$Ca_3Ru_2O_7$: Interplay among degrees of freedom and role of the exchange and correlation

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$Ca_3Ru_2O_7$ is an antiferromagnetic (AFM) polar metal and is considered a fascinating material because it displays a wide range of remarkable electronic phenomena such as colossal magnetoresistance, spin-wave and multiple phase transitions, among others. Understanding these phenomena has been a hard task due to several discrepancies among experiments and between experiment and theory [1]. Recent studies have given new perspectives about the origin of their phase transitions, evidencing that the wealth of the physical properties are governed by spin-orbit interactions (SOI), strong correlations and structural distortions. However, the role of fundamental interactions such as Coulomb and SOI has not been clarified yet [1-2]. In this research, we study the electronic structure of $Ca_3Ru_2O_7$ through ab-initio calculations, and we discuss the interplay among magnetism, Coulomb interaction, spin-orbit coupling and lattice degrees of freedom using different exchange and correlation approximations. Besides, we explore different paths to manipulate the magnetic states of this compound (see Fig.1) through lattice deformation, aiming to evidence novel quantum phases and propose new experiments.

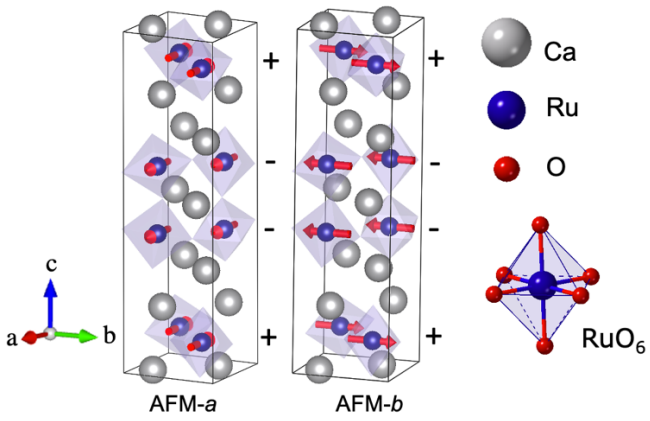

Figure 1: $Ca_3Ru_2O_7$ in two antiferromagnetic phases, AFM-a and AFM-b, with ferromagnetic coupling within the layers and antiferromagnetic coupling between the bilayers. The +/- signs represent the relative orientation of the Ru in-plane magnetic moments.

[1] Igor Markovíc, *et al*. Proceedings of the National Academy of Sciences, 117(27):15524–15529, 2020.
[2] Danilo Puggioni, *et al*. Physical Review Research, 2(2):023141, 2020