Functional Polycyclic Scaffolds and Their Charged States

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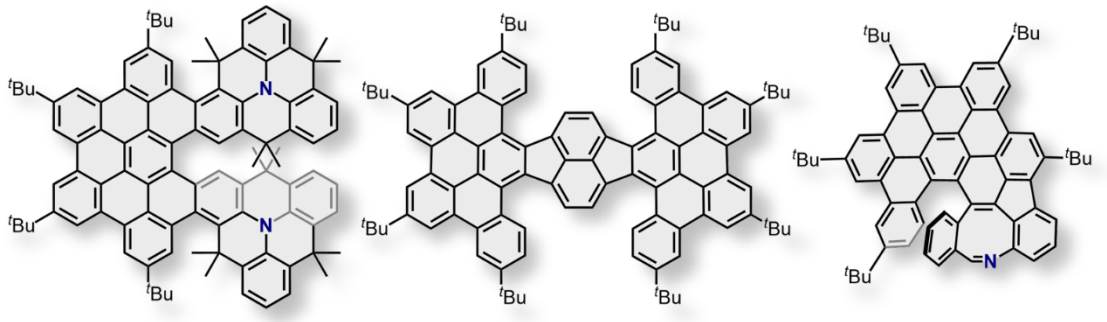
We use the selective incorporation of non-benzenoid rings and heteroatoms into the sp^2-carbon-based polycyclic scaffolds to efficiently modulate their structural, optoelectronic, and materials properties.

While the embedding of π-conjugated 5-membered rings facilitates electron uptake through the formation of aromatic cyclopentadienyl anion-like subunits, the 8-membered cyclooctatetraene with its characteristic saddle-shaped geometry imparts amphoteric redox activity through aromatic stabilization of the respective 6π-electron dication and 10π-electron dianion. The 7-membered cycloheptatriene units provide for the generation of an aromatic tropylium cation with negative curvature.

In addition, the nitrogen readily adopts a planar sp^2-hybridized geometry to provide for efficient electronic communication of its lone pair with the surrounding π-system. Such a nitrogen center can be reversibly oxidized to the corresponding radical cation with superior stability due to efficient spin and charge delocalization throughout the π-conjugated framework.

As discussed in this talk, this approach yields a wide variety of unprecedented polycyclic scaffolds with exciting properties that are of interest both as valuable objects for fundamental studies and as functional materials for diverse applications.



References

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