From MD simulations on large Biomolecules to DFT calculations on small systems

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The study of large biomolecular systems represents always a tough compromise between accuracy and computational cost. It is necessary to correctly sample the conformational space of the biomolecule and, for that, force field methods are usually a good choice. However, for the study the biochemical reactions, electronic structure methods are required (for a relevant part of the biomolecule).

Several examples will be presented in which the problem about the function of a biomolecule was tackled through a combination of different sized models using different computational approaches: Classical molecular dynamics simulations of the whole enzymes with explicit solvent, enhanced sampling MD, ONIOM medium sized models, DFT calculations on small models.

The enzymes that will be discussed are oxidoreductases (thioredoxin family enzymes, iron-sulfur metalloproteins, aldehyde oxidase), polymerases (reverse transcriptase, RNAP II), and a DNA repair enzyme.