Electronic Structure Properties of [*n*]Cyclacenes: Semi-Empirical and Wave Function Approaches

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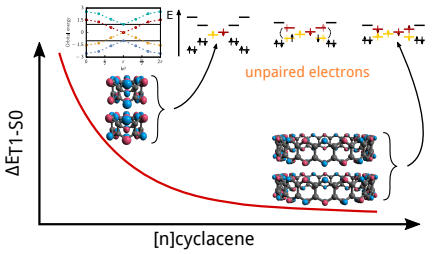

Cyclacenes have been subject of studies for the last 30 years and are still under active investigation because of their complicated electronic structure and their potential applications[1, 2]. Similarly to their "cousins" systems, the linear polyacenes, theoretical investigations have been proved difficult from a methodological perspective, which resulted in contradicting results. In this contribution, the investigation of different properties such as the total position spread tensor (TPS) and the singlet-triplet energy gap (ST gap) as a function of the system size will be presented at different levels of theory, namely by a semi-empirical Hückel approach and by wave function theory[2, 3]. The obtained results show a decreasing ST gap and an increasing radical character with increasing system size, which is in agreement with the most recent results obtained using TAO-DFT[1].

[1] C.-S. Wu, P.-Y. Lee, J.-D. Chai, *Nat. Sci. Rep.* **6**, 37249 (2016).

[2] S. Battaglia, N. Faginas-Lago, D. Andrae, S. Evangelisti, T. Leininger, *J. Phys. Chem. A* **121**, 3746 (2017).

[3] S. Battaglia, H.-A. Le, G. L. Bendazzoli, N. Faginas-Lago, S. Evangelisti, T. Leininger, *in preparation*.