Multiradical 1D and 2D conjugated polymers: novel platforms to control electron pairing, spin, and topological physics

Isaac Alcón
Institute of Theoretical and Computational Chemistry, Department of Materials Science and Physical Chemistry, Universitat de Barcelona, C/ de Martí i Franquès, 1-11, Les Corts, 08028, Barcelona, Spain
ialcon@ub.edu

Today, 1D and 2D carbon nanomaterials are receiving increasing attention for nanoelectronics, spintronics and quantum technologies.[1] This is partly due to their structural and chemical versatility, thanks to organic synthesis, leading to highly tunable electronic and magnetic properties. In this talk I will focus on carbon nanomaterials made of π-conjugated organic radicals (**Figure 1**). More concretely, I will summarize the progress in the design, modelling and realization of triarilmethyl (TAM) 1D and 2D conjugated polymers (1DCPs, 2DCPs, respectively). TAMs host a π-conjugated unpaired electron, and so are promising building blocks to tailor exotic quantum phenomena with atomic precision. I will briefly explain our theoretical predictions on the complex electronic structure of TAM 2DCPs,[2] the possibility to induced π-electron-pairing by stretching these 2D materials (**Figure 1**),[3] the emergence of magnetic frustration in mixed-valence TAM 2DCPs,[4] and the experimental efforts towards the synthesis of TAM 2DCPs.[5] Finally, I will also show more recent work on how to engineer topological phases via aryl-ring twisting in TAM 1DCPs,[6] also discussing potential implications for their 2D counterparts.

References

[1] H. Wang, H. S. Wang, C. Ma, L. Chen, C. Jiang, C. Chen, X. Xie, A. P. Li, X. Wang. *Nature Reviews Physics*, 3 (2021) 791–802
[2] I. Alcón, F. Viñes, I. de P. R. Moreira, S. T. Bromley, *Nat Commun*, *8* (2017) 1957
[3] I. Alcón, R. Santiago, J. Ribas-Arino, M. Deumal, I. de P. R. Moreira, S. T. Bromley, *Nat Commun*, *12* (2021) 1705
[4] I. Alcón, J. Ribas-Ariño, I. de P. R. Moreira, S. T. Bromley, *J Am Chem Soc*, *145* (2023) 5674–5683
[5] S. Wu, M. Li, H. Phan, D. Wang, T. S. Herng, J. Ding, Z. Lu, J. Wu, *Angewandte Chemie International Edition*, *57* (2018) 8007–8011
[6] I. Alcón, L. M. Canonico, N. Papior, J. Garcia, A. W. Cummings, J. Tremblay, M. Pruneda, M. Brandbyge, B. Paulus, S. Roche, *Adv Funct Mater*, 34 (2024) 2409174

Figures

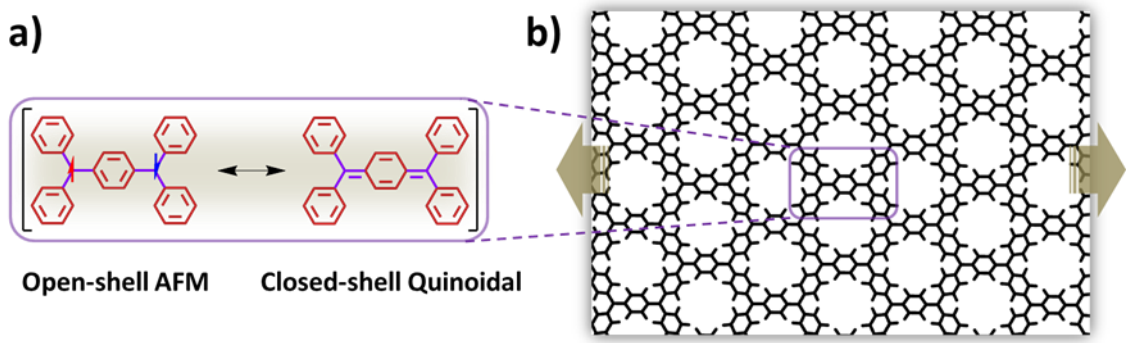

Figure 1: Some TAM 2DCPs may be understood as the 2D version of well-known organic bi-radicals (a). However, 2DCPs permit controlling molecular-scale properties, such as π-electron-pairing (a), via external means: e.g. uniaxial strain (b).[3]