

Materials Science and Technology Division

“First-Principles Many-body methods in Condensed Matter Theory: Recent developments and perspectives”

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10:00 a.m.
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ABSTRACT

Today, first principles (ab-initio) methods offer quantitative understanding of quantum many-body systems such as atoms, molecules and solids. Recent developments in the theory, algorithms and in computer power have placed these methods at a unique position to deepen our understanding of condensed matter.

In the seminar, a brief introduction to the modern ab-initio methods will given, with emphasis on Density Functional Theory (DFT) and quantum Monte Carlo (QMC) methods. While DFT methods provide a good description of large classes of systems, they also carry some uncertainty in the quality of their results (in particular for highly correlated materials). A more systematic approach is offered by the promising QMC methods, which deal directly with interacting system of electrons and nuclei. While QMC methods are the most accurate methods available for systems of more than few atoms, they are also computationally more demanding. However, with the advent of petascale computing facilities [such as the one at the National Center for Computational Sciences (NCCS)], the QMC approach has the potential to become the most viable ab-initio method.

In the remainder of the talk, I will describe some applications of QMC methods to real materials and outline possible applications that range from the electronic structure of transition and inner transition element compounds to the study the ultra-cold atoms and polar molecules. The open theoretical problems in the QMC methodology will be also discussed. Finally, I will present some challenges as well as perspectives on the long-term goals in the field.

Host: Fernando Reboredo (576-5346)

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