Contribution ID: **65** Type: **Poster Presentation**

Aiida-Muon: Automated Computational Workflows for Muon Sites and Hyperfine Calculations

Muon spin rotation and relaxation spectroscopy is a well established experimental probe used to investigate the properties of a wide range of condensed matter systems. However, beyond the properties revealed directly by the best fit parameters of the experiment, computational methods can effectively quantify the microscopic interactions underlying the experimentally observed signal, thus substantially boosting the predictive power of this technique. These computations remain challenging for non-experts due to limited familiarity with the method, and even for those well-versed in DFT, they are cumbersome to manage manually because of the large number of calculations involved.
To address this issue, we present an efficient set of algorithms and workflows [1] accompanied by an intuitive graphical user interface [2] devoted to the automation of this task. In particular, we adopt the so-called DFT+μ procedure and devise an automated strategy to obtain candidate muon stopping sites, their hyperfine interactions and polarization spectra. We validate the implementation on well-studied compounds including the Kagome-structured superconductors, particularly showing the effectiveness of our protocol in terms of accuracy and simplicity of use.

References
[1] I. J. Onuorah, et. al, Digital Discovery, 4, 523-538, 2025.
[2] X. Wang, E. Bainglass, M. Bonacci, et. al., “Making atomistic materials calculations accessible with the AiiDAlab Quantum ESPRESSO app”, in preparation, 2025.

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Funding Agency

Ministero dell’Università e della Ricerca, Finanziato dall’Unione europea (NextGenerationEu), Italia Domani è il Piano Nazionale di Ripresa e Resilienza (PNRR) italiano

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Session Classification: Poster session 2

Track Classification: Superconductivity