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Simulated electrolyte-metal interfaces – Li_3PO_4 and Li[1] XIAO XU, YAOJUN A. DU, N.A.W. HOLZWARTH, Wake Forest U. — There has recently been a lot of interest in solid electrolyte materials such as LiPON developed at Oak Ridge National Laboratory[2] for use in Li-ion batteries and other technologies. We report on the results of our model calculations on idealized interfaces between Li_3PO_4 and Li metal, studying the structural stability and the ion mobility, using first-principles density functional techniques with the *PWscf* and *pwpaw* codes.[3] Starting with a supercell constructed from Li_3PO_4 in its crystalline γ-phase structure and several layers of Li metal, we used optimization and molecular dynamics techniques to find several meta-stable configurations. The qualitative features of the results are consistent with experimental evidence that the electrolyte is quite stable with respect to Li metal.[4] In addition to stability analyses, we plan to study Li-ion diffusion across the interface.

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[2]J. B. Bates, N. J. Dudney, and co-workers, *Solid State Ionics*, **53-56**, 647-654 (1992).
[3]http://www.pwscf.org and http://pwpaw.wfu.edu.
[4]N. J. Dudney in Gholam-Abbas Nazri and Gianfranco Pistoia, Eds., *Lithium Batteries: Science and Technology*, Chapt. 20, pp. 623−642, Kluwer Academic Publishers, 2004. ISBN 1-4020-7628-2.

N. A. W. Holzwarth
Wake Forest University

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