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Calculating muon sites and couplings from a high-throughput modelling perspective

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In muon spin spectroscopy, the knowledge of muon implantation sites and hyperfine couplings is of importance to the analysis of the experimental data. Over the past decade there has been significant progress in calculating muon sites using first-principles methods such as density functional theory (DFT) [1,2]. However, the protocols required for muon calculations are both resource and task intensive. They are performed sequentially in steps with strenuous human intervention required to track, coordinate and analyse these calculations. The recent advent of the DFT-based high-throughput (HT) approach and the development of dedicated frameworks has opened the possibility of performing this type of sequential large-scale calculations in an efficient way. Here, we present our efforts towards the design and implementation of workflows within the AiiDA integrated platform for high-throughput DFT-based muon calculations aimed at i) the design of a user-friendly approach available to every muon user; ii) benchmarking the scope of sustainable DFT calculations. We started from identifying material selection criteria to exclude the well-known harder cases. We have benchmarked the workflow at its current stage over 16 magnetic compounds. Our preliminary benchmark results demonstrated the feasibility of this plan and have further allowed us to understand the workflow capabilities, its limitations and the likely improvements to be considered for more accurate results of the calculated muon properties. These improvements include; taking into account the muon charge states and spotting the right compromise between sustainable and accurate treatment of electronic correlation effects.

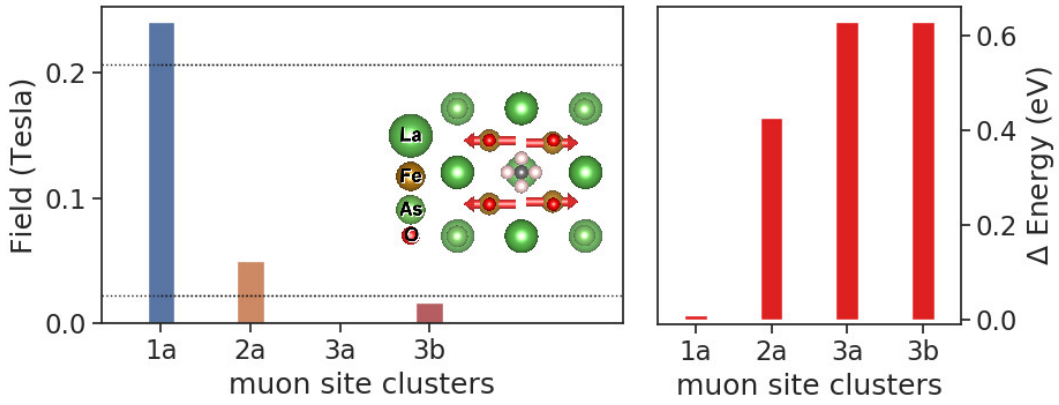

Figure 1: Typical workflow results: In this case for LaFeAsO [3].

References

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[3] M. M. Isah *et al.*, Ph.D. thesis, University of Parma (2022)

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