

Studying excited states in biomolecules with quantum Monte Carlo: A polarizing issue

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We will employ here quantum Monte Carlo methods to compute the excitation energies of realistic photosensitive biomolecules and combine the method with a variety of hybrid schemes commonly used to describe such complex systems. Using the prototypical examples of rhodopsin and green fluorescent protein, we will illustrate the difficulties one encounters in reconciling theory and experiments when modeling the protein-chromophore coupling via (static or responsive) electrostatic embedding. Our calculations clearly demonstrate that, ultimately, faithfully capturing the effects of the environment in these systems would require the quantum treatment of very large photoexcited regions.