Polarizable Density Embedding for Proteins: Excited States in Complex Environments

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In this talk I will review recent progress within the polarizable embedding (PE) and polarizable density embedding (PDE) methods [1-8]. These computational models have both been developed with the aim of enabling calculations of general molecular response properties for large and complex systems, *e.g.* proteins. The PE model builds on the concepts from mixed quantum mechanics / molecular mechanics (QM/MM) schemes, whereas the PDE model is an extension and is formulated within the general framework of QM/QM/MM models. Both models thus represent focused models in which different parts of a large molecular system are described using different levels of approximations. A key concept associated with the PE/PDE models is the introduction of quantum mechanical response theory in combination with polarizable force fields (in PE). This allows for calculation and simulation of general molecular properties, *i.e.* properties relevant for optical and magnetic spectroscopies. We will discuss some recent applications of the PE/PDE models aimed at elucidating optical and magnetic properties of both solute-solvent and heterogeneous molecular systems highlighting the general flexibility and accuracy of this computational model. Finally, we will show how the PDE model recently has been extended to the case of covalently bonded environments, *e.g.* proteins.

References

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