Effect of pressure and U parameter on the electronic properties of rutile RuO_2

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RuO_2 in the rutile phase is considered to be nonmagnetic. Several calculations based on density functional theory have found this as a metallic and nonmagnetic compound. Consideration of the on site Coulomb interaction in the PBE+U calculations and the polarized neutron scattering measurements have revealed, antiferromagnetic behaviour recently [1]. Therefore it is vital to investigate the electronic properties of RuO_2 following the DFT and DFT+U approaches. We present the effect of U on the Fermi surface, two-dimensional electron momentum density (2D-EMD) distribution and the anisotropies in the one dimensional EMD. The effect of pressure is also examined on these properties.

We deploy the full-potential linearized augmented plane wave (FP-LAPW) method founded on the DFT [2]. The on-site Coulomb repulsion is added via the Hubbard U term following a standard theoretical formalism. We consider both PBE and the PBE+U calculations. The rutile structure of RuO_2 belongs to the space group $P4_2/mnm$. There are two formula units in its unit cell. The Perdew-Becke-Ernzerohf (PBE) *ansatz* based on the GGA is considered to treat exchange and correlation part of the Kohn-Sham Hamiltonian. The plane wave cut-off parameter *rgkmax* was set to 7. The Birch-Murnaghan equation of state is applied to find the lattice constant and the bulk modulus. Both the two and one directional electron momentum density (EMD) can be studied theoretically vis-a-vis experimentally. The 2D-ACAR and the Compton profile (CP) spectroscopies measure these electronic properties. The calculation of a CP due to valence electrons, is performed, along a specific crystallographic direction. The length of **H+k**, that is, *hkmax*=25 was sufficient to get the valence electrons by normalizing each directional CP in the range of 0 to 10 a.u. The grid size 16 × 16 × 16 is taken for the **k** points. To get the CP of a poly-crystalline material, the spherical average is required. That is computed taking average of the three directional Compton profiles (DCP) [3].

The E(V) curve is shown in Fig.1. The E(V) data coupled with the Birch-Murnaghan equation of state gives a=4.55 Å, c=3.095 Å and B=289.55 GPa. These are in very good agreement with the experimental data[1,4,5]. Electronic band structure reveals that rutile is metallic under ambient conditions.

We examine the effect of pressure on the 2D-EMD and the DCPs of the rutile along the (100), (110) and the (001) directions. So the effect of pressure on the DCPs, 2D-EMD along the three principal directions will be presented. We will also discuss the effect of pressure on the anisotropies and the Fermi surface. The valence electron Compton profiles were found sensitive to the applied pressure in our earlier study [6].

The effect of PBE+U calculations is also examined on the one dimensional EMD. In CuO_2 and related compounds also, it is found that this correction plays important role in describing the EMD particularly due to the *d* electrons [3]. These effects include the self-interaction correction of the localized *d* electrons and hence affect the EMD in the low as well as intermediate range of momentum.

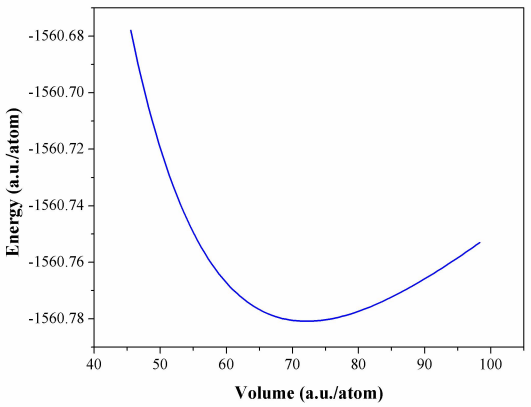

Figure 1. Total energy curve of the rutile phase of RuO_2.

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[1] T. Berlijn et al, *Phy. Rev. Lett* 2017, **118,** 077201.
[2] http://elk.sourceforge.net/
[3] V. Maurya and K.B. Joshi, *J. Phys. Chem. A* 2019, **123**, 1999.
[4] N. Mehtougui, D. Rached, R. Khenata, H. Rached. M. Rabah and S. Bin-Omran, *Mat. Sci. in Semicond. Processing* 2012, **15**, 331.
[5] J. S. Tse, D. D. Klug, K. Uehara, Z. Q. Li, J. Haines and J. M. Leger, *Phys. Rev. B* 2000, **61**, 10029.
[6] K.B. Joshi, B.K. Sharma, U. Paliwal and B. Barbiellini, *J. Mat. Sci.* 2012, **47**, 7549.