

Abstract Submitted  
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**First principles calculations of interfacial magnetism in CrO<sub>2</sub>-SnO<sub>2</sub> rutile junctions.** MAIRBEK CHSHIEV, KRISHNA CHETRY, ARUNAVA GUPTA, WILLIAM H. BUTLER, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL — Rutile oxides possess a wide range of interesting properties including the half metallic behavior of CrO<sub>2</sub> which has been shown both theoretically and experimentally to have essentially 100% spin polarization. For this reason, CrO<sub>2</sub> has attracted interest as an electrode material for fabrication of spin-valve structures and tunnel junctions with extremely high magnetoresistance ratios. SnO<sub>2</sub> is considered to be an ideal candidate for such magnetic tunnel junctions since it is an insulator with the same rutile crystal structure as CrO<sub>2</sub>. Understanding of the atomic configuration and magnetic structure at the interfaces is important for obtaining high magnetoresistance ratios because of possible mixing of Cr and Sn interfacial atoms. We report first-principles studies of the role of the magnetic structure for different interfacial intermixing configurations between Cr and Sn atoms for supercells in the (100) and (110) directions. The calculations were performed using the Vienna ab-initio simulation program (VASP) within the Generalized Gradient Approximation (GGA) to Density Functional Theory (DFT).

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