Effect of Supercell Calculation on Muon Sites in La$_2$CuO$_4$

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The muon spin relaxation (μSR) is a powerful tool for investigating the electronic states of Cu-based high-T_c superconducting oxides. It is important to understand the μSR data of the base material, La$_2$CuO$_4$ (LCO), especially in the magnetically ordered states, as it provides an insight to the other phases of this material. Although the μSR data can provide information on the local magnetic fields at the muon site, it is not so easy to obtain the details of the electronic structure surrounding the muons, which is the origin of the local fields at the muon site. This is because, we need to have the exact information on where the muon is located inside the material. Several attempts have been made to tackle this problem in the past.[1–3)] However, a unified method to obtain the muon positions inside the material has not yet been established.

In this study, the effect of supercell calculation on muon sites inside La$_2$CuO$_4$ system were investigated. DFT method was applied to determine possible muon sites in LCO. To account for the correlation energy of the strongly localized copper $3d$ orbitals, we employed Hubbard correction within our calculations (DFT + U) with the Hubbard parameter $U = 10$ eV, which opens the gap in the Fermi level of the system (2.6 eV) showing an insulating nature as predicted in the experiments. Three minimum potentials were found at positions near the apical and planar oxygens, which correspond well to the μSR experimental results shown in Fig. 1. These three positions (M1, M2, and M3) were set to be the initial muon positions on a $4 \times 2 \times 4$ LCO supercell for subsequent calculations in order to include the effect of local deformations caused by the presence of muons inside the material, as the inclusion of lattice deformations were found to be important to simulate the muon presence in the system realistically. The local deformations induced by muons on each site is shown in Fig. 2. From our current results, it was observed that M1 and M3 relaxation will affect the position of Cu inside the octahedra and the nearest planar oxygen. M2 relaxation only affects the nearest planar oxygen in the system without shifting the Cu atoms. It was also observed from our calculation that the magnetic moment on the nearest Cu atom is changed by the presence of a muon. The initial value of 0.7 μ_B in the case without the muon system is slightly lowered by the presence of muon. However, these local deformations do not change the insulating and antiferromagnetic nature for our material.
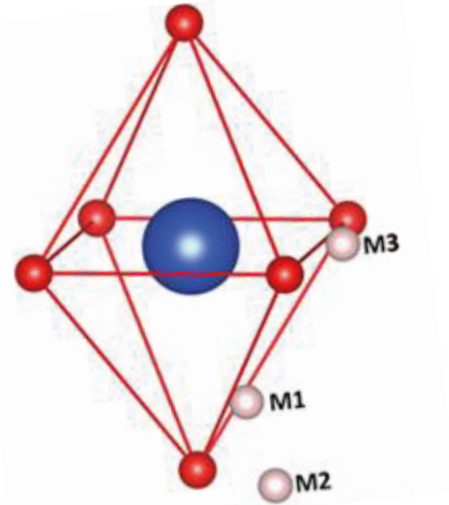

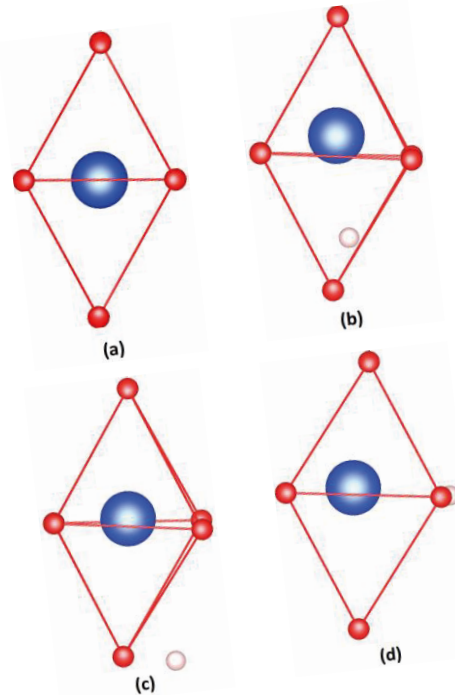Fig. 1. Three minimum positions observed by the DFT method (muon positions are enlarged for clarity).

Fig. 2. Comparison of CuO$_6$ octahedra after relaxation (a) Without muon (b) M1 (c) M2 (d) M3.

References
1) R. Saito, *et al.*, Physica (Utrecht) C **185–189**, 1217 (1991).
2) S. B. Sulaiman, *et al.*, Phys. Rev. B **49**, 9879 (1994).
3) H. U. Suter, *et al.*, Physica (Utrecht) B **326**, 329 (2003).

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