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Challenges and advances in QM/MM methods for studies of energetics and dynamics of biological systems

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QM/MM approaches have become a popular tool in studies of large systems, yet the use of such approaches in accurate evaluations of reaction rates in proteins and solutions is very challenging. Unfortunately, quantitative studies require a combination of accurate (ab intitio based) potential surfaces and the ability of extensive sampling for proper evaluation of activation free energies and transmission factors. Our strategies for overcoming these problems are based on the use of an EVB potential surface as reference potential for ab initio sampling. The use of this powerful approach for studies of the redox potential of blue copper proteins and related problems, the autoionization of water in water and some enzymatic reactions will be described, emphasizing the requirements of stable and reliable results for biological processes.