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Uncompensated magnetization and structural phase transitions at Cr_2O_3 (0001) surface: Theory ALEKSANDER WYSOCKI, Department of Physics and Astronomy, University of Nebraska Lincoln, SIQI SHI, Department of Physics, Zhejiang Sci-Tech University, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska Lincoln — Active research is currently aimed at achieving voltage-controlled magnetic functionality in nanostructures. While multiferroics attract most attention in this respect, magnetoelectric Cr_2O_3 offers an alternative route. Here we show that the Cr_2O_3 (0001) surface (in the single antiferromagnetic domain state) has an unusual feature of having an uncompensated magnetization, which persists even if the surface is rough. This magnetization persists up to the bulk Néel temperature. Reversible isothermal electrical switching of exchange bias field utilizing this feature was demonstrated experimentally [1]. We further investigate the termination of the Cr_2O_3 (0001) surface using total energy calculations and identify two competing sites for surface Cr atoms. We build a surface configurational Hamiltonian using supercell calculations and study its thermodynamics using the Monte Carlo method. An ordering phase transition from 1×1 to $\sqrt{3} \times \sqrt{3}$ structure is found in agreement with LEED measurements [2].

[1] X. He *et al.*, contributed abstract MAR10-2009-006536.
[2] M. Bender *et al.*, JPCM **7**, 5289 (1995).

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