Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

The Electronic Structures and Diffusion Kinetics of Li, Na, and Mg Intercalated TiO_2 Anatase and TiO_2 (B) HANDAN YILDIRIM, JEFFREY P. GREELEY, Purdue University School of Chemical Engineering — Large-scale electrochemical storage that would allow wider use of renewable electricity not only requires new and advanced electrode materials for Li ion batteries, but also beyond-Li technologies such as Na and Mg ion batteries. This grand challenge puts forward the necessity for designing efficient electrode materials providing suitable energetics and rapid diffusion kinetics. In this contribution, we evaluate TiO_2 anatase and TiO_2 (B) as attractive candidates for anodes in Li, Na, and Mg batteries due to their low cost, non-toxicity, cycling stability, reasonable capacity, and high operating potential. While the TiO_2 anatase is discussed as promising material for Li storage, structurally, TiO_2 (B) with large interlayer spacing can be considered as a good electro-active material for Na intercalation. We will report the results of the first principles calculations using generalized gradient approximation (GGA) for Li, Na, and Mg intercalation at low concentration. The differences in the electronic and atomic structures obtained using GGA, Hubbard "+U" correction (GGA+U), and Heyd, Scuseria, and Ernzerhof (HSE) hybrid functional will be reported, and the importance of the "+U" correction for modeling the electronic structure of the intercalated TiO_2 will be discussed. The detailed information on the differences in the diffusion mechanisms and barriers will also be reported for each ion in both structures.

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Date submitted: 14 Nov 2014 Electronic form version 1.4