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Electronic and magnetic properties of ring-shaped and chiral molecules from first-principles

Molecular magnets are systems of great technological appeal for a broad range of applications.
In the first part of my poster I discuss the magnetic properties of two ring-shaped molecular magnets with eight transition metal atoms: Cr_8 and V_8, as obtained from ab initio Hubbard-corrected DFT calculations. Our results highlight a significant difference between the two systems, with V's partially occupied 3d states amplifying the effects of curvature on the magnetic properties through anisotropies and Dzyaloshinskii-Moriya chiral couplings.
The second half of the poster focuses on the relationship between structural chirality and its effects on electronic and transport properties. Fully relativistic ab initio calculations were able to reveal an interesting interplay between structural and electrons' chirality and, in particular, the possible occurrence of spin-polarised currents. This fundamental connection could contribute to explain the origin of Dzyaloshinskii-Moriya couplings and also the chirality-induced spin selectivity these systems exhibit in transport phenomena.

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