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Combined Quantum Mechanical and Molecular Mechanical Modelling of Biomolecular Interactions

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Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Methods have been proved as a powerful computational technique in modelling enzyme mechanisms and biomolecular interactions. For systems as large as solvated proteins the method synergizes the advantages of both the Quantum mechanical (QM) and the Molecular Mechanical (MM) methods. A QM method is needed in order to model changes in the electronic structure including reaction mechanisms and is applicable to systems as big as a few hundreds of atoms. The MM method is applied for representation of the rest of the system and usually treats hundreds of thousands of atoms.

The QM/MM method uses the advantages of both the QM and the MM methods and hence its accuracy is due to the QM method and the speed up is due to the MM method. This volume of Advances in Protein Chemistry and Structural Biology contains comprehensive reviews covering current method developments and applications of the QM/MM method in modelling biomolecular systems.

Cover image: QM/MM-MD simulations using PUPIL interface. The figure shows the Cu-Ferritin cage as a basis to check multiple active zones simulation, and the HOMO orbital of the heme group in myoglobin protein. The calculation was done using the PUPIL interface between Amber and Gaussian. The image was prepared by Juan Torras, Benjamin P. Roberts, Gustavo M. Seabra, and Samuel B. Trickey, see chapter 1.

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