Large Scale Screening of Photochemical Transition Metal Centered Dyes

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Though many transition metal light harvesting dyes are in use, the search continues for more efficient and effective compounds to reduce make commercially viable light conversion and storage devices. Computational methods have been increasingly applied to understand the dyes currently in use and to aid in the search for improved light harvesting compounds. Semiempirical quantum chemistry methods have a well-deserved reputation for giving good quality results in a very short amount of computer time. The performance of newly optimized semiemirical basis sets are tested against a set of molecules whose geometries were optimized using a density functional theory (DFT) method. Beyond geometry, the main metric for light harvesting dyes is their UV/Visible spectra. Here we have developed a method to calculate approximate UV/Vis spectra using a modified PM7 semiempirical method. Using this re-parameterized method, a large set of transition metal centered light harvesters is screened, including expanded cage structures, electron donating and withdrawing groups, and various anchoring groups. These results clearly demonstrate the value of using semiempirical methods to screen chromophore geometries and excitations.