Triarylmethyl-based 1D Conjugated Polymers: A Highly Tunable Quantum Materials Platform

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One-dimensional conjugated polymers (1DCPs) that host periodic arrays of unpaired electrons are gaining increasing attention as atomically-precise correlated materials for future quantum technologies.[1-3] 1DCPs based on triarylmethyls (TAM) are particularly interesting, due to the persistent nature of TAM radicals and the possibility to control the delocalization of their unpaired electrons via different means.[4] Here, I will summarize recent density functional theory (DFT) studies where the unique electronic and magnetic tunability of TAM 1DCPs has been demonstrated. First, I will talk about the co-existence of competing electronic states in these systems: namely the multiradical antiferromagnetic (AFM) and the closed-shell quinoidal (QUI) states.[5] Then I will explain how the QUI configuration enables the realization of topologically trivial or non-trivial phases in TAM 1DCPs which, in turn, may be engineered via aryl-ring twist angles.[6] Finally, I will present our latest theoretical results where nitrogen-substitution has been used as a tool to engineer the quantum ground-state of the corresponding mixed-valence 1DCPs (see **Figure 1**).[7]

References

[1] Gröning, O. et al. Nature 560, (2018) 209–213
[2] Cirera, B. et al. Nat. Nanotechnol. 15, (2020) 437–443
[3] González-Herrero, H. *et al. Adv. Mater.* 33, (2021) 2104495
[4] Ratera, I. et al. Journal of Materials Chemistry C 9, (2021) 10610–10623
[5] Alcón, I. et al. RSC Advances 11, (2021) 20498–20506
[6] Alcón, I. et al. Adv. Funct. Mater. 34, (2024) 2409174
[7] Sánchez De La Cruz, L. K., et al. Phys. Chem. Chem. Phys. (2026) https://doi.org/10.1039/D5CP04664E

Figures

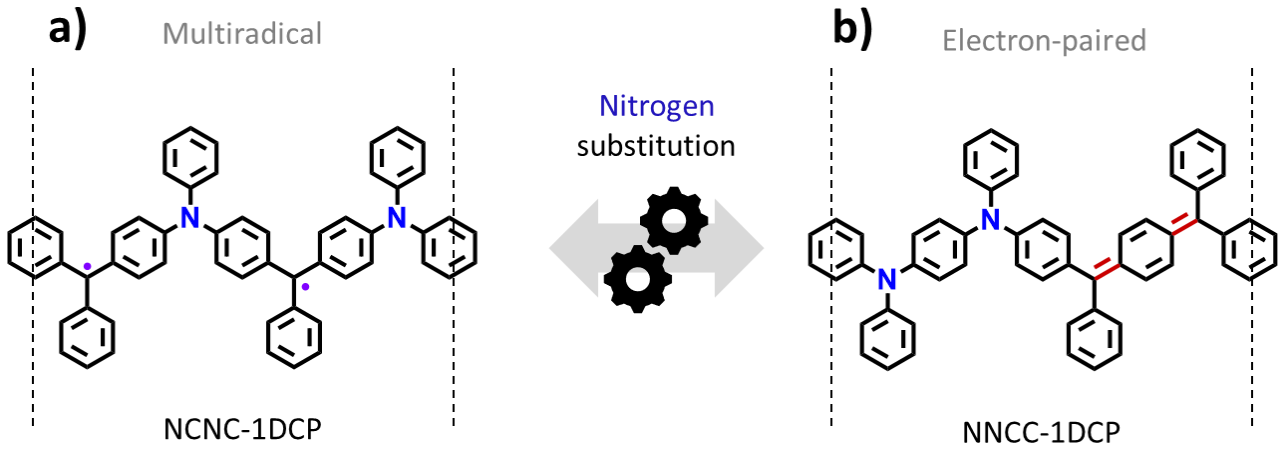

Figure 1: In TAM mixed-valence 1DCPs, a periodic nitrogen-substitution may be used to set **a)** a robust multiradical AFM ground-state or **b)** a closed-shell (electron-paired) QUI one.