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Total energy calculations for magnetic $La_{2/3}S_{1/3}rMnO_3/SrRuO_3$ bilayers YONGBIN LEE, BENJAMIN CAES, BRUCE HARMON, Ames Laboratory US DOE — . Recently positive exchange bias was reported for ferromagnetic $La_{2/3}Sr_{1/3}MnO_3/SrRuO_3$ (LSMO/SRO) bilayers which indicated anti-ferromagnetic exchange interaction across the interface [1]. To address the physical origin of this anti-ferromagnetic exchange interaction, we have performed first principles calculations with both ferro, and anti-ferromagnetic interface structures. We have found that the anti-ferromagnetic interface is preferred to ferromagnetic case energetically. The calculations indicate the interfacial O 2p orbitals and their interaction with Mn, Ru spin polarized 3d orbitals are critical for this anti-ferromagnetic interface preference. In this talk, we will discuss the total energy calculations with various magnetic structures near the interface. [1] X. Ke *et al.* Appl. Phys. Lett. **84**, 5458 (2004)

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