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Electronic structure and magnetic anisotropy of CrO_2 ANTONINA TOROPOVA, GABRIEL KOTLIAR, Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, SERGEJ SAVRASOV, Department of Physics, New Jersey Institute of Technology, VIKTOR OUDOVENKO[1], Bogoliubov Laboratory for Theoretical Physics, Joint Institute for Nuclear Research, Russia
— The problem of importance of strong correlations for the electronic structure, transport and magnetic properties of half–metallic ferromagnetic CrO_2 is addressed by performing density functional based electronic structure calculations in the local spin density approximation (LSDA) as well as using the LSDA+U method. In both schemes we compute electronic structure, optical conductivity and magnetic anisotropy energy for chromium dioxide. It is shown that the corresponding low–temperature experimental data are best fitted without accounting for the Hubbard U corrections. We conclude that the ordered phase of CrO_2 is weakly correlated.

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