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How DFT Calculations Contribute to μ^+SR Work on Battery Materials

Internal nuclear magnetic fields in various battery materials have been predicted using density functional theory (DFT) calculations to interpret the μ^+SR results, particularly for identifying the diffusing species responsible for the dynamic behavior observed. In materials where Li$^+$ and Na$^+$ ions are mobile, these cations readily change positions to minimize electrostatic repulsion with the implanted μ^+. As a result, the μ^+ sits at the bottom of a deep potential well, stabilizing itself through a “self-trapping” effect, making it a stable observer for detecting ion diffusion in battery materials. In contrast, in many metals and oxides, the implanted μ^+ diffuses even at low temperatures. In these materials, the local lattice distortion caused by the implanted μ^+ is relatively small compared to that in battery materials. To assess the stability of the implanted μ^+, we propose a ratio between the measured nuclear magnetic field distribution width (Δ^{exp}) and the DFT-predicted value without lattice relaxation (Δ^{min}), namely, $\Delta^{\mathrm{exp}}/\Delta^{\mathrm{min}}$, as an indicator of whether cations or μ^+ are diffusing. This indicator provides a comprehensive understanding of the diffusive behavior detected with μ^+SR in various materials, including battery materials, metals, and other oxides.

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