Metal-Insulator Transtion of V_2O_3 from Screened Hybrid Functional

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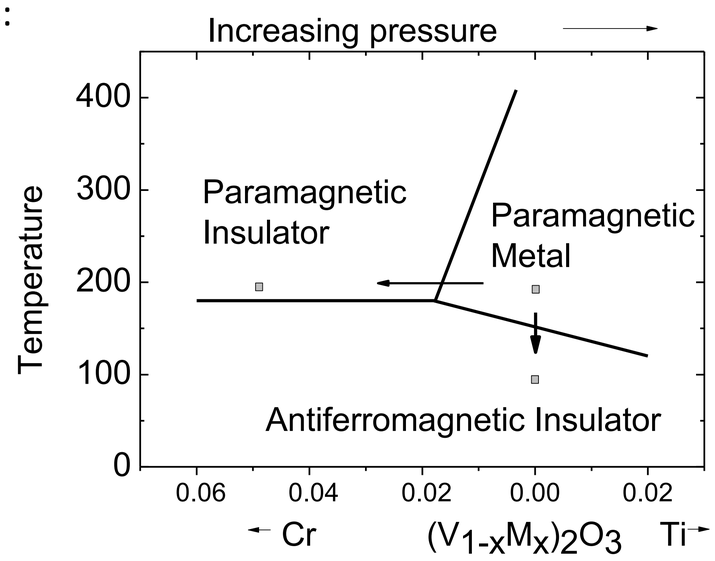
Introduction

After 40 years of experimental and theoretical investigation, vanadium sesquioxide V_2O_3 is still the subject of intense discussion because of the complicated phase transition routes[1]. Identified as the canonical Mott-Hubbard insulator at low temperatures, V_2O_3 could undergo several metal insulator phase transition by tuning temperature, pressure, and doping. The folllwing figure is its phase diagram showing the different phase transitions:

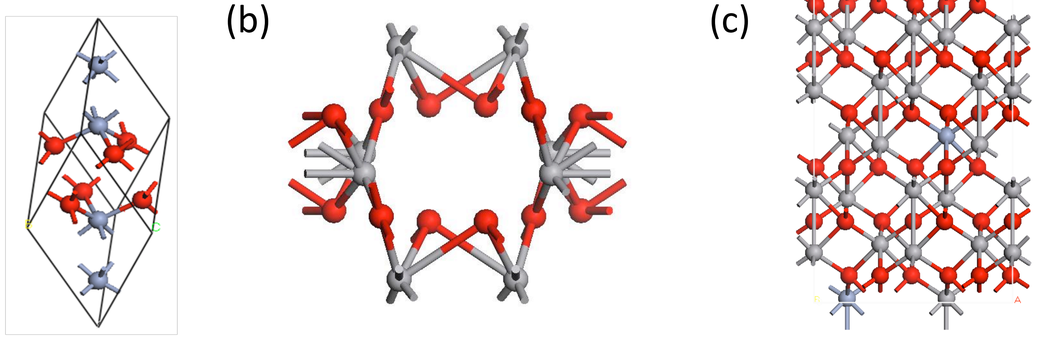


The electronic structures of vanadium sesquidoside in different phases have been calculated via screened exchange hybrid functional in this work.

Method

The screened exchanged functional is based on part of HF exchange potential where the exchange correlation energy explicitly depends on the orbital and includes the non-local parts[2]. The generalized Kohn-Sham scheme is used. The long-range exchange term is then screened by Thomas-Fermi exponential factor. The LDA local part is added to ensure that the hybrid functional is correct at homogeneous electron gas limit. The Thomas-Fermi screening vector is calculated by considering only the outer shell s, p, and d electrons to be valence.

(a) (b) (c)

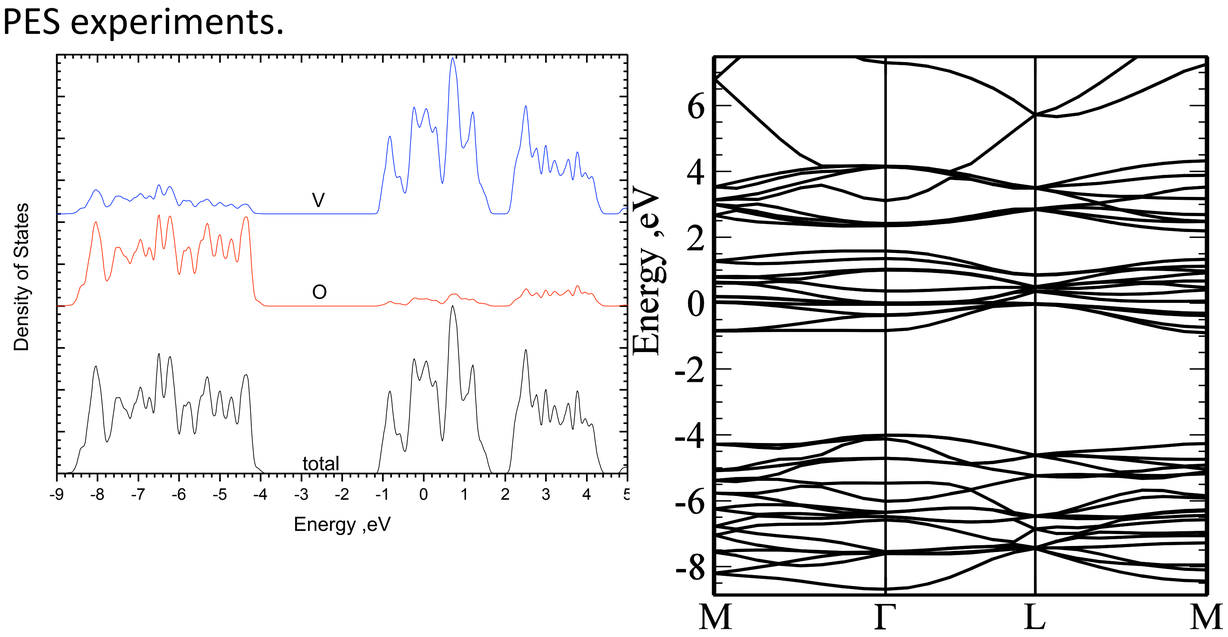


The primitive cell is used for calculation of the Paramagnetic Metallic phase(a) and Antiferromagnetic Insulating phase(b). For the Paramagnetic Insulating(PI) phase induced by Cr doping, a 120-atom supercell with 2 Cr atoms is used to reproduce the 4.8% Cr doping(c).

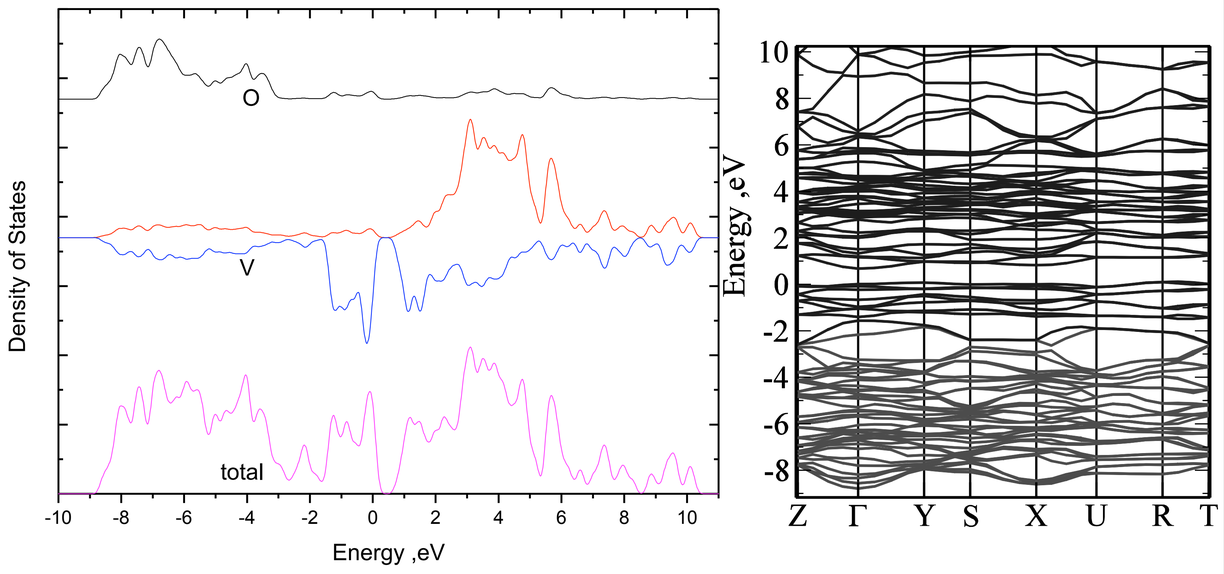
Results

1.Paramagnetic Metallic Phase

The Fermi level is set to be 0eV. The Fermi level lies within the V 3d states. The O 2p levels locate in between 4eV and 9 eV below the Fermi level, 1eV lower than the results from LDA DOS and are consistent with PES experiments.



2. Antiferromagnetic Insulating phase

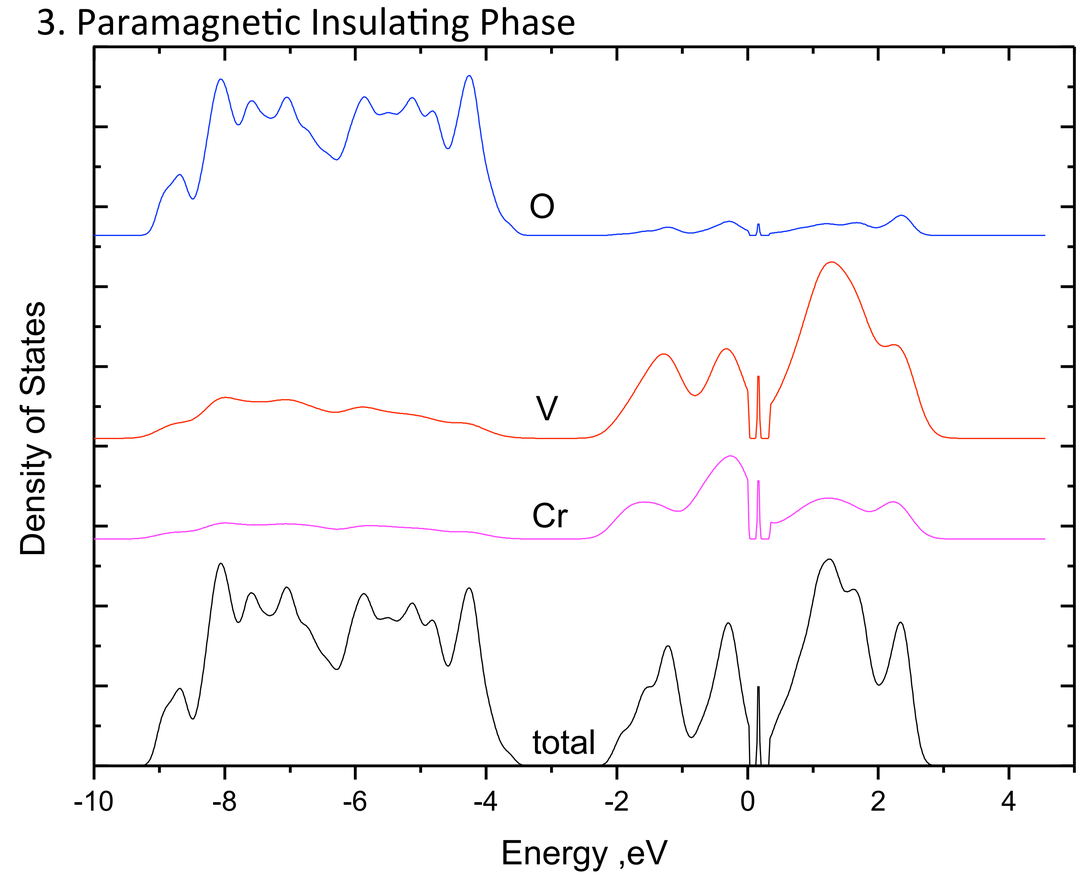


Calculated band gap compared with results from simulation:

	Optical Gap	LDA	LDA+U	GW	GW@LDA+U	SX
Eg(d) ,eV	0.5-0.66	0	0.60	0	0.943	0.76
Eg(id) ,eV					0.835	0.63

The O 2p orbital is still separated from the V 3d orbital but the hybridization between O 2p and V 3s is stronger compared with PM phase. Both the valence band and the conduction band edges are composed of V 3d orbital which confirms that at low temperature V_2O_3 is a Mott-Hubbard insulator. Compared with the PM phase, both the O 2p and V 3d states are broader.

3. Paramagnetic Insulating Phase



The band gap is 0.16eV which is consistent with the estimation of 0.1eV from PES experiments. The Cr partial DOS below the Fermi level is similar to that of V. The states from V and Cr are strongly hybridized. From the quasi particle spectrum we could estimate the U term to be the separation of the lower and upper Hubbard band, which is the V 3d bands in V_2O_3 systems. Our calculated U values from PM and PI phases support the constant-U scenario in the PM-PI phase transition.

Conclusion

Our calculation shows that screened exchange hybrid functional, as a parameter free generalised Kohn-Sham density functional, could describe the electronic structure of Mott insulator quite well. Moreover, we have shown for first time that the band theory could describe PM-PI transition in V2O3, a typical metal-insulator transition purely driven by electronic structural change

Reference

[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, J Robertson, Phys. Rev. B 82 085208 (2010).