Multiscale Modeling of Organic and Inorganic Nanostructures

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Current research in nanoscience and nanotechnology requires accurate computational tools at different length scale, to predict the electronic and the optical properties of different nanosystems, such as i) metal nanostructures, ii) semiconductor nanoparticles and iii) organic/inorganic interfaces.
i) Metal nanostructures, which can be used to increase the photoluminescence of emitters and in nanoplasmonics, requires a numerical solution Maxwell's equations [1];
ii) Semiconductor nanocrystals, which can be used for biological applications or in [opto]electronic devices, can be efficiently described using envelop function models [2];
iii) Organic-interfaces, which play a key role in [opto]electronic devices, are usually described within Density-Functional Theory (DFT) but conventional (e.g. local/semilocal) approximations to the exchange-correlation (XC) functional can show severe limitations. Orbital-dependent XC functionals can be used to correctly describe the energy-level alignment and the metal-molecule charge-transfer [3,4,5].

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