Abstract Submitted
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Electronic structure of square planar nickelates revisited: relationship to cuprates[1] ANTIA S. BOTANA, Argonne National Laboratory, VICTOR PARDO, Universidade de Santiago de Compostela, WARREN E. PICKETT, University of California Davis, MICHAEL R. NORMAN, Argonne National Laboratory — Based on ab initio calculations, a close connection between the Ruddlesden Popper layered nickelates and high temperature superconducting cuprates is established. The electronic structure of $La_4Ni_3O_8$ and $La_3Ni_2O_6$ is similar to that of cuprates not only in terms of filling of d-levels (close to d^9) but also because they show Ni^{1+}(S=1/2)/Ni^{2+}(S=0) stripe ordering. The Ni^{2+} ions are in a low-spin configuration (S=0) yielding an antiferromagnetic arrangement of Ni^{1+} (pseudo Cu^{2+}) S=1/2 ions like the long-sought spin-1/2 antiferromagnetic insulator analog of the cuprate parent materials. The analogy extends further with the main contribution to the bands near the Fermi energy coming from hybridized Ni-$d_{x^2-y^2}$ and O-p states [1]. These results bring renewed justification that layered nickelates of this type are cuprate analog systems that are promising for studying the interplay between structure, magnetism, and superconductivity. [1] A. S. Botana, V. Pardo, W. E. Pickett and M. R. Norman. Phys. Rev. B 94, 081105(R)(2016)

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