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Unusual valency and magnetic order in silver nickelates SERGEY STRELTSOV, Institute of Metal Physics, Ekaterinburg, Russia, M.D. JOHANNES, I.I. MAZIN, Naval Research Laboratory, D.I. KHOMSKII, II. Physikalisches Institut, Universität zu Köln, Köln, Germany — Ag_2NiO_2 forms as a triangular based layered nickelate, with a structure identical to the well-studied alkali nickelates $LiNiO_2$ or $NaNiO_2$, but with a double layer of Ag between the oxide planes. The metallic intercalant ions give rise to highly unusual valence state for silver: $Ag^{1/2+}$. We show that the reason for the underoxidation is that the two silver ions form extremely strong bonding-antibonding bands, pushing the lowest Ag-s derived band beneath the (filled) O p complex. This additionally preserves metallicity down to the lowest measured temperatures and gives rise to complex, competing magnetic interactions. The resulting spin fluctuations may explain the large discrepancy (too large for phonon renormalization) between calculated and measured linear specific heat coefficients. Our calculations do not support a controversial cooperative Jahn-Teller distortion, but a comparison with calculations and experiments for single-layer AgNiO2 suggests that magnetically driven charge disproportionation may instead explain the observed structural transition.

Michelle Johannes
Naval Research Laboratory

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