APPLICATION OF EFFECTIVE FRAGMENT POTENTIAL METHOS TO THE REDOX POTENTIAL OF GREEN FLUORESCENT PROTEIN

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Green fluorescent proteins (GFP) can be considered as a model for flurogenic dyes and are of importance in photovoltaic materials. It exhibits bright green fluorescence when exposed to blue light and has been an extremely powerful tool as non-invasive marker in living cells and extensibly used in molecular and cell biology. The understanding of the underlying electronic structure of these proteins and its chromophore is therefore crucial to the understanding of the mechanism for its optical properties.

The chromophore of the GFP is p-hydroxybenzylidene-imidazolinone (HBDI) and is embedded in the center of the β barrel of the GFP. Calculating redox potential of this chromophore is a challenging problem, especially in diverse solvents and protein environment. It is possible to carry out high-level accurate ab-initio calculation of ionization potential or electron affinity of the microsolvated chromophore or the bare chromophore. But, it is not possible to extend these calculations to bulk solvents due to the high computational cost. Effective fragment potential (EFP)[1,2] method gives us a convenient tool to understand such systems.

In our work, we have benchmarked the ionization energy and electron affinity of the microsolvated GFP chromophore calculated by combined EOM-IP-CCSD/EFP and EOM-EA-CCSD/EFP with the EOM-IP-CCSD and EOM-EA-CCSD calculations of the oxidized and reduced forms. We have carried out similar EFP-EOM-IP-CCSD and EFP-EOM-EA-CCSD calculations of ionization potential and electron affinity of GFP choromophore in bulk solvent generated by ab-initio molecular dynamics simulations.

[1] M. S. Gordon, L. Slipchenko, H. Li, J. H. Jensen, Annual Reports in Computational Chemistry, Volume 3, 177 (2007).
[2] D. Ghosh, D. Kosenkov, V. Vanovschi, C.F. Williams, J.M. Herbert, M.S. Gordon, M.W. Schmidt, L.V. Slipchenko, and A.I. Krylov, J. Phys. Chem. A 114, 12739 (2010).