An investigation of magnetism in ZrO$_2$ with low doping of transition metals

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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 9x9x9 K-mesh in a Monkhorst-Pack scheme. The calculation was carried out using a 2x2x2 supercell containing 96 atoms. Our results (Fig. 1) indicates that the doping with transition metals can modify significantly the magnetic properties of ZrO$_2$.

![Graph showing magnetic moment per transition metal ion](image)

Fig. 1 Magnetic moment per transition metal ion obtained from a Zr$_{1-x}$TM$_x$O$_2$ supercell with a low concentration of x
