Simple and efficient electrostatic embedding QM/MM method for modeling condensed phases using periodic boundary conditions

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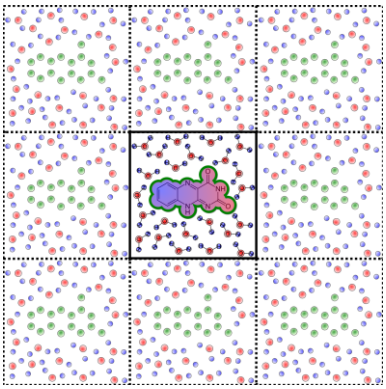

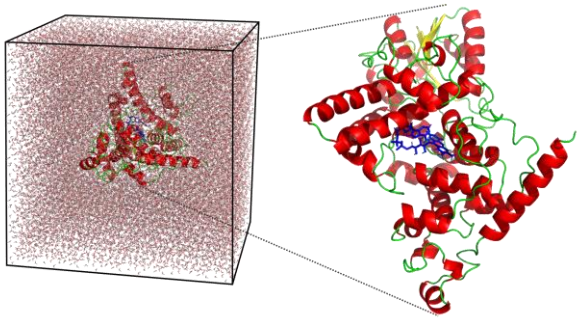

In this talk, I will present our recent development of a new, simple yet efficient electrostatic embedding Quantum Mechanical / Molecular Mechanics (QM/MM) model in Periodic Boundary Conditions (PBC).[1] Our method benefits from the *Nlog(N)* scaling of Smooth Particle Mesh Ewald (SPME),[2] for the treatment of long-range electrostatic interactions, and the advantages of Electrostatic Potential Fitted (ESPF) charge operators,[3] to approximately represent the QM density in replicas. This model allows the study of reactions and properties of condensed phase systems of arbitrary size.
To illustrate the efficiency of the method we have applied it to compute the lowest singlet excited state for a model of *Arabidopsis thaliana* cryptochrome 1 in water, which contains 93 000 atoms circa, using both Time-Dependent Density Functional Theory (TDDFT) and Restricted Open-Shell Kohn-Sham (ROKS), reproducing accurately the experimental absorption maximum.

[1] S. Bonfrate, N. Ferré, and M. Huix-Rotllant, J. Chem. Phys., **2023**, 158, 021101.
[2] U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee, and L. G. Pedersen, J. Chem. Phys., **1995**, 103, 8577.
[3] N. Ferré and J. G. Ángyán, Chem. Phys. Lett., **2002**, 356, 331.