Magnetic phases in the quasi-one dimensional $A_2Cr_3As_3$ (A=Na, K, Rb, Cs) superconductors

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Very recently, the $A_2Cr_3As_3$ (A=Na, K, Rb, Cs) [1] family of superconductors has been discovered. They are quasi-one-dimensional with double-walled nanotubes propagating along the c-axis and the Cr-atoms form triangles in the a-b plane, but the hybridization between different nanotubes is relevant [2,3]. Referring to the magnetism, theoretical investigations [4] suggest that the triangular geometry tends to frustrate antiferromagnetism. However, significant phonon instabilities have been found [5]. The Cr-triangles in the double walled subnanotubes $[(Cr_3As_3)^{2-}]_\infty$ are no longer equilateral, this could lead to an absence of frustration. Here we study the magnetism for the $A_2Cr_3As_3$ compounds and the parent compound KCr_3As_3 [6], by using density functional theory approach, in the cases of presence of the distortions in the Cr-triangles recently predicted [5]. We show that the strong interplay between the lattice and the spin degrees of freedom promotes a new collinear ferrimagnetic ground state within the chains [7]. We predict that in the region of parameters corresponding to a regime of moderate correlations the $A_2Cr_3As_3$ compounds are non-magnetic but on the verge of the magnetism, sustaining interchain ferromagnetic spin fluctuations while the intrachain spin fluctuations are antiferromagnetic. We also show that uniaxial strain is a viable tool to tune the non-magnetic phase towards an interchain ferromagnetic instability [8]. We are confident that this investigation can provide relevant insights about the interplay between superconductivity and magnetism in this class of materials.

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