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First-principles study of quantized muons in materials

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With advancements in muon science, muon spin rotation/relaxation/resonance (MuSR) has emerged as a standard tool for characterizing spin states and has found widespread application across various fields. The current first-principles methods of the muon, combining density functional theory with the point muon approximation (DFT+Mu) can efficiently predict muon positions and simulate phenomena such as hyperfine coupling but yet they overlook the significant quantum effects due to the muon's lighter mass. To address these issues, this poster proposes to integrate advanced first-principles computational approaches, including two-component density functional theory and quantum Monte Carlo and aims to conduct comprehensive research on the quantum effect of the muon. It is found that considering the quantum properties of muons is necessary and meaningful for the MuSR spectra analysis.

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