Hybrid QM/MM Dynamics of Complex Systems within the AMOEBA Polarizable Embedding

Daniele Loco,[a] Louis Lagardère[a,b], Filippo Lipparini[c], Benedetta Mennucci[c], Jean-Philip Piquemal[a]

[a] *Sorbonne Université, CNRS, Laboratoire de Chimie Théorique, 75252 Cedex 05 Paris, France* [b] *Sorbonne Université, Institut des Sciences du Calcul et des Données, Paris, France*
[c] *Dipartimento di Chimica e Chimica Industriale, Università di Pisa, via G. Moruzzi 13, I-56124 Pisa, Italy*
daniele.loco@lct.jussieu.fr

In recent years lots of efforts have been devoted in the field of classical molecular dynamics (MD) for the development of force fields that explicitly account for polarization, but still efficient for the study of large systems. They include many-body effects, improving, in principle, flexibility and accuracy. Such improvement is still not enough for the description of many important phenomena in molecular sciences, such as chemical reactivity and photoinduced processes, due to their intrinsic quantum nature. In that respect, Hybrid Quantum Mechanics/Classical methods represents a very promising strategy as They combines the computational efficiency of a classical model with the required quantum description of the subsystem of interest.

In the last years we developed a Born-Oppenheimer (BO) hybrid QM/MM MD strategy, based on the coupling[1, 2] of Density Functional Theory (DFT) and the polarizable AMOEBA[1] force field. This approach involves the interplay between the Gaussian and Tinker suite of programs through a variational formalism allowing for a self-consistent relaxation of both the AMOEBA induced dipoles and the DFT electronic density at each MD step.

In this contribution we will present some new advances in the implementation of the code, and some recent applications involving molecular systems embedded in complex environments, such as DNA or protein matrices.

References

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