Solvent Effects on Electronic Excited States

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The effective fragment potential (EFP) is a general model potential that is based in quantum mechanics. Recently, the EFP method has been interfaced with several quantum mechanics (QM) methods for excited electronic states, including CI singles (CIS), CIS with perturbative double excitations (CIS(D)), time-dependent density functional theory (TDDFT), equations of motion (EOM) coupled cluster (CCSD(T) theory, multi-reference perturbation theory (MRPT), and multi-reference CI (MRCI). In studying solvent effects on excited states, an interesting question is how important it is to include the response of the solvent method to the excited state electron density. A detailed analysis of the contributors to excited state solvent effects has been developed to address this question. Theoretical considerations, as well as applications of the EFP method to a variety of applications in excited state chemistry will be discussed.