
Molecules in Motion: Simulating the Operating Mechanisms of Photoactive Molecules

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In this talk, I will recount my quest to understand two practically important classes of photoactive molecules:

- Molecular solar thermal energy storage (MOST) is an emerging technology for the capture, storage, and controlled release of energy from solar radiation with the use of photoswitches - compounds which can be reversibly interconverted between two or more states through the action of light. Derivatives of norbornadiene (NBD) belong to the most promising candidates for the energy-storing material. Presently, I will discuss a computational investigation of the operating mechanism of NBD molecular switches with a push-pull substitution pattern, which combine high energy storage densities with good photoisomerization quantum yields.
- Aminobenzonitriles are model systems for intramolecular charge transfer, and for dual fluorescence. Their photophysics has been the subject of a long-standing controversy. I will outline how computer simulations of time-resolved spectra have helped tie in the available experimental data with the predictions of theory.