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Simulation of Li ion diffusion near electrolyte-metal interface – Li_3PO_4 and Li[1] YAOJUN DU, XIAO XU, N.A.W. HOLZWARTH, Wake Forest U. — Motivated by recent technological interest in Li_3PO_4-based electrolytes developed at Oak Ridge National Laboratory[2] for use in rechargeable solid-state batteries and other technologies, we have used first-principles modeling techniques to study Li ion diffusion near idealized interfaces between Li_3PO_4 and Li metal. Using the nudged elastic band method, migration energy barriers for Li ion diffusion across interfaces in different crystallographic directions are calculated for both vacancy and interstitialcy mechanisms. Preliminary results find interface migration barriers as low as 0.2 eV and 0.26 eV for the vacancy and interstitialcy mechanisms, respectively. This suggests that interface diffusion barriers are likely to be comparable or lower than the corresponding migration barriers within crystalline Li_3PO_4.[3]

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[2]J. B. Bates, N. J. Dudney, and co-workers, *Solid State Ionics*, **53-56**, 647-654 (1992).
[3]Y. A. Du and N. A. W. Holzwarth, *Phys. Rev. B*, **76**, 174302 (2007).

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