

Calculation of the properties of organic photovoltaics: charge separation and recombination

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This computer-based laboratory exercise looks at the critical properties of a model donoracceptor dyad. It utilizes a computationally efficient computational method, CNDO, to perform the electronic structure calculations either on a laptop PC or else on the internet at the NANO HUB. The basic aspects of molecular orbital calculations are considered, as well as some advanced applications such as multi-reference configuration interaction. These are used to provide a qualitative description of aromatic and quinonoid molecules as well as to make quantitative predictions about light absorption and emission, charge separation and recombination, and intersystem crossing. At the end, a diagram is produced encompassing the calculated energetics and kinetics of the primary photochemical processes of the dyad. Most significantly, the critical role of the condensed-phase environment in controlling the properties is stressed, as is the relationship between spectroscopic and electrochemical observations.