Abstract Submitted for the OSF16 Meeting of The American Physical Society

Strain effects in the electronic structure of  $CrN^1$  TOMAS ROJAS SOLORZANO, SERGIO E. ULLOA, Ohio University — Chromium nitride (CrN) has a promising future for its resistance to corrosion and hardness, and fascinating magnetic and electronic properties. CrN presents a phase transition in which the crystal structure, magnetic ordering, and electronic properties change at a (Neel) temperature 280K. Thin films from different labs exhibit different conductance behavior at low temperature. We performed ab initio calculations using the LSDA+U method, and estimate the interaction between the Cr-3d and N-2p orbitals, by analyzing the band structure. We also calculate effective masses and investigate the effect of strain fields in the electronic structure to understand the electronic behavior near the phase transition.

<sup>1</sup>Supported by NSF DMR-1508325

Tomas Rojas Ohio University

Date submitted: 11 Sep 2016

Electronic form version 1.4