

Towards new 2D quantum materials from single-layer chemically-expanded graphenic lattices

Stefan T. Bromley¹

Isaac Alcón, Raul Santiago, Jordi Ribas, Mercè Deumal, Ibério de P.R. Moreira

¹University of Barcelona / ICREA, Barcelona, Spain

s.bromley@ub.edu

Graphene displays a weakly correlated semimetallic electronic structure associated with its extended π -system of highly delocalised electrons. Early theoretical proposals to increase the electronic correlation in graphene suggested expanding the graphenic lattice to induce increased electron-localisation and the emergence of new gapped electronic states (e.g. antiferromagnetic/AFM). For pristine graphene, the high in-plane strains required to induce such states-are experimentally unattainable. An alternative approach is to “insert” additional carbon atoms between the trigonal sp^2 nodes of the 2D honeycomb lattice (i.e. chemically expanding the graphenic lattice). This procedure leads to a family of 2D materials known as graphynes. We have recently shown that many graphynes indeed display non-graphenic correlated gapped AFM states [1]. Such correlated graphynes are, however, chemically reactive and difficult to stabilize. Here, we focus on a class materials based on protected trigonal sp^2 carbon nodes. This can be achieved by using persistent radical building blocks (e.g. triphenylmethyl radicals) to construct such 2D materials (i.e. 2D covalent organic radical frameworks – 2D CORFs) in a bottom-up fashion. We show that the resulting chemically-expanded graphenic materials have the potential to exhibit a range of correlated electronic states (e.g. AFM Mott insulator, quantum spin liquid, exotic magnetic states) which, moreover, can be tuned by mechanical and chemical means [2,3,4]. 2D CORFs could thus provide a new single-layered materials platform for future carbon-based quantum technologies.

References

- [1] G. Lleopart, M. Lopez-Suarez, I. de P. R. Moreira, S. T. Bromley, *J. Chem. Phys.* 157 (2022), 214704.
- [2] I. Alcón, J. Ribas-Arino, Ibério de P.R. Moreira, S. T. Bromley, *J. Am. Chem. Soc.* 145 (2023) 5674.
- [3] I. Alcón, R. Santiago, J. Ribas-Arino, M. Deumal, I. de P. R. Moreira, S. T. Bromley, *Nat. Commun.* 12 (2021) 1705.
- [4] R. Santiago, I. Alcón, J. Ribas - Arino, M. Deumal, I. de P. R. Moreira, S. T. Bromley, *Adv. Funct. Mater.* (2021) 31, 202004584

Figures

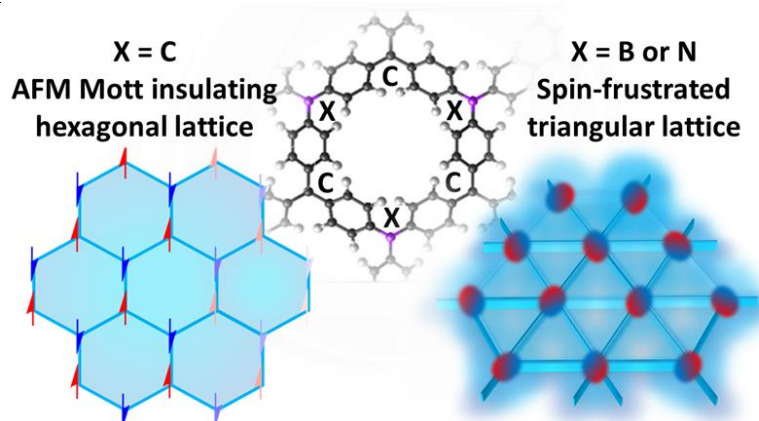


Figure 1: AFM Mott insulating / spin-frustrated states in chemically-expanded graphenic lattices [2].