Multilayer Approach to the IP-EOM-DLPNO-CCSD Method: Theory, Implementation, and Application

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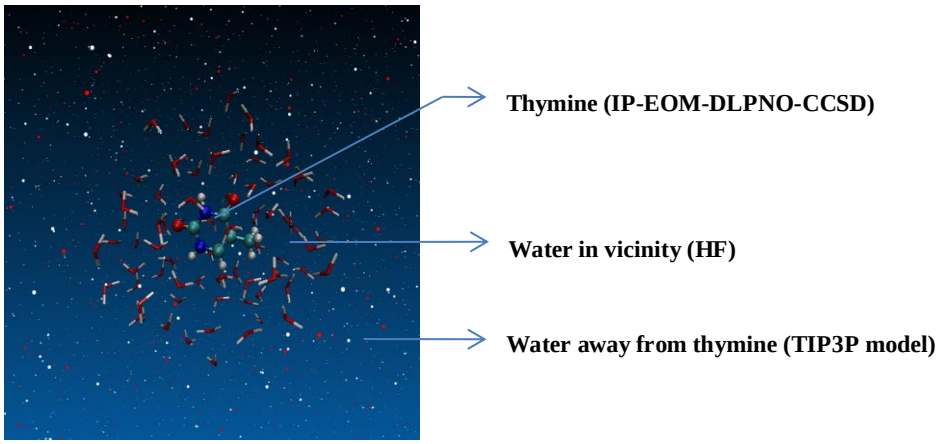

Three layer approach for studying the effect of bulk water on the IP & EA of Thymine

Many important chemical and biological processes take place in excited states. In the condensed phase, the surrounding environment plays a very crucial role in controlling and modulating such processes. However, a proper modeling of such environmental effects has always been a challenging task when it comes to the excited state instead of ground state as the excitation process involves a significant rearrangement of the wave function of the central fragment and the environment. We have developed a multi-layer scheme within the framework of EOM-CCSD method. The present scheme relies on the orbital localization to distinguish between different fragments within the system. The method is free from traditional problems of QM/MM method like over-polarization and cutting through the bonds. The resulting implementation is near black box and easy to use and is incorporated in a freely available quantum chemistry software. The accuracy and efficiency of the method is demonstrated by calculating ionization energies and electron affinities of solvated NABs, and DNA strand.

$$\hat{R}_k = \sum_{i,a} r_i^a \, a^+ i + \frac{1}{4} \sum_{i,j,a,b} r_{i_1 j_1}^{a_1 b_1} a_1^+ \, b_1^+ j_1 i_1$$

References:

[1] Sparta, M.; Retegan, M.; Pinski, P.; Riplinger, C.; Becker, U.; Neese, F. *J. Chem. Theory Comput.* **2017**, *13* (7),3198-3207

[2] Haldar, S.; Riplinger, C.; Demoulin, B.; Neese, F.; Izsák, R.; Dutta, A. K. *J. Chem. Theory Comput.* **2019**, DOI: 10.1021/acs.jctc.8b01263