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Molecular correlated insulating state in low-valence layered nickelates VICTOR PARDO, WARREN E. PICKETT, University of California Davis — In recent years, there has been an effort on artificially creating Fermi surfaces that resemble those of the superconducting cuprates. A Ni^{3+}:d^7 (one e_g electron) configuration can be made into the electron-like analog of the d^9 (one e_g hole) cuprate electronic structure.[1] Another cleaner alternative would be to grow low-valence Ni^{+}:d^9 compounds, which have recently become available through synthesis[2] of members of the series $La_{n+1}Ni_nO_{2n+2}$. We present LDA+U calculations on the layered compounds $La_4Ni_3O_8$ [3] and $La_3Ni_2O_6$, with three and two NiO_2 layers, respectively. Electron count implies very low Ni formal valencies: 1.33+ and 1.5+, respectively. If charge order is present, Ni^{+}:d^9 could occur in a geometry similar to that of the cuprates. However, this is not the case. Both compounds are insulators, which we can attribute to quantum confinement in the NiO_2 tri/bi-layers. The only states close to the Fermi level are Ni $d_{3z^2-r^2}$, which couple along the c-axis (Ni trimers or dimers). The insulating behavior must be viewed from a molecular orbital viewpoint, after AFM order within layers has narrowed the bands. Insulating behavior is that of a "molecular" Mott insulator rather than a charge-ordered insulator.

[1] J. Chaloupka and G. Khaliullin, *PRL* **100**, 016404 (2008).
[2] V. V. Poltavets *et al.*, *Phys. Rev. Lett.* **102**, 046405 (2009).
[3] V. Pardo and W.E. Pickett, arXiv:1008.2707.

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