Contribution ID: **328** Type: **Poster**

Using the TCDFT method to determine muon quantum effects

Thursday, 1 September 2022 18:40 (20 minutes)

In calculations supporting μSR, it is important to deal with muon quantum effects. In previous studies, people have gone beyond the point-like muon approximation by using methods such as vibrational analysis of the zero point motion and path-integral molecular dynamics.[1-3] We now use a new method called Two-component DFT (TCDFT), which treats the muon as a fully quantized particle with its own wave-function.[4] By modifying the Quantum Espresso DFT code[5], we have included the potential generated by a muon trial wave-function into the DFT calculation of electronic structure and optimum geometry. Once we have the crystal and electron structures, the new muon wave-function can be calculated by solving its Schrödinger equation via a finite difference method. Repeating iteratively the two-component calculation, we could get a self-consistent result for both the electron and muon wave-functions.
Due to many-body quantum effects, we need to use the Quantum Monte Carlo method to simulate the correlation energy and pair-correlation function. The former is used for the TCDFT calculation and the latter is used for coupling the individual wave-functions of the muon and electrons when calculating a specified physical quantity. In this work, we have already applied the new method to some ferromagnetic systems (Fe, Co, Ni) and the calculations are now being extended to some examples of semiconductors (Diamond, Si, Ge) and single molecules (TCNQ and acetone). From the results obtained so far, we have calculated muon hyperfine contact fields, which agree well with experiments and show good potential for further application of the method to other materials.
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Session Classification: Posters

Track Classification: Site calculations