Contribution ID: **146**   Type: **Poster Presentation**

Muon Behavior and Its Influence on Lithium Ion Diffusion in Cathode Materials Using Machine Learning Potentials

The µSR experiment has been used to measure diffusion coefficients and activation energies of ions in cathode materials such as LiCoO2. [1] However, direct determination can be challenging due to the use of models such as the Kubo-Toyabe dynamic 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 LiCoO2 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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Session Classification: Poster Session 1

Track Classification: Energy storage materials