

Excited state gradients in polarizable QM/MM models: an induced dipole formulation

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Charge and structural properties of electronically excited states in embedded systems are strongly affected by the environment. Multiscale approaches where different levels of theory are combined in a single calculation, have shown to properly describe such effects combining accuracy with computational efficiency.

Here we present an extension of a fully polarizable QM/MM scheme to analytic excited state gradients following a Lagrangian approach [1, 2]. Time-dependent density functional theory is used as the QM method of choice, whereas the classical environment is treated in terms of a polarizable force-field, where the polarization is included through induced dipoles [3]. The method is applied to study of formation and relaxation of the bright excited state of an organic dye (DAPI) intercalated in a DNA pocket. The results indicate the non negligible effect of polarization between the DAPI and DNA pocket, in determining the fluorescence properties of the embedded dye [4].

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