Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Hybrid QM/MM simulations of liquids with molecule exchange[1]

NOAM BERNSTEIN, Naval Research Laboratory, CSILLA VARNAI, University of Cambridge, IVAN SOLT, MONIKA FUXREITER, Hungarian Academy of Sciences, GABOR CSANYI, University of Cambridge — Many chemical reactions occur in a solvent, including essentially all biologically relevant ones. To describe these reactions accurately, one needs both a quantum mechanical (QM) description of the reaction site, as well as a large number of solvent molecule which affect the reaction via their electrostatic fields and free energy effects of their long-range structure. We present results of hybrid simulations that embed a density-functional theory QM region in a solvent region described with the CHARMM interatomic potential. Forces in the QM region are accurate, due to the use of force mixing and buffer regions. The methods allows for diffusion of molecules into and out of the QM region, a capability that improves the description of the local structure, and is essential for reactions where the transport of products is important for determining the reaction rate. We present results of the method on the structure of pure water, and dissolved ions. For pure water we show that the structure in the QM region reproduces the full QM results, and that it changes smoothly to the full MM result away from the QM region. We also show the structure of water around a dissolved Cl^- ion.

[1]This work partly funded by ONR contracts N00014-09-WX-2-1302 and N00014-09-1-1046, and the EU-FP7 ADGLASS Consortium.

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Date submitted: 28 Oct 2009 Electronic form version 1.4