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Predicting Hidden bulk phases in $Sr_3Ru_2O_7$ from surface phases[1]
PABLO RIVERO, CHEN CHEN, ROYING JIN, Louisiana State Univ - Baton Rouge, VINCENT MEUNIER, Rensselaer Polytechnic Institute, E. W. PLUMMER, WILLIAM SHELTON, Louisiana State Univ - Baton Rouge — Double-layered $Sr_3Ru_2O_7$ has received phenomenal attention as it exhibits an overabundance of exotic phases when perturbed. Recently it has been shown that the surface of this material displays significantly different properties than in the bulk due to the surface induced tilt of the RuO_6 octahedra [1]. Here we report detailed first principles calculations of the surface structure, and the structure property relationship. Tilt of the octahedra drive the surface into a much less conducting state than in the bulk due in part to the different electronic properties of the two Ru atoms in the first RuO_2 layer of the bilayer. The broken symmetry at the surface causes a tilt and enhanced rotation of the octahedra only present in the first (surface) bilayer. Theoretically the surface is ferromagnetically ordered but the stability with respect to the antiferromagnetic phase is small ($\simeq$ 11 meV). We have calculated the bulk properties under uniaxial pressure, which induces a tilt and drives the bulk into an antiferromagnetic-insulating state. [1] C. Chen, W. Chen, J. Kim, V. B. Nascimento, Z. Diao, J. Teng, Biao Hu, Guorong Li, Fangyang Liu, Jiandi Zhang, Rongying Jin, and E. W. Plummer, Phys. Rev. B 94, 085420 (2016).

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