

Abstract Submitted
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Electron doping of SmNiO₃ from first principles MICHELE KOTIUGA, KARIN M. RABE, Department of Physics and Astronomy, Rutgers, The State University of New Jersey — Rare earth nickelates have rich phase diagrams involving charge, orbital and magnetic order. In past experimental work, doping SmNiO₃ with interstitial hydrogen at room temperature has resulted in a new insulating state, characterized by a large change in the resistivity [1]. In this work we use the first-principles density functional theory (DFT) + U method to study the effect of added electrons on the crystal and electronic structure of SmNiO₃. We consider added electron concentrations of $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$ and 1 electron per Ni, starting from various low energy structures of pure SmNiO₃, which include either an oxygen-octahedron shape distortion or a breathing distortion characteristic of disproportionation. We analyze the changes in the local crystal and electronic structure and magnetic ordering, and relate the changes to the changes in optical and transport properties observed experimentally.

[1] J. Shi, Y. Zhou, S. Ramanathan, Nat Comm 5, 4860 (2014)

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