Screening Singlet Fission (SF) via Accessible Spectroscopic Methods in Acene-Derived Semiconductors

Kudrimoti, Avneesh (School: Paul Laurence Dunbar High School)

Traditional silicon solar cells are limited to approximately 33% efficiency, proposed by the Shockley-Queisser limit. Singlet fission (SF), a process in which one singlet exciton splits into two triplet excitons, offers a promising pathway to surpass this limitation, doubling charge carriers generated per absorbed photon. However, identifying SF-active materials requires specialized and expensive instrumentation. This study investigates if accessible spectroscopy can serve as a quicker screening method for SF in triisopropylsilylethynyl (TIPS)-functionalized acene semiconductors, reducing the samples passed onto expensive SF tests. Stock solutions of TIPS-pentacene, TIPS-tetracene, TIPS-anthracene, TIPS-benzodithiophene, and diphenyl-substituted derivatives were prepared in tetrahydrofuran (THF). UV-Vis spectroscopy was used to determine extinction coefficients and concentrations. Fluorescence spectroscopy was conducted across varying concentrations. Integrated emission intensities were plotted against calculated concentrations. Linear regression analysis was performed before and after correcting for reabsorption effects. While all compounds exhibit increasing reabsorption at higher concentrations, SF-active materials display greater first-peak emission shifts and greater departures from linear emission patterns compared to SF-inactive compounds. After accounting for reabsorption, SF-active materials maintain stronger nonlinearity, while SF-inactive compounds deviate from linearity at lower concentrations. These findings suggest that concentration-dependent fluorescence can serve as an accessible preliminary indicator of singlet fission activity. Expanding this method to a broader range of materials could establish a cost-effective screening framework for SF.

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