Metal-Insulator Transition of V_2O_3 from Screened Hybrid Functional

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The electronic structure of vanadium sesqui-oxide (V_2O_3) in different phases has been calculated by the screened exchange hybrid functional. After 40 years of experimental and theoretical investigation, V_2O_3 is still the subject of intense discussion because of the complicated phase transitions [1]. V_2O_3 is a canonical Mott-Hubbard insulator at low temperature, and can undergo several metal-insulator transitions by varying the temperature, pressure or doping. Here, different transitions have been examined by the screened exchange (sX) hybrid functional. This functional mixes a Thomas-Fermi screened Hartree-Fock exchange into the local-density approximation (LDA) to correct the band gap and localization error of density functional theory [2]. As a generalized Kohn-Sham functional, sX can be used for energy minimization and structural relaxation. This allows a single shot calculation of structure and electronic structure of systems in which bond length variations may contribute to the metal-insulator transition or to other complex phenomena such as multiferroic behavior. This contrasts with perturbative methods such as GW or dynamic mean field theory (DMFT) which only operate on a pre-defined structure. Here, we show that sX can reproduce the paramagnetic metal phase of V_2O_3 in the corundum structure, the antiferromagnetic insulating phase in the monoclinic structure, and the paramagnetic phase via Cr doping, without adjustable parameters. The electronic structure of the high temperature metallic phase and the low temperature insulating phase is in good agreement with the photoemission spectra [3]. Furthermore we have relaxed a Cr-doped V_2O_3 corundum structure supercell to realize the doping induced paramagnetic insulating phase with a 0.15eV energy gap from first principle calculation for the first time. We show that the metal insulator transition induced by crystal structure change and doping could be explained in the framework of band theory. The hybrid sX functional can describe the electronic structure change when the Hubbard correlation energy is comparable to the band energy.

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[1] S. Lupi *et al.*, Nat. Commun. **1**, 105 (2010); S. Y. Ezhov, V. I. Anisimov, D. I. Khomskii, and G. A. Sawatzky, Phys. Rev. Lett. **83**, 4136 (1999).

[2] S. J. Clark and J. Robertson, Phys. Rev. B **82** 085208 (2010).

[3] S. K. Mo *et al.*, Phys. Rev. B **74**, 165101 (2006); H. Fujiwara *et al.*, Phys. Rev. B **84**, 075117 (2011).

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