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QM/MM Study of the Structural and Spectroscopic Properties of Monomeric Red Fluorescent Proteins

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The interest in the study and development of red fluorescent proteins (RFPs) has increased during the last years due to their many applications in biochemistry and biomedicine. We report here a combined quantum mechanical / molecular mechanical (QM/MM) study of the monomeric red fluorescent proteins DsRed.M1,[1] mStrawberry[2] and mOrange[2] using as QM component the self-consistent charge density functional tight-binding (SCC-DFTB)[3] method in molecular dynamics simulations and hybrid density functional theory in QM/MM geometry optimizations. We consider different variants of the chromophores as well as different protonation states of environmental residues. The QM/MM calculations provide an insight into the role of nearby residues concerning their interactions with the chromophore and their influence on structural and spectroscopic properties.Vertical excitation energies are computed using DFT/MRCI[4] and TDDFT as QM methods for the study of the spectra.

References

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