Pseudo Jahn-Teller mediated ferromagnetic to antiferromagnetic crossover in d^9-ion (Cu^{2+}, Ag^{2+}) layered perovskites

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Oxide and fluoride layered-perovskites containing d^9-ions (Cu^{2+}, Ag^{2+}) display, suprinsingly, quite different geometric and magnetic structures. Here, we describe the electronic states of these systems using first- and second-principles simulations and we interpret these results using (i) electrostatics and (ii) a valence-bond model that allows us to address both superexchange and pseudo Jahn-Teller at the same time. This model indicates that a high-symmetry tetragonal configuration favors the kind of antiferromagnetic state characteristic of oxides while systems with an orthorhombic distortion beyond a threshold (usually involving a 0.1Å movement of the ligands), typical of fluorides, display a ferromagnetic state.

Inspired by pseudo Jahn-Teller effect we explore what would happen when epitaxial strain is applied, which would favor higher symmetry. Our simulations show that for a compressive strain of 5.1% it is possible for fluoride systems to transition to an antiferromagnetic state that closely resembles those of high-Tc oxide superconductors.

The authors acknowledge financial support from Grant PGC2018-096955-B-C41 funded by MCIN/AEI/ 10.13039/501100011033 and by "ERDF A way of making Europe", by the European Union.

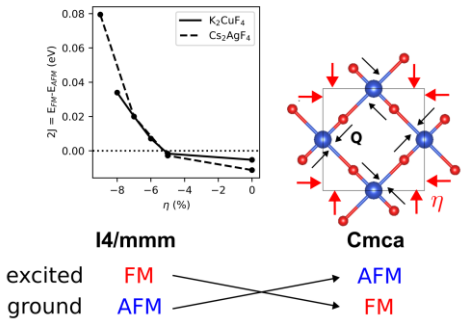

Figure caption: Strain triggers ferromagnet-antiferromagnetic crossover