Automated Generation and Theoretical Predictions for Potential Near-Infrared (NIR) Dye Sensitized Solar Cells: Novel Theoretical Dye Properties

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Abstract

Dye-sensitized solar cells (DSCs) are simple to synthesize, low in cost, and tunable for usage. This makes them exciting candidates to replace silicon solar cells, which are difficult to manufacture and problematic to deploy. Additionally, they are susceptible to damage in extreme environments. Differently, DSCs are flexible and easily repaired making them ideal candidates for various applications. Current DSC technologies could be improved by varying the structure of the organic dye molecule in order to provide longer wavelength absorption in organic molecules. The triple donor method is one of the most common synthesis strategies for DSC construction. This method involves the combination of an electron donor, backbone, and electron acceptor to create the dye. Computational chemistry has the capability to automate this process by combining the three structures virtually and to provide the optical properties for the resulting dyes. The present work has analyzed over 2000 potential dyes in such a process. The theoretical dyes undergo B3LYP/6-311G(d,p) geometry optimizations, and the absorption properties are computed with CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p) and PBE0/6-311G(d,p). In every instance, CAM-B3LYP excitation energies are higher in energy than the benchmark, and PBE0 is higher. The combination of TD-DFT methods and a least squares fit (LSF) model are combined to produce a predicted value. Moreover, this computational methodology opens the door for faster utilization in novel applications such as human spaceflight and planetary colonization.