Highlights

RESEARCH AREA 2 - **Functional and Complex Materials for Innovative Electronics and Sensing** - 2022

"Curved Magnetism in CrI_3"

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PHYSICAL REVIEW LETTERS 128 (2022) 177202

Curved magnets attract considerable interest for their unusually rich phase diagram, often encompassing exotic (e.g., topological or chiral) spin states. Strain gradients can strongly impact magnetism via a curvature-induced modification of the spin coupling parameters, commonly referred to as flexomagnetism. Micromagnetic simulations are playing a central role in the theoretical understanding of such phenomena; their predictive power, however, rests on the availability of reliable model parameters to describe a given material or nanostructure. We used noncollinear magnetic calculations within Density Functional Theory (DFT), with and without spin-orbit coupling (SOC), to investigate the interplay of curvature and magnetism in monolayer CrI_3. Besides revealing a crossover between two spin states of distinct symmetry, our calculations demonstrate that the effects of SOC are essential for a quantitatively (and sometimes even qualitatively) accurate description of the flexomagnetic coupling parameters.

This work has been supported by the Swedish Research Council (Grant no. 2018-06807), MICINN-Spain (Grant no. PID2019–108573GB-C22), Severo Ochoa FUNFUTURE center of excellence (CEX2019-000917-S), Generalitat de Catalunya (Grant No. 2017 SGR1506), the EU Horizon 2020 program ERC (Grant no. 724529), PRIN-MIUR projects (Grant No. 2017Z8TS5B and Grant No. 2017YCTB59) and NFFA-MIUR Italy project.

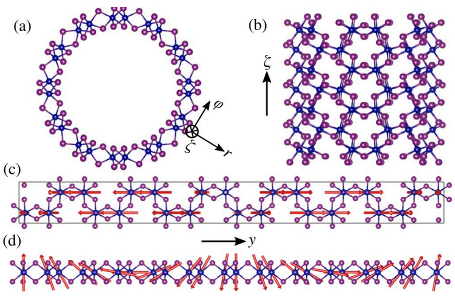

Fig. 1: Curvature effects are studied in CrI3 nanotubes using cylindrical coordinates (a), (b). A ferromagnetic state in the nanotube takes the form of a spiral in this reference frame, as when unrolling the nanotube (c),(d).

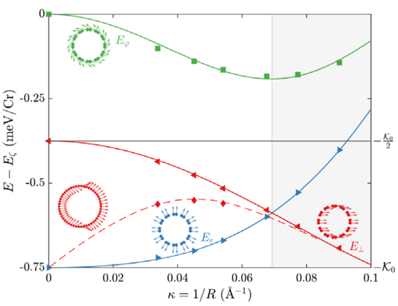

Fig. 2: Energies of magnetic states with spins along radial, tangential and azimuthal direction as a function of curvature. Points are DFT energies, lines display the continuum model results. Dashed line shows the energy of a two-domain state.

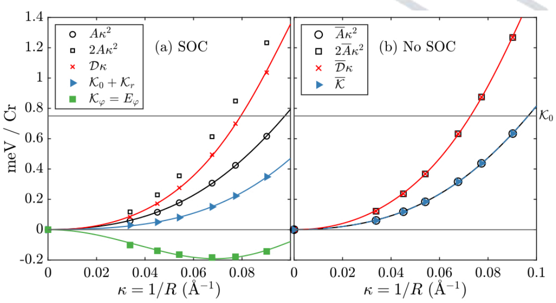

Fig. 3: Energy contributions of spin-coupling parameters $A\kappa^2$ (exchange), $D\kappa$ (Dzyaloshinskii-Moriya), $\mathcal{K}$ (anisotropy) obtained by mapping DFT results with (a) and without SOC (b) onto the continuous model, revealing the impact of relativistic effects on the curvilinear spin Hamiltonian.