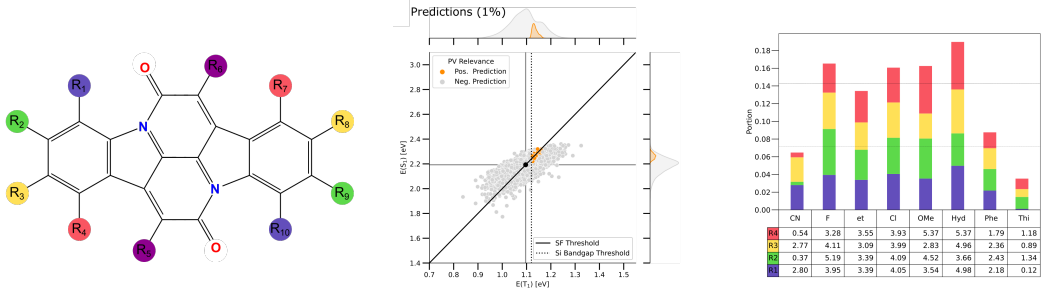
Electronic Structure Informatics of Singlet Fission in Indigoids

([1]*Department of Applied Chemistry, Chuo University*, [2]*Institute for Molecular Science, Okazaki*) ○Fabian Weber,[1] Hirotoshi Mori[1,2]

Keywords: Electronic Structure Informatics, Singlet Fission, Molecular Design, Machine Learning

To design photovoltaic cells that may go beyond the Shockley-Queisser limit, singlet fission (SF) has been identified as a potential upgrade to existing photovoltaic cell technology.[1] In SF, a singlet excited state located on one monomer can transition into a dimeric state of coupled triplets, which eventually decouples to yield two excited triplet states of lower energy from one photon. When the SF material's first triplet energy lies above the photovoltaic semiconductor's band gap this opens the possibility to exceed 100% internal quantum efficiency.[2] Even though several organic compounds have been identified as SF materials already, designing long-lived and efficient SF materials poses a large challenge: While it is widely agreed that there must exist an energetic requirement with respect to the excited states, the molecular design principles that promote SF are not yet fully understood.

To discover such common rules in SF molecules, in this work a chemical subspace of cibalackrot[3] with over 4 million molecules was studied, combining techniques of high throughput screening with predictions of excitation energies from machine learning. Choosing specific energy requirements, we first identify a number of potential SF molecules with triplet excitation energies above the silicon band gap and then proceed to extract common design rules using machine learning classification techniques. It is found that in cibalackrot-type molecules, there are direct correlations between the energetic condition and the atomic charges, as well as spin density in specific aromatic rings of the molecule.



1) M.C. Hanna, A.J. Nozik, *J. Appl. Phys.* **2006**, *100*, 074510. 2) M.C. Beard, J.C. Johnson, J.M. Luther, A.J. Nozik, *Phil. Trans. R. Soc. A* **2015**, *373*, 20140412. 3) W. Zeng, O. El Bakouri, D.W. Szczepanik, H. Bronstein, H. Ottosson, *Chem. Sci.* **2021**, *12*, 6159.