QM/MM/MC Calculations of Organic and Enzymatic Reactions in Solution with the PDDG/PM3 Hamiltonian.

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The development of QM/MM methodology has allowed the study of organic and enzymatic reactions in solution in detail, precision and extents previously impractical by either QM or MM calculations. This talk will initially center on the need, development and implementation of the PDDG/PM3 Hamiltonian in the framework of QM/MM/MC simulations. Subsequently, some applications of this method to the calculation of several interesting organic and enzymatic reactions in solution will be discussed with emphasis on the structural and energetic results and their mechanistic implications.