INTRAMOLECULAR CHARGE TRANSFER STATES IN THE CONDENSED PHASE

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Time-Dependent Density Functional Theory (TDDFT) with long range corrected functionals[a] can give accurate results for the energies of electronically excited states involving Intramolecular Charge Transfer (ICT) in large molecules. If this is combined with a Molecular Mechanics (MM) representation of the surrounding solvent this technique can be used to interpret the results of condensed phase UV-Vis Spectroscopy. Often the MM region is represented by a set of point charges, however this means that the solvent cannot repolarize to adapt to the new charge distribution as a result of ICT and so the excitation energies to ICT states are overestimated. To solve this problem an algorithm that interfaces TDDFT with the polarizable force-field AMOEBA is presented; the effect of solvation on charge transfer in species such as 4,4'dimethylaminobenzonitrile (DMABN) is discussed.

[a] M.A. Rohrdanz, K.M. Martins, and J.M. Herbert, *J. Chem. Phys.* **130** 034107 (2008).