

## Transport properties of fluorite RuO<sub>2</sub>

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Under ambient conditions RuO<sub>2</sub> is found in the rutile phase. Several calculations based on density functional theory have found pressure induced transition to the fluorite phase. Now it has become possible to couple the E-k curve of a compound with the Boltzmann transport equations to find the transport coefficients such as Seebeck coefficient, power factor and the electrical conductivity [1]. Such calculations are performed under the constant relaxation time approximation and the rigid band model wherein it is assumed that band structure does not change with temperature and doping.

We apply the full-potential linearized augmented plane wave (FP-LAPW) method founded on the DFT [2]. The fluorite structure of RuO<sub>2</sub> belongs to the space group  $Fm\bar{3}m$ . 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 E(V) data coupled with the Birch-Murnaghan equation of state gives  $a=4.915$  Å and  $B=318$  GPa. These are in very good agreement with the other calculations [1,3,4]. Electronic bands structure reveals that fluorite phase is a semiconductor with indirect gap of 0.43 eV which is in good agreement with earlier results.

So due to a reasonable band gap and high bulk modulus it is worthwhile to compute thermoelectric properties of the fluorite. For this, eigen-energies at about 8000 k-points were calculated and used to compute transport coefficients using the BoltzTrap [1,5]. The Seebeck coefficient, power factor, and the electrical conductivity will be presented and effect of pressure will be seen on these properties. The rank of fluorite shall be assessed on the EFF scale proposed recently to see performance of thermoelectric materials.

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