Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-Principles Study of LiPON Solid Electrolyte SANTOSH K.C., Department of Physics, University of Texas at Dallas, Richardson, Tx 75080, KA XIONG, KYEONGJAE CHO, Department of Material Science & Engineering, University of Texas at Dallas, Richardson, Tx 75080 — There has been much interest in the thin-film solid electrolyte for solid state battery and ionics applications. LiPON is a representative material developed by Oak Ridge National Laboratory [1]. In this work, we use first principles calculations based on the density functional theory to investigate the Li- ion migration mechanisms of LiPON family materials [2]. We investigate atomic structures, electronic structures and defect formation energies of these materials. To determine the migration path of Li diffusion, the activation energies are calculated. This study helps us to understand fundamental mechanisms of Li-ion migration and to improve Li ion conductivity in the solid electrolytes.

[1] Patil et al, Material Research Bulletin, 43 (2008) 1913-1942.
[2] Yaojun A. Du and N. A. W. Holzwarth, Physical Review B, 81 (2010).

Santosh K.C.
Dept of Physics, University of Texas at Dallas, Richardson, Tx 75080

Date submitted: 23 Nov 2010 Electronic form version 1.4