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Charge-ordering transitions without charge differentiation[1]

YUNDI QUAN, University of California Davis, VICTOR PARDO, Departamento de Fisica Aplicada, Universidade Santiago de Compostela, Spain, WARREN PICKETT, University of California Davis — The distorted perovskite nickelate system $RNiO_3$ (R=rare earth except La) undergoes a metal-insulator transition (MIT) at a temperature that varies smoothly with the R ionic radius. This MIT is accompanied by structural transition which leads to two inequivalent Ni sites in the cell, and has been explained by charge ordering (CO): charge is transferred between the Ni1 and Ni2 sites in a long-range ordered fashion. Experimental data on core binding energies, ionic radii, and Mossbauer shifts are interpreted in terms of Ni cation charges of $3\pm\delta$ with, for example, $\delta \approx 0.3$ for $YNiO_3$. Making use of first principles DFT results and a new approach not invoking integration of the charge density, we find[2] that the Ni $3d$ occupation is identical (to high accuracy) for the two Ni sites. We also present results for other compounds (La_2VCuO_6, $YNiO_3$, $CaFeO_3$, $AgNiO_2$, V_4O_7), all of which have distinct "charge states" that have identical $3d$ occupation. This quantitative procedure will be discussed and some implications will be outlined.

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[2] Y. Quan, V. Pardo, and W. E. Pickett, Phys. Rev. Lett. (2012, in press)

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