

Abstract Submitted
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Li⁺ ion diffusion in nanoscale alumina coatings MICHELLE JOHANNES, NOAM BERNSTEIN, Naval Research Lab — Nanoscale coatings of alumina are used to stabilize surfaces for a variety of technologies. Diffusion of ions through these coatings is of primary importance: in some cases, diffusion is unwanted (e.g. corrosion) and in others (e.g. electrode materials), it is necessary. In this work DFT and AIMD calculations are used to investigate Li⁺ ion diffusion through a nano-layer of alumina, examining the phase (alpha, gamma, and amorphous), ion concentration, and electron count dependence. We look at the role of the surface itself in promoting diffusion. One of our main findings is that as the number of ions or charge increases, the diffusivity rises. We show how our data can explain electrochemical data from coated LiCoO₂ cathodes and may point toward better and more efficient coatings for stabilizing electrodes.

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