

Computational Screening for New Generation Photovoltaic Materials

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Abstract

The present study is devoted to singlet fission chromophores – a rare kind of molecules, which, upon excitation, may double the charge carriers in a solar cell, overcome the Shockley–Queisser limit and boost the development of new generation organic based solar cells. In order to find new potential singlet fission chromophores, we have developed computational screening procedure implementing quantum-chemical approaches, machine learning algorithms and chemometrics methods. The singlet fission propensity of the molecules is rated based on their diradical character. In order to prove our concept for finding new photovoltaics chromophores, we have created an open-access database. The computational screening procedure allows us fast preselection of potential singlet fission candidates, as well as to explore in detail the structure-properties relationships and to define new strategies for the design of such materials.

Keywords: singlet fission, excited states, semi-empirical, diradical character

Short biography

Dr. Julia Romanova is an assistant professor at the Department of Inorganic Chemistry of the Faculty of Chemistry and Pharmacy, University of Sofia. Her research interests are in the field of applied computational chemistry with special focus on organic and organometallic compounds with attractive optical, magnetic and conducting properties. Assist. Prof. Julia Romanova has co-authored 1 patent, 23 research papers and 3 book chapters. In 2011, she was received the national 'Eureka' Foundation Award for exceptional achievements in science for her work as an early-stage researcher. In the period 2012-2017 she gained international research experience working as a postdoctoral and research fellow at the University of Surrey (UK) and the University of Namur (Belgium). Assist. Prof. Julia Romanova was a fellow of the German Academic Exchange Service at the Max Plank Institute for Polymer research (Germany, 2006) and a fellow of the French Government at the University of Upper Alsace (France, 2007-2010). In 2019, she won a L'Oréal-UNESCO fellowship for Women in Science, Bulgaria.

