Fabio Della Sala, *Institute of Nanoscience (CNR) and Center for Biomolecular Nanotechnologies (IIT) Lecce (Italy)*

Modeling nanostructures at different length scales: electronic and optical properties

Abstract:
Current research in nanoscience and nanotechnology requires accurate computational tools to predict the electronic and the optical properties of different nanosystems, in particular:
i) Metal nanoparticles(MNPs), which can be used to increase the photoluminescence of emitters, requires a full numerical solution Maxwell's equations on a grid [1,2];
ii) Semiconductor nanocrystals, which can be used for biological applications or in optoelectronic devices, can be efficiently described using envelop function models [3,4];
iii) First-principles atomistic modeling can be achieved for nanostructures (e.g. organic molecules) less than 100-1000 atoms. Density-Functional Theory(DFT) is here the method of choice, but conventional (e.g. local/semilocal) approximations to the exchange-correlation(XC) functional show severe problems. Orbital-dependent XC functionals, in particular the efficient Localized Hartree-Fock(LHF) method [5,6,7] can be used to obtain more accurate energy levels and to correctly describe the energy-level alignment in organic-metal interfaces [8-9].
iv) For larger systems, such as biological molecules, a full-principles treatment can be obtained using the Frozen Density Embedding methods [10] which allows the determination of the properties of the whole system from its (embedded) subsystems.
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