

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ab-Initio Molecular Dynamics Study of the Concentration Dependent Diffusivity of Lithium Ions in Acetonitrile Electrolyte using the van der Waals Density Functional¹ KEITH RAY, Lawrence Livermore National Laboratory, ZHENXING WANG, ISAAK DANIELS, University of Kansas, DAVID OLMSTED, University of California, Berkeley, BRIAN LAIRD, University of Kansas, MARK ASTA, University of California, Berkeley — Pseudocapacitors are devices that store electrical energy faradaically, but feature fast reactions/intercalations enabling high power applications. Power density may be improved by utilizing electrolytes with fast Li ion diffusion. In this study we utilize ab-initio molecular dynamics to elucidate the solvation structure as well as the vibrational and diffusion dynamics of Li ions in the acetonitrile electrolyte. Acetonitrile is a promising electrolyte for energy storage applications due to its lower viscosity and higher ionic conductivity when compared to other battery electrolytes such as ethylene carbonate and propylene carbonate. Interestingly, the trends in the Li ion concentration dependent diffusivity are calculated to be qualitatively different depending on whether the PBE or vdW-DF density functional is used.

¹This work was supported as part of the Molecularly Engineered Energy Materials (MEEM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0001342.

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Date submitted: 14 Nov 2014

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