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 as \( m_s = 0.11J +4.52\mu_B \) and \( m_s = 0.03U+4.52\mu_B \). So, the relation of J and U parameter is obtained, it is obviously, \( J = -0.24U+1.346 \text{ eV} \).

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 investigated both experimentally and theoretically. Among these materials, the most potentially applicable material being investigated both experimentally and theoretically. Among these materials, the most potentially applicable material being investigated both experimentally and theoretically.

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 parameter 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
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.

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.

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

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

\[ m_s = 0.03U + 4.52 \mu_B \quad (2) \]

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

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. 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.

In table 1 shown our calculation the values of spin magnetic moments were 4.37 \(\mu_B\) (\(U=1.0\) eV, \(J=0\) eV) to 4.67 \(\mu_B\) (\(U=5.0\) eV, \(J=1.0\) 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 \(\mu_B\). 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:

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

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 4.59\(\mu_B\) and 4.61\(\mu_B\), respectively. While our calculation it be equal to 4.58\(\mu_B\) 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 \(J = -0.249U +1.346\text{ eV}\).
TABLE I
CALCULATED THE SPIN MAGNETIC MOMENT $m_s$ ($\mu_B$), EXCHANGE INTERACTION $J$ (eV) AND THE COULOMB INTERACTION $U$ (eV).

<table>
<thead>
<tr>
<th>Methods</th>
<th>$U$ (eV)</th>
<th>$J$ (eV)</th>
<th>$m_s$ ($\mu_B$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>This Work</td>
<td>0 – 6</td>
<td>0 – 1.0</td>
<td>4.37- 4.67</td>
</tr>
<tr>
<td>Experiment [4]</td>
<td>-</td>
<td>-</td>
<td>4.58</td>
</tr>
<tr>
<td>SIC-LSDA-ASA[6]</td>
<td>-</td>
<td>-</td>
<td>4.64</td>
</tr>
<tr>
<td>Constrained LSDA[7]</td>
<td>6.9</td>
<td>0.86</td>
<td>4.61</td>
</tr>
<tr>
<td>LDA+U$d+$$p$[9]</td>
<td>6.9</td>
<td>0.86</td>
<td>4.59</td>
</tr>
<tr>
<td>Hybrid[10]</td>
<td>-</td>
<td>-</td>
<td>4.46</td>
</tr>
<tr>
<td>LSIC[12]</td>
<td>-</td>
<td>-</td>
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</tr>
<tr>
<td>EXX[13]</td>
<td>-</td>
<td>-</td>
<td>4.81</td>
</tr>
</tbody>
</table>

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.

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