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Magnetism of bulk $Cr_2O_3$and its (0001) surface: An ab initio study SIQI SHI, Department of Physics, Center for Optoelectronics Materials and Devices, Zhejiang Sci-Tech University, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska Lincoln — Magnetic properties of bulk Cr_2O_3 and its (0001) surface are studied using the LSDA+U method. Magnetic energies are well fitted by the Heisenberg model and the Neel temperature is calculated using the quantum pair-cluster approximation. Very good agreement with experiment is found for the equilibrium volume, spectral density, local magnetic moment, band gap, and the Neel temperature. The stable (0001) surface is known to be terminated by a Cr semilayer [1], but its detailed structure is unknown. We identify two competing surface sites. The configurational surface Hamiltonian is constructed from supercells and the structural thermodynamics is studied. We find that in a wide range of temperatures about 1/3 of Cr atoms are below the oxygen layer and that there is a ordering phase transition from $\sqrt{3} \times \sqrt{3}$ to 1×1 structure. Further, we find that (0001) surface has a unique feature of having an uncompensated magnetic moment that is not destroyed by surface roughness. This phenomenon makes Cr_2O_3 a promising exchange bias application. [1] M. Bender, *et. al.* J. Phys.: Condens. Matter **7**, 5289 (1995). .

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