MFCC-PDE: Polarizable Density Embedding for large biomolecules

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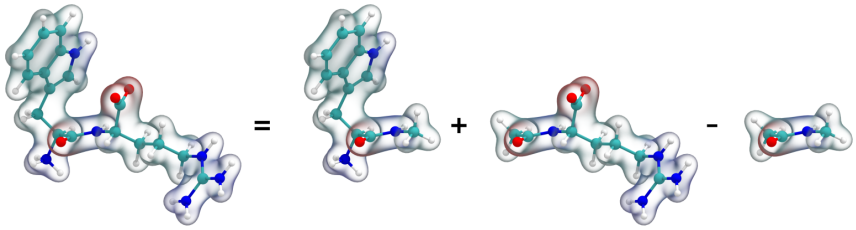
Polarizable Density Embedding[1,2] (PDE) is an extension of the well-established Polarizable Embedding (PE) model. The PDE model replaces the approximate multipole expansion in PE with exact quantum-mechanical electrostatics and further models non-electrostatic (Pauli) repulsion. Crucially, the inclusion of non-electrostatic repulsion solves the problem of electron spill-out[2] in QM/MM simulations. Both PE and PDE use the same classical description of polarization with a classical induced dipole model, which allows for a very efficient and accurate inclusion of the mutual polarization.
PDE has so far been restricted to treat solute-solvent systems, but we have now extended the model to cover much larger systems by applying a completely general Molecular Fractionation with Conjugate Caps (MFCC) strategy. The MFCC procedure is applied on a Fock matrix level

$$F^X_{\mu\nu} = \sum_{f=1}^{N_f} F^{X,f}_{\mu\nu} - \sum_{c=1}^{N_c} F^{X,c}_{\mu\nu}, \tag{1}$$

where X refers to the contribution from either the fragment density or repulsion operator. The resulting model, MFCC-PDE, is applicable to a wide range of systems, including proteins, DNA, lipids and supramolecular assemblies. MFCC-PDE is implemented in the Dalton program and is formulated within the general framework of response theory, which allows for the calculation of a wide range of molecular properties, e.g., excitation energies and multi-photon absorption strengths.



References

[1] J. M. H. Olsen, C. Steinmann, K. Ruud, and J. Kongsted, *J. Phys. Chem. A* **119**, 5344 (2015).

[2] P. Reinholdt, J. Kongsted, and J. M. H. Olsen, *J. Phys. Chem. Lett.* **8**, 5949 (2017).