Photo-processes in biological systems – Need for hybrid QM/MM with polarization

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Photo-processes in biology are fundamental to life itself, e.g., photosynthesis and light harvesting. However, accurate description of such processes is challenging, especially considering the need to depict the complex environment with sufficient accuracy. It requires a large number of degrees of freedom to be described and therefore, become impossible for any ab initio or purely quantum mechanical method. Hybrid quantum mechanical molecular mechanical (QM/MM) methods, that combine the accuracy of quantum mechanical methods and the speed and versatility of molecular mechanical methods, are used for these systems. Effective fragment potential (EFP) is a sophisticated, polarizable and non-empirical molecular mechanical method that is capable of treating the long range electrostatics and short range non-covalent interactions with sufficient accuracy. On the other hand, these systems are multi-reference in nature, and therefore, multireference electronic structure methods, such as spin flip MP2 and equation-of-motion coupled cluster or MP2 (EOM-CC or EOM-MP2) need to be used. We have developed hybrid methods based on EFP and EOM-MP2. In this talk, I will present some applications of the hybrid techniques to understand the excited state processes, especially in biological systems. I will also discuss our work on developing polarizable force fields based on machine learning techniques that can be applied to biological systems.

References

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