

Abstract Submitted
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First-principles study of the electronic structure of NiS and NiO¹
JOAQUIN NOYOLA, MENG TAO, QIMING ZHANG, University of Texas at Arlington — First-principles calculations of the electronic structure of NiS and NiO are performed. The exchange-correlation schemes of GGA, DFT+U and hybrid functional have been applied. The resulting band structures for each scheme are compared and analyzed to assess the reliability of the GGA, DFT+U, and hybrid functional.

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