Materials Science and Technology Division

Materials Theory Seminar

"Electronic Structure of Nanosystems from First-Principles Theories"

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Abstract:

Density-functional theory (DFT) has evolved into a mature and reliable theory for predicting the electronic properties of weakly and moderately correlated systems. DFT can be cast into a first-principles theoretical framework, which requires a minimum of information from experimental measurements. As a result, it is now the theory of choice for investigating the electronic properties of new materials and devices. One difficulty though is that first-principles DFT calculations often require heavy numerical calculations, especially for nanostructures containing hundreds or thousands of atoms. A real-space approach to DFT has been proposed in order to tackle this problem. Some of the latest developments of the real-space DFT method will be presented in this talk. Three applications will be discussed: the electronic properties and energetics of silicon nanocrystals with up to 7 nm in size; the evolution of magnetization in iron clusters Fe_n (n < 400); and the optical properties of CdSe pyramidal nanocrystals. The last application illustrates a known limitation of DFT: the optical properties of semiconductors are often dominated by excitonic and other many-body effects, which are not accurately described within DFT. These effects are taken into account within a many-body formulation, based on the one-electron Green's function and the electron-hole propagator. DFT calculations presented in this talk have been done using the PARSEC code.

Host: Fernando Reboredo