

## Dipolar linkers as electric field responsive switches for magnetic 2D organic materials

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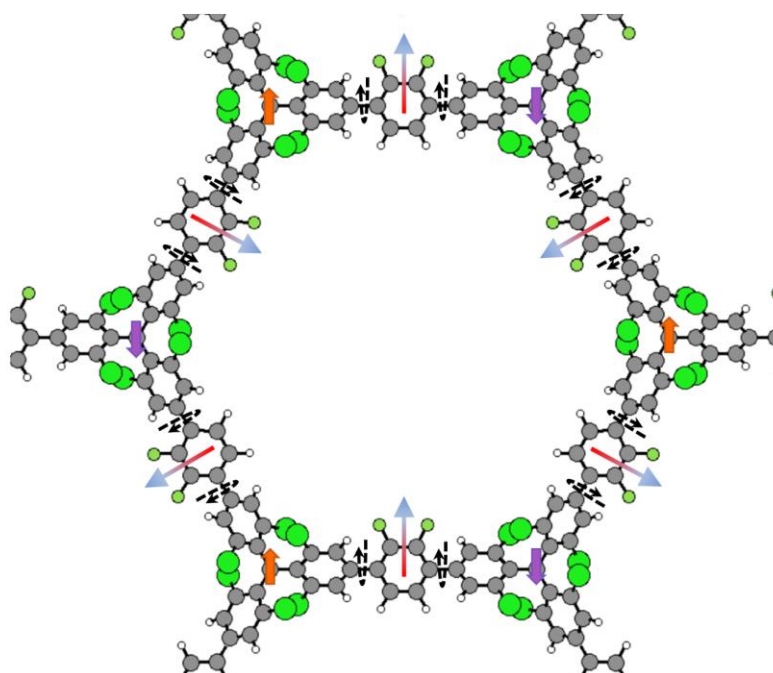
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A 2D-covalent organic radical framework (2D-CORF) has been chemical-designed from polychlorotriphenylmethyl (PTM) spin-localized radical nodes joined by difluorobenzene dipolar linkers. Density functional theory (DFT) calculations have shown that the linker conformation with respect to the material plane modifies the exchange spin coupling between PTMs, achieving a maximum  $J$  coupling variation of  $75 \text{ cm}^{-1}$ . A set of moderate electric fields have been applied to an isolated diradical excised from the extended 2D-network, revealing significant conformational changes of the linker with respect to the zero-field case, due to the coupling of the linker dipole moment and the electric field. These variations enable electric field induced conformational control [1]. Consequently, the proposed 2D-CORF is a responsive material with intrinsic switches in its structure. Extended 2D-material DFT calculations reveal flat bands whose low dispersion is independent of the linker conformation, a signature of its Mott insulator behaviour. The high spin-localization in the extended 2D-CORF system leads to it having very similar zero field behaviour to the isolated diradical. The strong analogy between molecular and extended system mean that the properties of the latter can largely be understood by relatively computationally inexpensive calculations of the former.

### References

- [1] K. Jutglar, R. Santiago, J. Ribas, S. Bromley Phys. Chem. Chem. Phys. 23, (2021), 3844

### Figures



**Figure 1:** 2D-CORF made of PTM spin centers and dipolar difluorobenzene linkers.