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An example to use DFT and muSR to real electronic states of La2CuO4

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We are carrying out DFT investigations in conjunction with muSR measurements in order to reveal electronic states of strongly corelated systems, organic molecular systems and battery materials. As our first step, we tried to creproduce muSR results on the mother material of the La-based high-Tc superconducting oxide, La2CuO4 (LCO), which is a typical strongly correlated system. There were some early muSR results showing the appearance of the muon-spin precession due to the formation of a long-range ordered state of Cu spins. However, all of DFT and computational studies have failed to reproduce the muSR results on LCO and we could not achieve realistic feature of Cu spins from muSR for a long time. We tackled this problem by using DFT calculations with the electronic-correlation functional GGA+U assuming a supercell model with only one muon. Since our computational model was too big for a standard PC, we needed to use a supercomputing system with GPU units and many core numbers. I am going to report how to manage our DFT calculations to reproduce muSR results on LCO and how we reveal Cu-spin states. Through this study, we found some new problems regarding how to handle DFT calculations. I will also report those new problems to be considered to use DFT to understand muSR results.

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