Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ab initio molecular dynamics study of liquid Li surfaces exposed to deuterium MOHAN CHEN, JUNCHAO XIA, ILGYOU SHIN, EMILY CARTER, Princeton University — We investigate the structure of liquid Li and its interactions with deuterium atoms using PROFESS (PRinceton Orbital-Free Electronic Structure Software) [1]. This linear-scaling orbital-free density functional theory method is a very fast quantum mechanics technique that allows one to perform ab initio molecular dynamics of metals for a large number of atoms and fairly long times. We adopt the WGC99 kinetic energy density functional that is very accurate for simple metals [2]. We use well validated bulk-derived local pseudopotentials [3] to describe the electron-ion interactions. Key properties of liquid Li will be presented and discussed, such as its bulk and surface structures, etc. Time permitting, we will discuss predictions related to adsorption and absorption of deuterium atoms into Li. This work provides new insights into understanding the surface structure of liquid Li using large-scale ab initio molecular dynamics methods. [1] L. Hung, C. Huang, I.Shin, G. Ho, V. L. Ligneres, and E. A. Carter, Comput. Phys. Comm., 181, 2208 (2010). [2] Y. A. Wang, N. Govind, and E. A. Carter, Phys. Rev. B, 60, 16350 (1999). Erratum: Phys. Rev. B, 64, 089903-1 (2001). [3] C. Huang and E. A. Carter, Phys. Chem. Chem. Phys., 10, 7109 (2008).

Mohan Chen
Princeton University

Date submitted: 09 Nov 2012 Electronic form version 1.4