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Muon behavior and its influence on lithium ion diffusion in cathode materials using machine learning potentials

A μ^+SR technique has been used to measure self-diffusion coefficients and activation energies of ions in cathode materials such as Li_xCoO_2. [1] However, direct determination can be challenging due to the use of models such as a dynamic Kubo-Toyabe function, as well as difficulties in distinguishing muon diffusion itself from Li^+ diffusion at high temperatures.

First principles calculations can overcome these limitations, but they are too demanding when it comes to performing the simulation while taking into account zero-point vibrations and crystal lattice deformations. In recent years, this problem has been mitigated by machine learning potential techniques, which have enabled large-scale simulations with hundreds of atoms and nano second. [2]

In this study, we applied this technique to Li_xCoO_2 and performed simulations incorporating muon quantum effects using the path integral method, while taking into account magnetic interactions based on DFT+U. We report new findings concerning the stable positions of muons and their effects on Li ion diffusion.

References:

1 J. Sugiyama et al., Phys. Rev. Lett., 103 (2009) 147601.

2 Y. Kataoka et al., Phys. Rev. Res. 6 (2024), 043224.

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