

An investigation of magnetism in ZrO_2 with low doping of transition metals

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

(1) *Instituto de Física de la Plata - CONICET – Argentina*

(2) *Laboratório de Simulação de Moléculas e Superfícies, Centro Brasileiro de Pesquisas Físicas CBPF, Rua Dr. Xavier Sigaud, 150 Urca, 22290-180, Rio de Janeiro, Brazil*

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

Dilute magnetic semiconductors materials have a significant importance because of their potential technological and industrial applications such as magnetic-optic and spintronic devices. In this work we investigate the magnetic properties of ZrO_2 in the monoclinic phase with a low doping concentration of transition metals as V, Cr, Mn, Fe, Co. The calculations were performed using Vienna ab-initio Simulation Package which employs Density Functional Theory and expand the electronic structure using plane wave basis set. Electron-ion interaction is described using the projector-augmented wave method (PAW) with plane waves up to energy cutoff at 500 eV and a Gaussian smearing with a smearing parameter of 0.2 eV. We have also adopted the GGA Perdew and Wang 91(GGA) and PBE exchange-correlation functional with Vosko Wilk and Nusair interpolation corrections. The integration was performed over $9 \times 9 \times 9$ K-mesh in a Monkhorst-Pack scheme. The calculation was carried out using a $2 \times 2 \times 2$ supercell containing 96 atoms. Our results (Fig. 1) indicates that the doping with transition metals can modify significantly the magnetic properties of ZrO_2 .

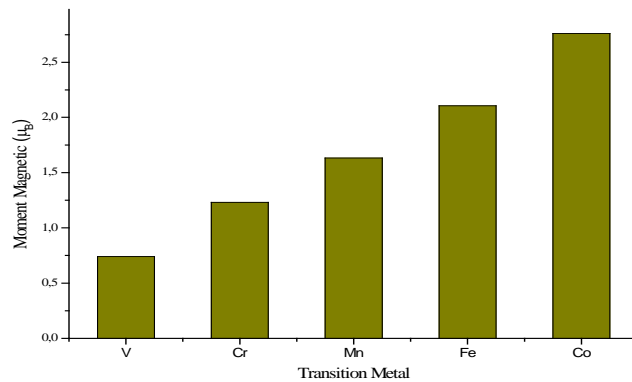


Fig. 1 Magnetic moment per transition metal ion obtained from a $Zr_{1-x}TM_xO_2$ supercell with a low concentration of x

[1] G. Kresse and J. Furthmüller, *Comput. Mat. Sci.* 6, 15-60 (1996).

