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First principal calculation of the magnetic properties and muon stopping site in metal oxide with different Electronic correlational Functionals

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For deeper understanding of exotic magnetic phenomena of condensed matters, the muon spin relaxation (μSR) measurement is a powerful experimental technique to probe local magnetic properties of condensed matters. In order to understand ⊠SR results, we are approaching to magnetic phenomena of by using the density functional theory (DFT) calculations. I am going to report our recent results of DFT investigations, especially on La2CuO4 and Nd2Ir2O7. Our challenges to those typical condensed matters are to investigate the DFT calculation results by changing the functional and compare with μSR results. We tested the local spin density functionals (LSDA), the generalized gradient approximation (GGA) including U as an adjustable parameter (DFT+U), and the strongly constrained and appropriately normed meta-GGA (SCAN) to discuss what electronic orbitals contribute to magnetic phenomena of La2CuO4 and Nd2Ir2O7 and which functional is the most suitable for each system.

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