Computational Insights into the Synthesis and Photophysics of Curved and Extended Nanographenes

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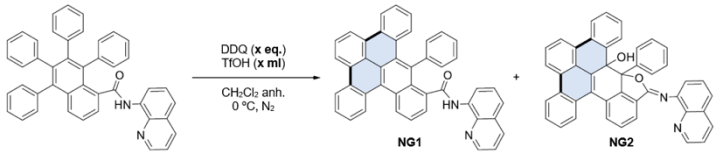
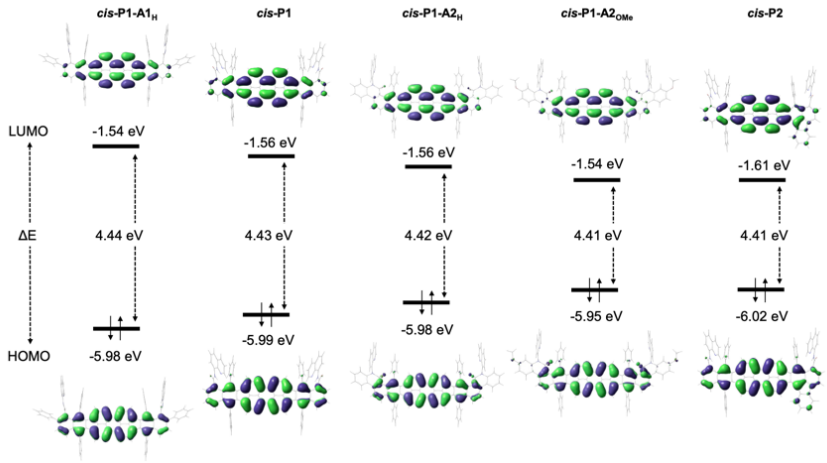
We present a computational study of the synthesis and photophysical behavior of novel nanographenes (NGs) developed via bottom-up Scholl ring fusion reactions. These reactions takes the advantage of aromatic homologation intermediates previously obtained by the *Ribas* group through Ni-catalyzed C(sp^2)–F activation.[1] While two distinct mechanistic pathways have been proposed for the Scholl reaction, its fundamental mechanism remains under debate.[2]



Here, we provide DFT-supported mechanistic insights into the formation of furanol-bearing NGs under moderately acidic conditions, comparing competing pathways and rationalizing their feasibility.[3]

In parallel, a shortcut to highly soluble, bent perylene-based NGs was developed via a two-step strategy starting from non-perylene homologation precursors. Thorough computational analysis elucidated the relationship between emission wavelengths and structural modifications, showcasing a rational design strategy for tuning photophysical properties in nanographenes.[4]



This work highlights the essential role of theoretical approaches in understanding structure–property relationships and guiding the rational design of nanographenes.

References

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(2) Rempala, P.; Kroulík, J.; King, B. T. Investigation of the Mechanism of the Intramolecular Scholl Reaction of Contiguous Phenylbenzenes. *The Journal of Organic Chemistry* **2006**, *71* (14), 5067-5081. DOI: 10.1021/jo0526744.

(3) Sala, J.; Capdevila, L.; Berga, C.; de Aquino, A.; Rodríguez, L.; Simon, S.; Ribas, X. Luminescent Chiral Furanol-PAHs via Straightforward Ni-Catalysed Csp2−F Functionalization: Mechanistic Insights into the Scholl Reaction. *Chemistry – A European Journal* **2023**, *n/a* (n/a), e202303200. DOI: https://doi.org/10.1002/chem.202303200.

(4) Capdevila, L.; Sala, J.; Berga, C.; de Aquino, A.; Parella, T.; Blancafort, L.; Rodríguez, L.; Simon, S.; Ribas, X. Shortcut to highly fluorescent perylene derivatives: from fluoranthene fissure coupling to late-stage aromatic extension - **2025** (Submitted)