First-principles study of the electronic structure of NiS, NiS₂, and Ni₃S₂ JOAQUIN NOYOLA, QIMING ZHANG, University of Texas at Arlington — First-principles study of the electronic structure of NiS, NiS₂, and Ni₃S₂ 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.