화학과 세미나

김형준 교수님
한양대학교 화학과

Heteroatom-Engineered Quantum Interference in Intramolecular Singlet Fission

Intramolecular singlet fission (iSF) is governed by the electronic coupling between the locally excited singlet and the multiexciton ^{1}(TT) state, and the covalent linker is the principal handle through which this coupling can be engineered. Here we show that heteroatom substitution in the linker acts as a quantum-interference (QI) switch that reroutes this coupling. Using RAS-2SF calculations on trimethylsilylethynyl-pentacene dimers, we find that nitrogen doping of a meta-phenylene linker leaves the fission energetics essentially unchanged while modulating the nonadiabatic coupling by up to eight-fold, with the effect determined by dopant position rather than dopant number. The magic-ratio-rule framework rationalizes this behaviour quantitatively: doping at the 2- and 6-positions contributes with opposite phase, so that 2,4-disubstitution amplifies transmission constructively whereas 2,6-disubstitution cancels exactly and restores the destructively interfering parent. Full-orbital transport-pathway analysis reproduces the same connectivity-based trends. Together these results establish heteroatom-controlled QI as a design principle for multiexciton formation kinetics, and suggest a route toward linkers engineered at the level of individual coupling pathways.

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