

Continuum solvation models for electronic dynamics and excitations in molecular solutes

S. Corni

Dipartimento di Scienze Chimiche, Università di Padova, Italy & CNR Istituto Nanoscienze, Modena, Italy

Continuum solvation models provide a computationally inexpensive way to include solvation effects in first principle calculations for molecules in solution. As such, they represent the standard approach for quantum chemical investigations of molecular solutes. From a theoretical point of view, their physically transparent formalism is also useful to inform developments of other multiscale approaches such as QM/MM methods with polarizable MM fields. Most relevantly for this contribution, they are also used to simulate phenomena where molecular electrons are dynamically perturbed and excited (e.g., by light in an optical spectroscopy). These applications, on one hand call for developments of continuum solvation models toward a real time description of solvation dynamics. On the other hand, they expose the consequences of core assumptions in continuum solvation (and polarizable QM/MM) models, and the role of the relative time scales of the solute and the solvent electronic responses. Formally similar problems are encountered in the description of the electronic dynamics of molecules interacting with environments more complex than solutions, such as plasmonic nanostructures (e.g., for surface enhanced spectroscopies and polaritonic chemistry). In this talk, I will present the work we performed in the last years to tackle the issues mentioned here, both from the theoretical and the computational points of view.