The Electronic Structures and Diffusion Kinetics of Li, Na, and Mg Intercalated TiO$_2$ Anatase and TiO$_2$ (B)  

HAN DAN 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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