Altermagnetism in π-conjugated covalent organic frameworks

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Altermagnetism is the name that received a new type of collinear magnetism[1,2] with promising applications in spintronics[3]. This spin broken-symmetric phase presents alternating moments and zero net magnetism but, unlike regular antiferromagnets, and similar to ferromagnets, there is no Kramers degeneracy in the bands structure[4]. For the altermagnetic phase to emerge, it is necessary that each magnetic block is related with the adjacent by a crystal rotation. The previous requirement hinders the possibility of altermagnetism in 2D frameworks made of open-shell nanographenes with just alternant rings. Here we show that it is possible to overcome this eventuality by including non-alternant rings with 7 carbon atoms in the magnetic block, which opens the possibility of designing D_{2h} nanographenes. As an example, we select the simple dibenzoheptalene, which has a S=1 ground state. Then, adjacent dibenzoheptalene units present antiferromagnetic coupling when connecting an hexagon with an heptagon via a covalent bond, hence showing altermagnetism when extended in a 2D π-magnetic framework. Additionally, we also explore the possibility of turning the system in a covalent organic framework by including linkers, which we expect to be more plausible in an eventual synthesis experiment.

References

[1] L.Smejkal, R.González-Hernández, T.Jungwirth, J.Sinova. Sci. Adv. 6, 23, eaaz8809 (2020)
[2] L.Smejkal, J.Sinova, T.Jungwirth. Phys.Rev.X 12, 031042 (2022)
[3] L.Smejkal, J.Sinova, T.Jungwirth. Phys.Rev.X 12, 040501 (2022)
[4] J.Krempasky et al. Nature 626: 517-522 (2024)

Figures

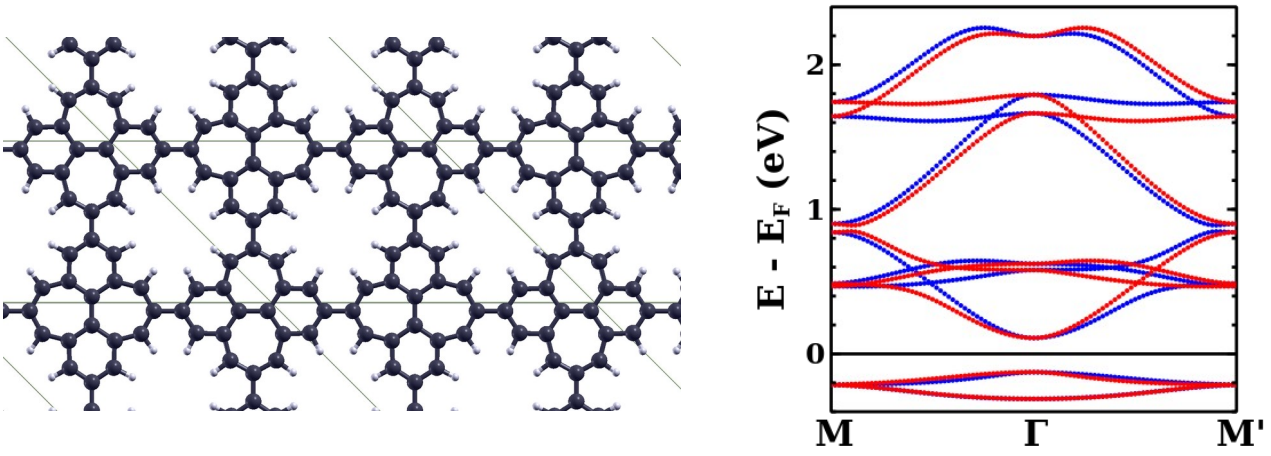

Figure 1: (Left) Relaxed dibenzoheptalene 2D crystal; (right) its corresponding spin polarized bands structure of the altermagnetic phase calculated with DFT.