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Impact of spin-orbit coupling on the magnetism of Sr_3MIrO_6 (M = Ni, Co) XUEDONG OU, HUA WU, Fudan University, LABORATORY FOR COMPUTATIONAL PHYSICAL SCIENCES TEAM — Recently, Iridates have recently drawn considerable attention due to their significant spin-orbit coupling (SOC) effect and possibly exotic properties [1]. In this work, we demonstrate, using density functional calculations, that the SOC of Ir^{4+} ions plays an essential role in determining the antiferromagnetism of hexagonal spin-chain materials Sr_3MIrO_6 (M=Ni, Co) by tuning the crystal-field level sequence and altering the Ir-M inter-orbital interactions. Owing to the SOC effect, the single t_{2g} hole of the Ir^{4+} ion resides on the e'_g upper branch and gives rise to the Ir^{4+}-M^{2+} antiferromagnetic coupling. In absence of the SOC, however, the single t_{2g} hole would occupy the crystal-field a_{1g} singlet instead, which would mediate an unreal ferromagnetic exchange This work clarifies the nature and the origin of the intra-chain Ising antiferromagnetism of Sr_3MIrO_6(M = Ni, Co) [2].

[1] B. J. Kim, et al., Phys. Rev. Lett. 101, 076402 (2008)
[2] X. Ou and H. Wu, Sci. Rep. 4, 4609 (2014); Phys. Rev. B 89, 035138 (2014).

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