Interplay Bewteen Diradical Character and Stability in Singlet Fission Chromophores

Vaska Petakova
Faculty of Chemistry and Pharmacy
Sofia University
Sofia 1164, Bulgaria
vaska.petakova@abv.bg

Joanna Stoycheva
Faculty of Chemistry and Pharmacy
Sofia University
Sofia 1164, Bulgaria
stoycheva.joanna@gmail.com

Alia Tadjer
Faculty of Chemistry and Pharmacy
Sofia University
Sofia 1164, Bulgaria
fhat@chem.uni-sofia.bg

Julia Romanova
Faculty of Chemistry and Pharmacy
Sofia University
Sofia 1164, Bulgaria
jromanova@chem.uni-sofia.bg

Abstract

It was recently demonstrated that molecules with low to intermediate diradical character are good candidates for singlet fission chromophores and are therefore promising for photovoltaics application. On the other hand, the diradical character can also be associated with low stability and high reactivity – undesired molecular features for practical utilization. Therefore, in order to reveal the relationship between diradical character – stability – singlet fission propensity, we have performed quantum-mechanical calculations on a series of *o*- and *p*-quinone methides. Most of the investigated compounds are reported in the literature and data on their stability and reactivity are available. The study allows us to conclude on the impact of molecular stability on the excited state properties and to explore the compromise between diradical character and singlet fission propensity from stability perspective.

Keywords: *computational modelling, excited states, photovoltaics*

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