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Nitrogen vacancy effects on the electronic structure of CrN[1]
TOMAS ROJAS, SERGIO E. ULLOA, Ohio University — Chromium nitride (CrN) is believed to be a small indirect gap semiconductor with interesting electronic and magnetic properties. It exhibits a phase transition at T 280K in which both the electronic and magnetic structures change from a paramagnetic cubic rock-salt to an antiferromagnetic orthorhombic structure. However, the transport properties of CrN thin films are not fully settled, exhibiting metallic and semiconducting behavior at low temperatures in different situations. In particular, the impact of nitrogen vacancies and other defects on the transport properties are yet to be analyzed in detail. We have performed ab initio calculations using the LSDA+U method to examine the effect of N vacancies in bulk CrN. By replacing or removing a nitrogen atom in an appropriately large supercell, we study the accompanying deformations of the lattice structure as well as the energetics and spatial distribution of the associated charge and spin distribution of the defect state. We also study and compare less likely defects such as Cr, N-N and Cr-N vacancies. Our results indicate that a high percentage of N vacancies results in a transition towards a metallic phase, which produces strong defects on the local magnetic arrangements and may even create a small absolute magnetization.

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