Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Computer modeling of crystalline electrolytes – lithium thiophosphates and phosphates[1] NICHOLAS LEPLEY, N.A.W. HOLZWARTH, Wake Forest University — During the last 5 years, lithium thiophosphate solid electrolyte materials have been developed[2] for use in all-solid-state rechargeable batteries. In particular, crystalline $Li_7P_3S_{11}$ has been characterized as a superionic conducting material having room temperature conductivities as high as 10^{-3} S/cm, which is 1000 times greater than that of the commercial solid electrolyte material LiPON. Building on our previous work,[3] we report computer modeling studies of this material as well as those of related phosphates and phosphonitrides. We present results on meta-stable crystal structures, formation energies, and mechanisms of Li ion migration. The calculational methods are based on density functional theory. The calculations were carried out using the Quantum Espresso (PWSCF) package.[4]

[1]Supported by NSF Grant DMR-0705239
[2]H. Yamane, M. Shibata, Y. Shimane, et al., *Solid State Ionics* **178**, 1162-1167 (2007).
[3]N. A. W. Holzwarth, N. D. Lepley, Y. A. Du, *J. Power Sources* (2010) [in press: doi:10.1016/j.jpowsour.2010.08.042]
[4]P. Giannozzi, S. Baroni, et al., *J. Phys.: Condens. Matter.* **21**, 394402 (2009); available from the website: http://www.pwscf.org/.

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Date submitted: 16 Nov 2010 Electronic form version 1.4