Princeton Institute for Computational Science (PICSciE) Colloquium:

Materials Properties from *ab-initio* Simulations: Recent Progress, New challenges and Open issues

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ABSTRACT:

In the past thirty years, the use of scientific computing has become pervasive in all disciplines: collection and interpretation of most experimental data is carried out using computers, and physical models in computable form, with various degrees of complexity and sophistication, are utilized in all fields of science. However, full prediction of physical and chemical phenomena based on the basic laws of Nature, using computer simulations, is a revolution still in the making, and it involves some formidable theoretical and computational challenges. We illustrate the progress and successes obtained in recent years in predicting fundamental properties of materials in condensed phases and at the nanoscale, using *ab-initio*, quantum simulations, in particular first principles molecular dynamics and Quantum Monte Carlo calculations. We also discuss open issues related to the validation of the approximate, first principles theories used in large scale simulations, and the resulting complex interplay between computation and experiment.