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Strain effects in the electronic structure of CrN[1] TOMAS ROJAS, 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 groups exhibit varied conductance behavior at low temperature. We have 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 near the optical gap (0.2 eV). We also calculate effective masses and investigate the effect of strain fields on the electronic structure. Our results show that for compressive strain 1.3% the band gap closes, suggesting that realistic strains could cause a significant change in the electronic structure and could contribute to explain under what experimental conditions the material has metallic behavior. The changes in the effective mass derived from our calculations show a large anisotropy, which would result in anisotropic charge carrier mobility. The mass anisotropy is found to be connected with the magnetic ordering in the lattice.

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