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Electron Doping of $SmNiO_3$ from First Principles

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Rare earth nickelates exhibit a rich temperature-composition phase diagram involving charge, orbital and magnetic ordering. Recent experimental work on samarium nickelate ($SmNiO_3$) has demonstrated that $SmNiO_3$ can be doped with interstitial hydrogen in a reversible manner, resulting in a large increase in resistivity and band gap [1]. To elucidate this behavior, we used the first-principles density functional theory (DFT) + U method to study the effect of added electrons on the crystal and electronic structure of $SmNiO_3$. Specifically, we relaxed starting structures obtained by adding electron concentrations of $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$, and 1 per Ni, compensated by a uniform positive background, to various low energy structures of pure $SmNiO_3$, which include either an oxygen-octahedron shape distortion or a breathing distortion characteristic of disproportionation. We find that the added electrons localize on the nickel sites resulting in a high spin Ni^{2+} configuration, leading to a large gap between the occupied and unoccupied e_g orbitals [2]. We also present results with the addition of hydrogen atoms at the same concentrations, optimizing their positions as part of the relaxation process, that show the same change in electronic structure and the band gap.

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[2] F. Zuo, P. Panda, M. Kotiuga, J. Li, M. G. Kang, C. Mazzoli, H. Zhou, A. Barbour, S. Wilkins, B. Narayanan, M. Cherukara, Z. Zhang, S. K. R. S. Sankaranarayanan, R. Comin, K. M. Rabe, K. Roy, and S. Ramanathan, ArXiv e-prints (2017), arXiv:1703.01209 [cond-mat.mtrl-sci].