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Apr 29: Antoine Kahn (Princeton) | **Jun 24:** Barbara Hissa (Beilstein) | **Aug 21:** Richard Kaner (UCLA)

📅 Wednesday, April 29th | 🕒 14:00 Israel Time (07:00 AM EDT)

Singlet Fission and Triplet Transfer to Si and Metal Halide Perovskites: the Key Role of Interface Electronic Structure

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This talk first gives a short review the process of “singlet fission plus triplet transfer” and its theoretical benefits in boosting the efficiency of solar cells beyond the Shockley-Queisser limit. Much work has been devoted to this process over the years, yet the transfer of singlet fission-generated triplet excitons into solar cell absorbers, and silicon (Si) and perovskites in particular, has remained elusive. Tetracene (Tc) is a prototypical molecular singlet fission (SF) material. Singlet excitons formed upon absorption of photons with energy $h\nu \geq 2.4$ eV in Tc can undergo fission, generating two triplet excitons with energy equal to 1.25 eV. We look at a recent investigation of SF and triplet transfer from Tc to Si and the lessons it provides on the critical importance of the electronic structure of the interface between the triplet generating organic and the semiconductor. A successful structure is achieved by inserting an ultrathin (1 nm) layer of zinc phthalocyanine (ZnPc) to create a double interface Tc/ ZnPc/Si.[1] The electronic structures of Tc and ZnPc, and the energy level alignment across the double interface are fully determined by ultra-violet and X-ray photoelectron and inverse photoemission spectroscopies (UPS, XPS, IPES). It reveals that ZnPc forms a ladder structure that insures a sequential charge transfer to the absorber. The triplet dissociates at the ZnPc/Si interface, the electron is transferred to the Si conduction band minimum (CBM), leaving the hole in the ZnPc highest occupied molecular orbital (HOMO), and forming an interface charge transfer state ZnPc+ - Si- with energy between the triplet energy and the Si energy gap. The hole is then injected from the ZnPc HOMO to the Si valence band maximum (VBM). External quantum efficiency (EQE) measurements confirm partial transfer of the triplets to Si. Turning to the perovskite absorber, a similar Tc/ZnPc/perovskite double interface is investigated. The perovskite, MA(Pb0.45Sn0.55)I3, is optimized for an energy gap of ~ 1.20 eV. In this case again, the ZnPc/perovskite interface is shown to sustain an interface charge transfer state with energy intermediate between the Tc triplet and the perovskite energy gap, and EQE measurements confirm partial transfer of triplets to the perovskite absorber.[2]. These two cases, Si and MA(Pb0.45Sn0.55)I3, strongly argue for the importance of the interface electronic structure in the delicate process of triplet transfer.

[1] N. Nagaya et al., Joule, 9, 101965 (2025)

[2] Y. Ren et al., Joule, (submitted, 2026)

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