NEW DEVELOPMENTS IN ADAPTIVE QM/MM: MOLECULAR SIMULATIONS OF AQUEOUS SYSTEMS

Rosa Bulo*

Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands
e-mail: r.e.bulo@uu.nl

We present the latest developments in multi-scale simulations of aqueous catalytic processes. Molecular dynamics simulations of chemical reactions in water can be significantly accelerated by exploiting the local nature of chemical reactivity, and describing a reactive region at the quantum mechanical (QM) level, while the environment is described at the more approximate molecular mechanical (MM) level. Difficulties arise due to the diffusive nature of the solution, involving water molecules that flow in and out of the reactive region during a molecular dynamics simulation. Adaptive QM/MM methods[1] allow molecules to change description as they flow across the border between the two regions. Here we present several new developments and challenges in the field, such as energy conserving simulations that yield accurate solvent structures, and accurate free energies for acid-base reactions.

1) R. E. Bulo, J. Sikkema, B. Ensing, L. Visscher, J. Chem. Theory Comput., **5** (2009), 2212.