Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Li Diffusion Characteristics and Energetics in TiO_2 H. YILDIRIM, SUBRAMANIAN SANKARANARAYANAN, JEFF GREELEY, Argonne National Laboratory — We present the results of density functional theory-based calculations for the activation energies of Li diffusion in TiO_2 crystalline and amorphous structures. Additionally, molecular dynamics simulations using shell potential models are used to investigate the Li ion diffusion mechanisms for various titania morphology. The diffusion pathways and the corresponding energetics for each diffusion mechanism are further probed using the DFT-based Nudged Elastic Band Method. We will report the calculated diffusion energetics (MD and DFT) for each (Li-TiO_2) system and compare the atomic scale Li transport characteristics on crystalline and amorphous TiO_2 structures. We also discuss the effect of Li concentration on the diffusion energetics.

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Date submitted: 29 Nov 2010 Electronic form version 1.4