

Abstract Submitted  
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**DFT investigation of weak ferromagnetic and antiferroelectric properties of tetragonal BiCrO<sub>3</sub>**<sup>1</sup> LEONARD KLEINMAN, Dept. of Physics, University of Texas, Austin, TX 78712, JUN DING, Institute of Physics, CAS, Beijing 100190, China, YUGUI YAO, Dept. of Physics, Univ. of Texas, Austin, TX 78712 and Institute of Physics, CAS, Beijing 100190, China — The magnetic and ferroelectric properties of a very thick tetragonal BiCrO<sub>3</sub> film are studied using density functional theory. The experimental lattice constants were used but the atomic positions within the unit cell had to be calculated. This resulted in a centrosymmetric Pnma ground state, in agreement with the experimental antiferroelectric result. The magnetization is G type antiferromagnetic with a spin-orbit induced canting that is larger than the experimental value. A simple model of the local electric polarization of the Bi and their twelve surrounding oxygens is consistent with the experimental polarization induced by a large electric field. A comparison with experimental and calculated bulk BiCrO<sub>3</sub> in the C2/c structure will be given.

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