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Comparative first principles study for Li, Na, and Mg storage at rutile, anatase, bronze, and amorphous TiO2 KONSTANTINOS KOTSIS, FLEUR LEGRAIN, SERGEI MANZHOS, National University of Singapore — TiO2 has been studied very extensively and its applications in various fields, e.g. applications in energy storage and catalysis are well known [1, 2]. Crystalline, amorphous and amorphous/crystalline titania have emerged as anode materials for Li and post-Li batteries due to good capacity, high rates [2, 3], and safety. Which is why the electronic and atomic structures as well as the properties of various crystalline TiO2 phases have recently attracted much research interest. Amorphous TiO2 (a-TiO2) phase also looks promising based on the few available studies but is much less explored [3, 4, 5, 6]. We have previously shown that amorphization of Si improves storage energetics of Li, Na, Mg [7], and there are reasons to believe that a-TiO2 will achieve the same. At high rates of charge-discharge, capacitive contribution to the specific capacity of titania electrodes becomes significant [8, 9, 10]. Therefore, interfacial effects are critical for the performance of titania-based anodes and need to be understood. We present a comparative first principles study of Li, Na, and Mg storage at nanosheets (NS) of crystalline (anatase (101), rutile (110), and (B) (110) surfaces) and amorphous TiO2 and compare the results to Li, Na, Mg in the bulk.

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