Magnetic Carbon Tomas Heine

It is generally accepted that carbon is the most versatile element of the periodic table, and it offers a plethora of compounds ranging from biology to materials science. While the list of fascinating properties carbon materials offer is long, they are not yet famous for magnetism.

Indeed, most carbon materials are diamagnetic. Defects, dopants and dangling bonds can introduce paramagnetic centers without the potential to generate magnetic ordering. Recently reported magic-angle twisted bilayer graphene may become ferromagnetic due to a half-filled flat band at the fermi level and spin-orbit coupling [ACS Nano 21 (2021) 4299]. A spectacular early report on magnetic carbon in pressurized fullerenes [Nature 413 (2001) 716] was found to be caused by defects and the paper has been retracted five years later.

We propose an alternative concept to generate carbon materials with strongly coupled magnetic centers. Our materials are based on molecular triangulene and its derivatives, aromatic molecules intrinsically carrying one or two unpaired electrons. Using covalent linkages that preserve electron conjugation, we construct two-dimensional polymers with honeycomb-kagome lattice. The magnetic coupling between the monomers is facilitated by the linker groups. This has been examined in detail for the dimers [JACS 145 (2023) 19303]. When extending this concept to 2D polymers, we predict magnetic carbon materials with intriguing electronic structure that includes orbital ferromagnetism, while it maintains the Dirac and flat bands which are characteristic for the honeycomb-kagome lattice of the underlying 2D polymer.