Atomistic simulations for complex systems with chemical accuracy

Markus Meuwly

Chemistry Department, University of Basel, Klingelbergstrasse 80, CH-4056 Basel

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With recent advances in both, experiment and computer simulations, it has become possible to investigate the dynamics of small molecules in heterogeneous environments. This is of particular interest because small ligands can be used as an experimental probe to investigate the interior of proteins or other disordered materials.

Atomistic Simulations are an established computational method to investigate gas- and condensed-phase systems. Recent extensions to force fields incorporate more details in capturing electrostatic interactions and allow to more quantitatively understand particular processes. Here, I will describe some of these methods and their use to understand the energetics, [vibrational]spectroscopy and reactions in biological and physico-chemical systems. For myoglobin interacting with diatomic ligands the vibrational spectroscopy of the ligand[1,3,4,5] and its rebinding kinetics are long-standing problems in biophysics which continue to attract the attention of experimentalists and computational chemists. The relationship between spectroscopy and structure is an interesting problem in the physical chemistry of doped ices which play an important role in astrophysics.[2,3]

References