Hole localization in Li-doped antiferromagnetic MnO

<u>Yun-feng Zhu</u>*, Kuwahara Kazuhiro, and Hannes Raebiger Department of Physics, Yokohama National University, Yokohama, Japan. <u>zhu-yunfeng-ny@ynu.jp</u>

MnO is a Mott insulator that cannot be correctly described by conventional first principle calculation. Here we apply a self-interaction correction to density-functional theory and describe the hole localization in Li-doped antiferromagnetic (AFM) MnO. We use the exchange-correlation functional SCAN^[1] with the Hubbard U correction (U_{eff} = 2.5eV), combined with the hole state potential^[2],

$$V_{m,\sigma}^{hs} = \lambda (1 - n_{m,\sigma}/n_{host})$$

The Li-doped MnO is calculated in a supercell of 128 atoms including one Li atom.

We created the localized holes at Mn atoms around Li through orbital occupation initialization. It turns out that all the localized holes have lower energies and thus are more stable than delocalized hole state as shown in Figure 1, which indicates that localized holes are weakly bound to the Li. The second localized hole state has the lowest energy and is the most stable one among them. Localized hole



Figure 1. (a) The energy difference between localized hole and delocalized hole (b) The structure and the partial charge density of the hole around the closest Mn to Li.

induces split-off states in the energy gap from valence bands. Meanwhile, the crystall structure is distorted around the localized hole and the neighbouring O atoms are attracted towards the hole.

We also studied the transition dynamics between different localized holes. The transition can be either adiabatically keeping the hole spin or changing the hole spin non-adiabatically, as shown in Figure 2. The hopping energy is defined as the difference between the maxima and the intial energy along the transition path and it fits well with the experiment results of paramagnetic (PM) MnO^[3].



Figure 2. Transition between different localized holes

References

- 1. Jianwei Sun, Adrienn Ruzsinszky, John P. Perdew. Phys Rev Lett, 115, 036402.
- 2. Lany S, Zunger A. Phys Rev B, 2009, 80(8), 085202.
- 3. C. Crevecoeur, H.J. De Wit. J Phys Chem Solids, 1970, 31(4), 783-791.