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Effect of transient metals on spin density of β-MnO_2

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The effect of impurities on the spin density of β -MnO_2 crystal was theoretically investigated by the DV-X_α (Discrete variational X_α) method[1], which is a sort of the first principle molecular orbital method and use the Hartree-Fock-Slater approximation. The β-MnO_2 is a paramagnetic oxide semiconductor material having the energy band gap of 0.18 eV and a 3 loan-pair electrons in the 3d orbital of a cation. This material exhibits spin-only magnetism and has the magnetic ordering temperature of 94 K. Below this temperature its magnetism appears as antiferromagnetism.[2] The magnetic properties of the oxide vary with the number of 3d loan pair electrons in transient metals. In this study the cluster model of $Mn_{15}O_{56}$ was used as the basic model for electronic structure calculations. An Mn atom in the center of model was replaced to other transient metals in order to investigate the effect of the dopant addition. The spin density distribution of up- and down-spin, the energy levels of 3d electrons, the density of state, and the bond overlap population were calculated and analyzed in association with the magnetic properties.

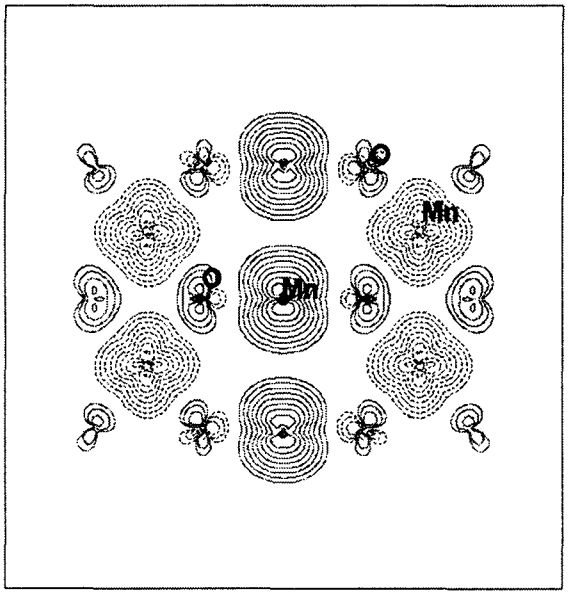

Fig.1 The difference spin density map shows antiferromagnetism along [110] direc

References

[1] H. Adachi, M. Tsukada and C. Satoko, J. Phys. Soc. Jpn. **45** (1978) p. 875

[2] C. N. R. Rao, FRS, J. Gopalakrishnan, New Directions in Solid State Chemistry (Cambridge University Press, Cambridge, 1986), p. 304