For high-throughput experimental workflows, I will discuss how we can leverage a fast forward algorithm known as "cluster correlation expansion" to augment experimental data for high-throughput recovery of hyperfine coupling constants for defects in semiconductors. For high-throughput computational workflows, I will discuss a new (relatively fast) algorithm to calculate electric polarization that circumvents a numerical branch selection issue that arises in functions of complex numbers.