

The Role of On-site Coulumb Interaction on Electronic Structure of FeO

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We report our density functional theory (DFT) calculation on FeO in order to describe the electronic properties of FeO. The DFT result calculation is known to be failed to describe the electronic properties of system with strong on-site Coulumb interaction such as FeO. Then, we introduce the Hubbard correction, U , in order to take into account the onsite coulumb interaction of d -electron at Fe-ion. The band structure and density of state (DOS) were calculated within DFU+U framework. The band gap of FeO from DFT+U calculation are comparable with experimental results.

Keywords: DFT, Hubbard, Energy gap

I. INTRODUCTION

The transition metal oxide (TMO) were very actively studied due to the rich of physical phenomena. FeO is one of the TMO system which is interesting due to the wide application and the large availability of natural iron sand in Indonesia [1]. The theoretical study of its electronic structure is done to support the experimental results. Based on band theory, if all band are full or empty then the system will be in the insulating state. On the other hand if band partially occupied, the system will be metallic state [2].

The density functional theory (DFT) calculation is very successful theory to solve the Schrödinger equation for many body system [3, 4]. The success of DFT on predicting energy level for metallic system [5]. On the hand, the DFT known to be failed to describe the insulator behavior of TMO system in the ground state. The local density approximation (LDA) and generalized gradient approximation (GGA) scheme is not able to treat the on-site Coulumb interaction of d -electron [2]. We studied the electronic structure by taking in to account the on-site coulumb interaction among d -electrons and study its effect on band structure and density of states (DOS) of FeO. This is the first step for estimate other physical properties from the calculation. The calculation results is compared with the available experimental data.

II. METHOD

The DFT calculation were done on the basis plane wave and pseudopotential approximation as implemented in Quantum Espresso [6]. The Perdew, Burke, Ernzerhof (PBE) approach of GGA exchange correlation function was used for all calculations [7]. The cut-off energy was set to be 50 Ry and K-point was divided in to $9 \times 9 \times 9$ mesh. The crystal structure is chosen to be rhombohedral with $a = 8.1900 \text{ \AA}$ and antiferromagnetic ordering of Fe-ion. The band structure and DOS were calculated with and without on-site coulumb interaction (U parameter). For the calculation with U , The U value was set to be 4.3 eV for Fe-ion [8].

III. RESULTS AND DISCUSSION

The figure 1 show the band structure and DOS of FeO with ignoring the on-site coulumb interaction ($U = 0$). The Fermi energy is 11.6426 eV and several band across this Fermi energy. This result suggested that FeO is metal in the ground state. On the other hand, the experimental results showed that FeO is insulator with energy gap $\approx 2.4 \text{ eV}$ [9]. The d -electron split into e_g at higher energy and t_{2g} at the lower energy state due to the octahedral crystal fields [10]. The hopping of unpaired electron in t_{2g} is prevented by on-site coulumb interactions which make FeO become insulator. The Antiferromagnetic ordering below Néel temperature $T_N = 198 \text{ K}$ is also observed in this system [11].

We then include Hubbard Parameter U in our DFT calculations to take in to account the on-site coulumb interactions. The U value is set to be 4.3 eV. We can observe the clear direct energy gap $\approx 2 \text{ eV}$ at the Γ point as shown in the figure 2. This result indicates in addition to the crystal field, the on-site coulumb interaction plays the key role to describe the electronic properties of FeO which opens the gap around Fermi level by splitting in to upper Hubbard band (UHB) and lower Hubbard band (LHB) [12].

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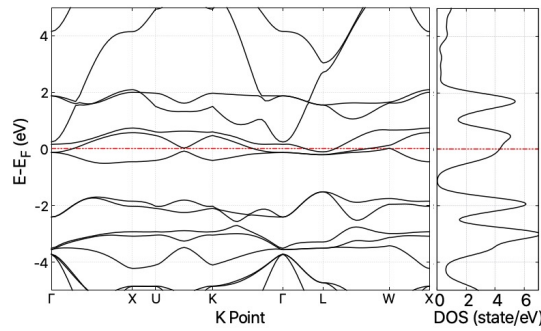


FIG. 1. The band structure dan DOS of FeO with $U = 0$ eV. There is no energy gap is observed

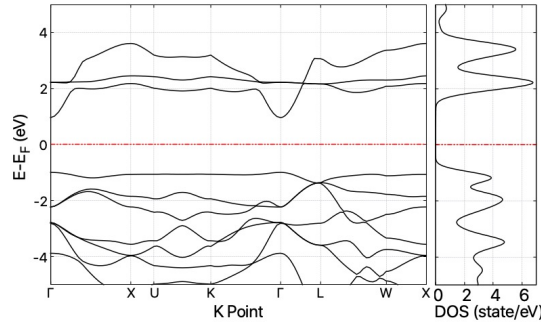


FIG. 2. The band structure and of FeO with $U = 4.3$ eV. The clear direct gap is observed at Γ point.

IV. CONCLUSION

We studied the role of the on-site coulomb interaction parameter, U , in electronic structure of FeO by DFT+ U Calculations. The value of $U = 4, 3$ eV give result that FeO in insulator in the ground state with $E_g \approx 2\text{eV}$ which match with the previous experimental results.

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