

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
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SPRING 2022

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GUEST SPEAKER

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TOPIC

The Prospect of Exciton Band Shape Engineering in Organic Materials: Perylene Diimide-Based
H_j- and hJ-Aggregates

ABSTRACT

The aggregated and crystalline phases of π -conjugated molecules and polymers continue to receive widespread attention as semiconducting materials for field effect transistors, light emitting diodes and solar cells. In such materials, the exciton band dispersion is a critical factor in determining the photophysical response and energy transport properties. In this talk the prospect of exciton band-shape engineering in organic materials is explored with applications made to π -stacks of perylene diimide chromophores.[1] In such stacks, the exciton band width and, in particular, the curvature at the band center, is determined by an interference between short-range coupling due to wave function overlap and long-range Coulomb coupling arising from transition dipole-dipole interactions.[2, 3] The crystal and solution phases of two perylene diimide (PDI) derivatives, N-phenyl PDI and tetraphenyl PDI are analyzed in detail.[1] In the crystal phases of both derivatives positive long-range coupling induces H-aggregate behavior, whereas counteracting short-range coupling induces J-aggregate behavior. As such, both derivatives display so-called HJ-aggregate properties. In N-phenyl PDI π -stacks, the stronger Coulomb coupling tilts the scales in favor of overall H-like behavior resulting in H_j-aggregates, characterized by a weak 0-0 vibronic photoluminescence (PL) peak, which increases with temperature. By contrast, in tetraphenyl PDI π -stacks, the short-range coupling dominates, resulting in hJ-aggregates, as characterized by dominant 0-0 emission. The prospect of band-shape engineering is discussed, for example, in terms of chemically induced or pressure- induced changes in molecular packing.

BIO

Frank Spano is a full professor at the Department of Chemistry at the Temple University. He has received his PhD from Princeton University in 1988 followed by postdoctoral research under the supervision of the Nobel laureate Prof. Shaul Mukamel. In his independent research, Prof. Spano has become known as a pioneer in developing theoretical models to describe molecular aggregates

and conjugated polymer photophysics and excited state dynamics. His group is particularly interested in how the complex interplay of long-range Coulomb exciton couplings, charge transfer, vibronic coupling, and disorder can be unraveled through the interpretation of well-defined spectral signatures.

References: [1] A. Oleson, T. Zhu, I.S. Dunn, D. Bialas, Y. Bai, W.Q. Zhang, M.J. Dai, D.R. Reichman, R. Tempelaar, L.B. Huang, F.C. Spano, Perylene Diimide-Based H_j- and h_J-Aggregates: The Prospect of Exciton Band Shape Engineering in Organic Materials, *Journal of Physical Chemistry C* 123 (2019) 20567-20578. [2] N.J. Hestand, F.C. Spano, Expanded Theory of H- and J- Molecular Aggregates: The Effects of Vibronic Coupling and Intermolecular Charge Transfer, *Chem. Rev.* 118 (2018) 7069–7163. [3] N.J. Hestand, F.C. Spano, Molecular Aggregate Photophysics beyond the Kasha Model: Novel Design Principles for Organic Materials, *Acc. Chem. Res.* 50 (2017) 341-350.

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