International Journal of Engineering, Mathematical and Physical Sciences
ISSN: 2517-9934
Vol:4, No:11, 2010

Effect of Exchange Interaction J on Magnetic Moment of MnO

C. Thassana and W. Techitdheera

***Abstract*—**This calculation focus on the effect of exchange interaction J and Coulomb interaction U on spin magnetic moments (m_s) of MnO by using the local spin density approximation plus the Coulomb interaction (LSDA+U) method within full potential linear muffin-tin orbital (FP-LMTO). Our calculated results indicated that the spin magnetic moments correlated to J and U. The relevant results exhibited the increasing spin magnetic moments with increasing exchange interaction and Coulomb interaction. Furthermore, equations of spin magnetic moment, which h good correspondence to the experimental data $4.58\mu_B$, are defined $m_s = 0.11J + 4.52\mu_B$ and $m_s = 0.03U + 4.52\mu_B$. So, the relation of J and U parameter is obtained, it is obviously, J = -0.249U+1.346 eV.

***Keywords*—**exchange interaction J, the Coulomb interaction U, spin magnetic moment, LSDA+U, MnO.

I. Introduction

OVER decades, electronic structure and magnetic properties of 3d-transition metal monoxides (TMO) such as MnO, FeO, CoO and NiO, have been extensively investigated both experimentally and theoretically. Among these materials,The most potentially applicable material being used in wide range of applications such as high-temperature superconductors, antiferromagnetic material [1], and electrochromic devices [2]. It is well recognized that MnO is a type II antiferromagnetic insulator with the Neel temperature (T_N) of 122K. At temperature above T_N, MnO has a cubic rocksalt (B1) structure and below T_N, the magnetic moments are aligned ferromagnetically on the (111) plane orientation[3]. The magnetic moment from experiment was $4.58\mu_B$[4], Meanwhile, theoretical studies on MnO have been accordingly carried out by various calculations including self-interaction corrected local spin density approximation (SIC-LSDA) [5,6], Constrained local density approximation (Constrained-LDA)[7], self-interaction corrected local density approximation plus Coulomb interaction (SIC-LDA+U)[8,9], hybrid approximation [10], Quasiparticle GW approximation (QP-GW[11]), LSIC[12], EXX [13] and so on. Moreover, these methods also differ on J and U parameter for instance J = 0.86 eV, U = 6.9eV[7], J = 0.9 eV , U = 4,6,8 eV[8]. The spin magnetic moments, which were calculated from this method, shown in the table 1. Compare to the experiment [4], both they overestimated [6,7,12,13] and underestimated [5,8,10].

Although the electronic and magnetic properties of MnO have been studies within LSDA+U method by many pioneered works, but the effect of exchange interaction J and Coulomb interaction U on magnetic properties and equation of spin magnetic, as a function of J or U, have not yet been investigated. Thereby, in this work, we report on the pioneered study focusing on the effect of the parameter U and J on spin magnetic moment of MnO by using the FP-LMTO within the LSDA+U method. First, the magnetic moments were calculated by J ranging from 0 – 1.0 eV. The calculation was conducted at constant U. The next calculation was carried out by varying the Coulomb interaction from 0 to 6 eV at constant exchange interaction. Finally, magnetic equations, as a function of J and U, and the relation of J and U were defined.

II. Computational Detail

In this work, the spin magnetic moments of MnO were calculated by using the local spin density approximation plus the Coulomb interaction (LSDA+U) method within the full potential linear muffin-tin orbital (FP-LMTO)[14], which is among the most accurate method for performing electronic structure and magnetic properties for 3-d transition metal monoxide.

All the calculations and methods are performed using the MSTUDIO 7.0 package [15]. The muffin-tin radii of Mn^{2+} and O^{2-} ions were 2.346 a.u. and 1.843 a.u., respectively. The lattice constant of MnO is 4.44 Å at normal pressure. While U and J parameter were defined $U = F^0$ and $J = (F^2+F^4)/14$ [16]. Our calculations, the effect of J and U on the spin magnetic moments of MnO were studied. Firstly, the spin magnetic moments, which the J and U were varied from 0 to 1.0 eV and 1.0 to 5.0 eV, were calculated. Finally, the relation of J and U parameter was obtained where the spin magnetic moment is $4.58\mu_B$ [4].

III. Results and Discussions

The value of the spin magnetic moments of MnO at normal pressure were calculated by self-consistently LSDA+U method. In Fig 1 is shown that the spin magnetic moments, as a function of J for all U, slightly increased with increasing of

C. Thassana is with Physics and General Science Program, Nakhon Ratchasima Rajabhat University, Nakhon Ratchasima, 30000 Thailand (corresponding author to provide phone: +66-44254000 ext 1303 fax: +66-44272939; e-mail: ct2709@gmail.com).

W. Techitdheera is with School of Applied Physics, King Mongkut's Institute of Technology Ladkrabang (KMITL), Bangkok, 10520 Thailand. (e-mail: Wdheera@gmail.com).

J. Since the exchange interactions should be analyzed by means of quantum theory, so it strongly concerns with spin-spin interactions. More specifically, on the atomic scale, the exchange interaction J tends to align neighbor spins so the spin magnetic moment increase with increasing of J. Moreover, our calculations show equation of the spin magnetic moment (m_s) and J was defined

$$m_s = 0.11J + 4.52\ \mu_B \quad (1)$$

where m_s and J represent the spin magnetic moment and exchange interaction, respectively.

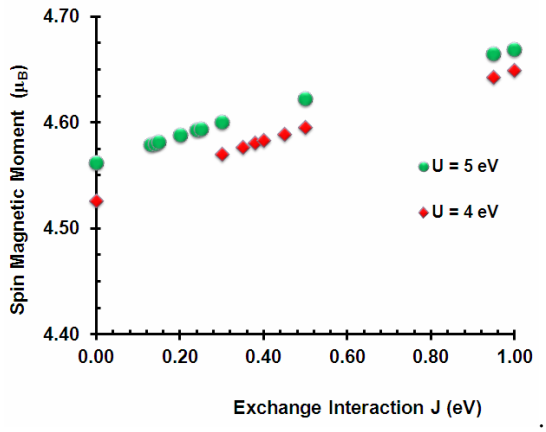

Fig. 1. represents the spin magnetic moment of MnO depend on the exchange interaction J for U = 4 and 5 eV .

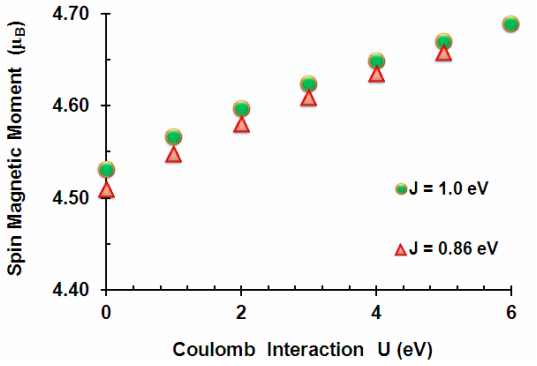

Fig. 2. Represents the spin magnetic moment of MnO depend on U for J = 0.86 and 1.0 eV.

Furthermore, the spin magnetic moment also depend on U as shown in Fig 2. Our results were shown the spin magnetic moments are proportional to the Coulomb interaction U. Since U enhances the electron localization, which leads to magnetic moment gain.

In addition, equation of the spin magnetic moment (m_s) and U was defined

$$m_s = 0.03U + 4.52\ \mu_B. \quad (2)$$

where m_s and U represent the spin magnetic moment and the Coulomb interaction, respectively.

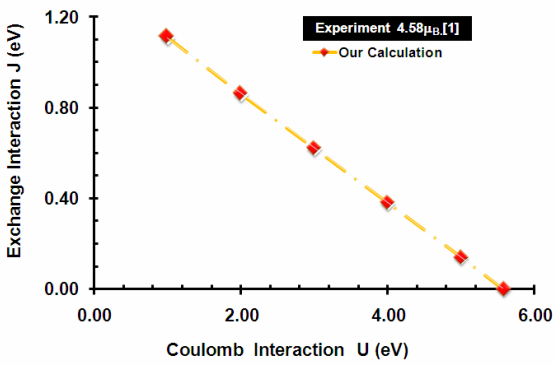

Fig. 3. represents the relation of U and J where the spin magnetic moment is 4.58μ_B.

In table 1 shown our calculation the values of spin magnetic moments were 4.37μ_B. (U=1.0 eV, J=0 eV) to 4.67 μ_B. (U=5.0eV, J=1.0 eV). Therefore we can conclude that the spin magnetic moment depend on both U and J. In Fig 3. shown the relation of U and J where the spin magnetic moment is 4.58 μ_B[4], We found that J linearly decreased about 0.249 with increasing of U 1.0 eV. Hence, the relation of J and U was obtained :

$$J = -0.249\ U + 1.346\ \text{eV}. \quad (3)$$

However, the values of spin magnetic moment, were calculated by using LDA+U^{p+d} [9] and Constrained LSDA[7] which both methods used U of 6.9 eV and J of 0.86 eV were 4.59μ_B and 4.61μ_B, respectively. While our calculation it be equal to 4.58μB we use J as 0.86 eV and 2 eV of U.

IV. Conclusions

Effect of the exchange interaction J and Coulomb interaction U on the spin magnetic moment of MnO was studied by using the local density approximation plus the Coulomb interaction method within the full potential linear muffin-tin orbital. Our results revealed that the value of the spin magnetic moments are depend on J and U. Furthermore we can define $m_s = 0.11J + 4.52\ \mu_B$ and $m_s = 0.03U + 4.52\ \mu_B$ In addition, the relation of exchange interaction J and Coulomb interaction U is defined J = -0.249U+1.346eV.

TABLE I
CALCULATED THE SPIN MAGNETIC MOMENT m_s (μ_B), EXCHANGE INTERACTION J (eV) AND THE COULOMB INTERACTION U (eV).

Methods	U (eV)	J (eV)	m_s (μ_B)
This Work	0 – 6	0 – 1.0	4.37- 4.67
Experiment [4]	-	-	4.58
SIC-LSDA-ASA[6]	-	-	4.64
Constrained LSDA[7]	6.9	0.86	4.61
LDA+U^{d+p}[9]	6.9	0.86	4.59
Hybrid [10]	-	-	4.46
QP+GW[11]	-	-	4.50
LSIC[12]	-	-	4.63
EXX[13]	-	-	4.81

ACKNOWLEDGMENT

The authors thank Physics and General Science Program, Nakhon Ratchasima Rajabhat University, Nakhon Ratchasima, Thailand and School of Applied Physics, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand for their facilities support.

REFERENCES

[1] M. Rubinstein, R.H. Kodama and S.A. Makhlouf, "Electron Spin Resonance Study of NiO Antiferromagnetic Nanoparticles" , J Magn Magn Mater. 234,289 (2001).
[2] H. Liu, W. Zheng, X. Yan, and B. Feng, J. Alloy Compd. 462, 356(2008).
[3] C.G. Shull, W.A. Strauser, and E.O. Wollan, "Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances" ,J. Phys. Rev. 83, 333 (1951).
[4] A.K. Cheetham and D.A. Hope, "Magnetic ordering and exchange effects in the antiferromagnetic solid solutions MnxNi1-xO", J. Phys. Rev B., 27, pp 6964-6967, 1983.
[5] A. Svane Du and O. Gunnarsson, "Transition-Metal Oxide in the Self-Interaction-Corrected Density-Functional Formalism", J. Lett.65,vol 9, pp 1148-1151, 1990.
[6] Z. Szotek, and .W.M. Temmerman, " Applicaton of the self-interaction correction to transition-metal oxides", J. Phys. Rev. B.47, vol 7, 4029-4032, 1992.
[7] V.I. Anisimov, J Zaanen and O.K Anderson, " Band Theory and Mott insulators: Hubbard U instead of Stoner I ", J. Phys. Rev. B, 44, vol 3, pp 943-954, 1991.
[8] D.W. Boukhvalov, A.I. Lichtenstein and V.I. Anisimov, " Effect of local Coulomb interactions on the electronic structure and exchange interactions in Mn12 magnetic molecules ", J Phys. Rev. B.65, pp 184435-1- 1184435-6, 2002.
[9] I.A. Nekrasov, M.A. Korotin and F. V.I. Anisimov, "cond-mat 0009107v1", 2008.
[10] F.Tran, P. Blaha, K. Schwarz and P. Novak, "Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides", J. Phys. Rev. B. 74, 2006, pp 155108 -155117.
[11] C. Rodl, F. Fuchs, J. Furthmuller and F. Bechstedt, "Quasiparticle band structures of the antiferromagnetic transition-metal oxides MnO, FeO, CoO, and NiO ", J. Phys. Rev. B.79, pp 235114-235121, 2009.
[12] G. Fisher, M. Dane, W. Temmerman and W. Hergert, " Exchange coupling in transition metal monoxide : Electronic structure calculations", J. Phys. Rev.B 80, pp 014408-1- 014408-11, 2009.
[13] E. Engel, and R.N. Schmid, " Insulating Ground States of Transition-Metal Monoxides from Exact Exchange " , J. Phys. Rev. Lett 103, pp 036404-1-036404-4, 2009.
[14] S.Y. Savasov, "Linear-response theory and lattice dynamics: A muffin-tin-orbital approach " J. Phys. Rev. B54 (1996).
[15] http://www.physics.ucdavis.edu/~mindlab/MaterialResearch/MINDLab/index_general.htm
[16] S.K. Kwon and B.I. Min, "Unquenched large orbital magnetic moment in NiO" J. Phys. Rev. B 62, 73(2000)