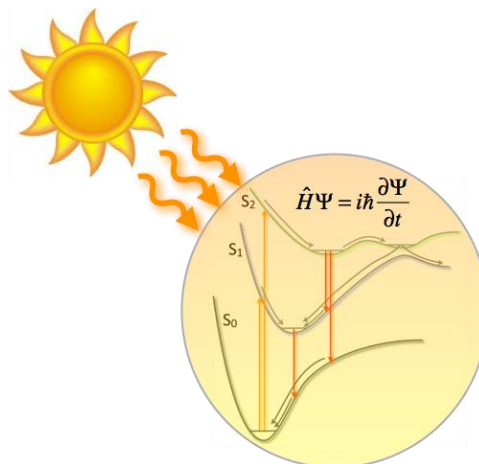


Quantum Mechanical Simulations of Electronic Excited States of Chromophores for Renewable Energy Applications

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Our research focuses on the theoretical simulation of the photochemistry of complex chromophores with applications in materials and energy science. To this goal, we are developing 1) accurate electronic structure methods based primarily on coupled cluster theory, and 2) multiscale models that are able to combine multiple levels of theory (quantum and classical mechanics) to describe environmental effects.



REU students will be involved in the theoretical simulation of absorption and emission spectra of promising chromophores for solar energy harvesting. This involves the calculation of energy minima in both ground and excited states, and of transition energies and properties. Students will use state-of-the-art quantum chemistry software, including the new methods developed in our group. Projects in methods and software development are also available for interested students. This work will provide training in electronic structure calculations and the use of the relative software, together with the opportunity to study the photochemistry of promising molecular systems.