Functional Polycyclic Aromatics: Tailored Organic Materials for Light and Charge

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Polycyclic aromatic frameworks offer a powerful route to organic materials that manage both charge and excited states, but practical deployment requires controlling stability, energy levels, and intermolecular photophysics. I will outline a broader research theme that couples molecular architecture engineering with programmable chromophore assembly to translate π-systems into function.

First, I will address stability and band-gap tuning in PAH-like semiconductors by heteroatom incorporation and targeted benzannulation, introducing a new indoloindolizine class in which ring fusion patterns modulate frontier orbitals in ways that challenge simple "more conjugation = smaller gap" expectations. Guided by aromaticity principles, π-expansion and fusion topology provide a rational handle to tailor HOMO–LUMO gaps and optoelectronic behavior.[1]

Second, I will expand the design space with furan-based polycyclic systems, leveraging the heteroaromatic core to access π-extended architectures with distinctive electronic structures and high modularity.[2] In particular, we developed furan-based helicenes with an intrinsic push–pull character, providing a tunable platform for chiroptical emitters that deliver circularly polarized luminescence (CPL).

Third, I will move beyond isolated chromophores to well-defined multichromophore architectures that exploit through-space coupling and precise geometry to steer excited-state pathways. Using scaffolds such as hexaphenylbenzene and porphyrins, we created acene oligomers that enable efficient singlet fission and quintet-state formation, accelerate triplet–triplet annihilation upconversion by bypassing diffusion-limited steps, and support controlled singlet-oxygen handling relevant to photocatalysis and photomedicine.[3,4,5]

Together, these directions establish a unified design strategy for tailored organic materials for light and charge, linking synthetic structure control to device-relevant electronic and photonic function.

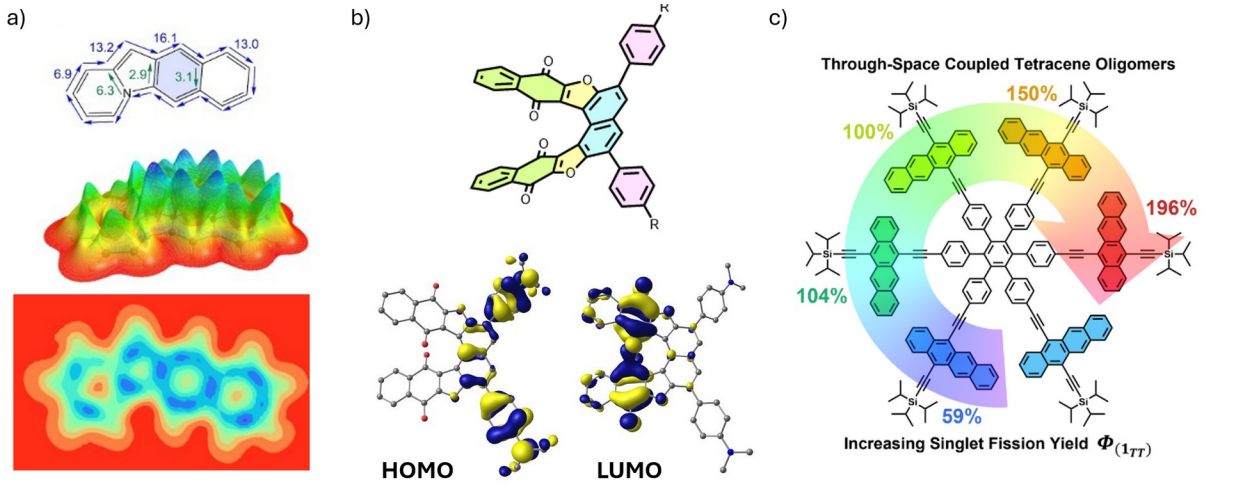

Figure 1: a) Indoloindolizines, b) furane-based helicenes, c) tetracene oligomers.

References

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