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DFT Investigations on Magnetic Properties with Muon in La_2CuO_4 by Using LSDA+U Functional

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The mother material of the La-based high-Tc superconducting oxides, La₂CuO₄(LCO), which family of materials possesses a d9 electronic configuration for copper ions, acts as a three-dimensional antiferromagnetic Mott insulator. LCO has been well investigated experimentally and theoretically in the past, but there are still questions on electromagnetic states to be investigated. The on-site Coulomb potential, U, on the Cu site plays a key role for magnetic properties forming the covalent state of electronic orbitals between Cu and O. We are performing first-principles calculations based on the density functional theory (DFT) to investigate the covalent state and discuss experimental results by using muons. One important key issue for this problem is what kind of electronic correlation functional should be chosen for calculations. In our presentation, we report detail DFT calculation results on LCO by using the Local Spin Density Approximation (LSDA) functional with the Vienna ab-initio simulation package (VASP) to investigate structural and magnetic properties of LCO.
The calculated magnetics moment of Cu in the antiferromagnetically ordered state with the spin direction along the b-axis without the muon is 0.491 μ_B, which was agreed upon well with the neutron scattering experiment. We found that the calculated band structure and the density of states indicated that U significantly influenced the hybridization of Cu-3d with O-2p orbitals at the valence and conduction bands influencing the band-gap energy. After adding the muon into the calculation model, it was confirmed that the muon deformed the local crystal structure around the preferable muon position and drastically reduced the magnetic moment of Cu near by the muon changing surrounding electronic states. We are now trying to investigate this situation by using other functionals and will report the results in our presentation.

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