MAR06-2005-005887

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Reaction Path Reaction path potential for complex biomolecular systems derived from mixed QM/MM methods[1]

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The reaction path potential (RPP) follows the ideas from the reaction path Hamiltonian of Miller, Handy and Adams for gas phase reactions but is designed specifically for large systems described with QM/MM methods. RPP is an analytical energy expression of the combined QM/MM potential energy along the minimum energy path (J. Chem. Phys. 121, 89, 2004). An expansion around the minimum energy path is made in both the nuclear and the electronic degrees of freedom for the QM subsystem, while the interaction between the QM and MM subsystems is described as the interaction of the MM charges with polarizable QM charges. The input data for constructing the reaction path potential are energies, frequencies and electron density response properties of the QM subsystem. RPP provides a potential energy surface for rigorous statistical mechanics and mixed quantum/classical reaction dynamics calculations of complex systems, as will be shown for several enzymes. Recent further development in determining QM/MM free energy reaction paths will also be presented.

[1]in collaboration with Zhenyu Lu, Hao Hu and Steven Burger