Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

One-shot calculation of the Electronic Structure across the Metal Insulator Transitions in V_2O_3 by Hybrid Density Functional JOHN ROBERTSON, YUZHENG GUO, Cambridge University — We present the first calculation of the electronic structure of V_2O_3 in its different phases using the screened exchange (sX) hybrid functional [1]. The sX functional reproduces the observed band gaps, magnetic moments and photoemission spectra of the corundum paramagnetic metal (PM) phase, the monoclinic anti-ferromagnetic insulating (AFI) phase, and the corundum Cr-doped paramagnetic insulating (PI) phase. The PI phase has a 0.15eV band gap in good agreement with experiment. Using the generalised Kohn-Sham nature of the hybrid functional, a fully relaxed supercell model of the Cr-doped V_2O_3 PI phase is calculated, and it shows that the local strain field around Cr atoms is the driving force for the PI-PM transition. This illustrates that hybrid functionals that fix the exchange interaction can give a good, one-shot description of single particle spectra, and are efficient enough compared to DMFT or GW to treat the complex electron-lattice interactions that occur in the more interesting systems.

[1] S J Clark, J Robertson, Phys Rev B 82 085208 (2010)

John Robertson
Cambridge University

Date submitted: 16 Nov 2012 Electronic form version 1.4