

Unlocking New Opportunities for the Photovoltaic Materials Market

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Abstract

Singlet fission (SF) is a photophysical process, occurring in organic materials and having the potential to boost the solar cells' efficiency. Our study aims at guiding the way for molecular design of compounds, capable of SF. Doping of quinoid structures with Se or/and N-atoms turns out to be a productive strategy for that. Through functionalization and pH modulation, we succeeded to establish rules that link the molecular characteristics to the SF proclivity. Quantum chemical calculations at an appropriate level of theory show that all modelled structures satisfy the conditions, required for a successful fission of singlet excitons.

Keywords: *singlet fission, organic photovoltaics, quantum chemistry, materials*