Abstract Submitted
for the TSS12 Meeting of
The American Physical Society

First-principles study of the electronic structure of NiS, NiS_2, and Ni_3S_2 JOAQUIN NOYOLA, QIMING ZHANG, University of Texas at Arlington — First-principles study of the electronic structure of NiS, NiS_2, and Ni_3S_2 are performed. DFT+U and HSE hybrid functional are used as the primary exchange-correlation schemes. The resulting electronic structures at various phases are analyzed, and the results compared with previous experimental and theoretical work.

Joaquin Noyola
University of Texas at Arlington

Date submitted: 21 Feb 2012 Electronic form version 1.4