An investigation of ZrO_2 doped with Ca and Sc

Solano, J. G.[1,2] , Gil Rebaza, A. V.[3] and C. A. Taft [2]

(1) Laboratorio de Simulação de Moléculas e Superfices, Centro Brasileiro de Pesquisas Físicas CBPF,Rua Dr. Xavier Sigaud,150 Urca, 22290-180, Rio de Janeiro, Brazil

(2) 1) Laboratorio de colisiones atómicas, Universidad Nacional de Rosario, Facultad de Ciencias Exactas, Ingenieria y Agrimensura, Av. Pelegrini 250, 2000, Rosario-Argentina.

(3) Laboratorio de colisiones atómicas, Universidad Nacional de Rosario, Facultad de Ciencias Exactas, Ingenieria y Agrimensura, Av. Pelegrini 250, 2000, Rosario-Argentina

We have used the plane wave pseudopotential method of Vasp to investigate doped ZrO_2 with Ca and Sc in the cubic, tetragonal and monoclinic phases. Our calculations are performed in the framework of density functional theory using the Ultrasoft Pseudopotential and Projector Augmented Wave with the Perdew and Wang 91 (GGA) and PBE approximation to the exchange correlation functional. One of the relevant effects is the stabilization of the most symmetric phases increasing the ionic conductivity. This is particularly important in ceramic materials used in gas sensors and solid oxide fuell cells. When zirconia is combined with other materials such as CaO and ScO_3 the cubic phase is stabilized at lower temperatures. We have investigated the electronic and structural properties for cubic, tetragonal and monoclinic ZrO_2 doped with Ca and Sc having different percentages of concentrations, i.e 25% and 12.5 % for Ca and 33% and 14% for Sc. The density of states indicate a gap > 3.0 eV required for application of cell fuels. For each case we observed modifications of the electronic structure compared with the pure material. We also observed an increase of the gap for the systems doped with Ca and a reduction for the systems doped with Sc. With each type of doping we observed changes in the unit cell, bulk modulus, in the valence and conduction bands as well as the charge densities.

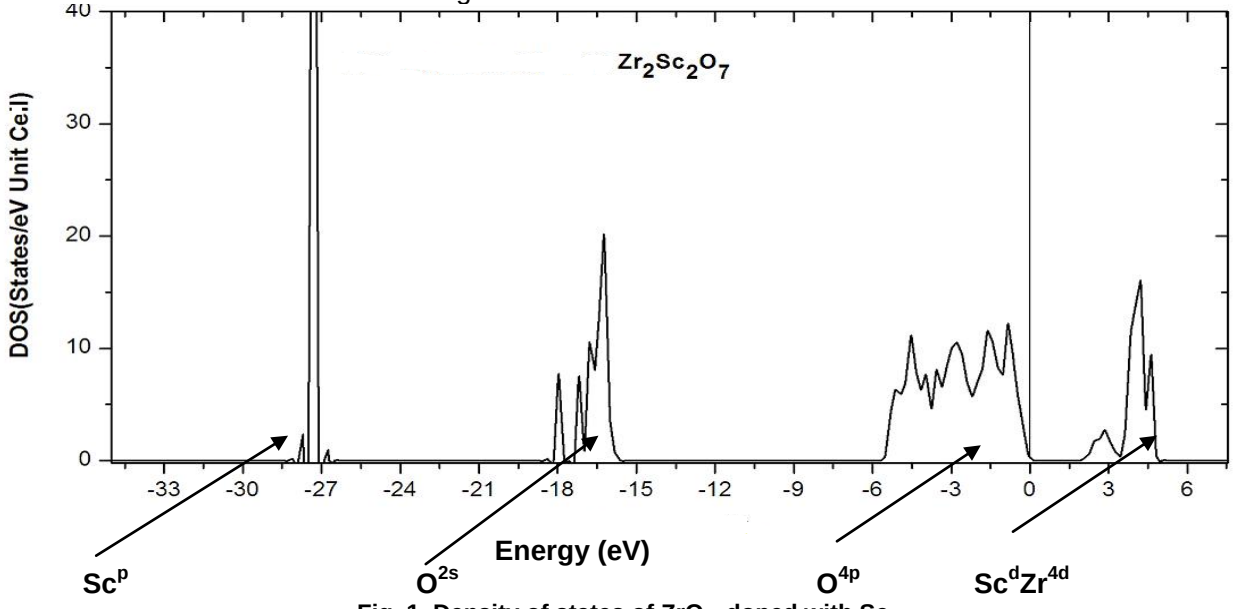

Fig. 1 Density of states of ZrO_2 doped with Sc

References

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