Muon User Meeting - 2024



Contribution ID: 29

Type: not specified

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

Thursday, 5 September 2024 15:00 (15 minutes)

For deeper understanding of exotic magnetic phenomena of condensed matters, the muon spin relaxation (μ SR) measurement is a powerful experimental technique to probe local magnetic properties of condensed matters. In order to understand \boxtimes 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 μ SR 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.

Primary author: Ms CHAROENPHON, Supparat (RIKEN)Presenter: Ms CHAROENPHON, Supparat (RIKEN)Session Classification: Science Session