CORE-CM SEMINAR
Michigan State University — Department of Chemistry

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Systematically improvable multiscale methods for correlated electron systems

Abstract:

The development of numerical methods capable of simulating realistic materials with strongly correlated electrons, with controllable errors, is a central challenge in quantum chemistry. Here we describe a framework for a general multiscale method based on embedding a self-energy of a strongly correlated subsystem into a self-energy generated by a method able to treat large weakly correlated systems approximately. As an example, we present the embedding of an exact diagonalization self-energy into a self-energy generated from self-consistent second order perturbation theory.

Finally, I would like mention our newest development that is stochastic embedding framework where the weakly correlated part is modeled by quantum Monte Carlo and can describe a realistic solid with thousands of orbitals and electrons. Subsequently, we embed the strongly correlated part of the self-energy into the stochastic self-energy for the weakly correlated part.

Thursday, December 3, 2015
12:00 PM
Room 1400 – BPS
Professor Ben Levine – Host

Accommodations for persons with disabilities may be requested by calling the Chemistry Department at (517) 355-9715, X191 two days prior to the event to ensure sufficient time to make arrangements. Requests received after this date will be met when possible.