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Different behavior of lithium interaction with SiO2 and Al2O3¹ YUFENG ZHAO, CHUNMEI BAN, National Renewable Energy Laboratory, BRANDEN B. KAPPES, Colorado School of Mines, QIANG XU, CHAIWAT EN-GTRAKUL, National Renewable Energy Laboratory, CRISTIAN V. CIOBANU, Colorado School of Mines, ANNE C. DILLON, National Renewable Energy Laboratory — Lithiation of SiO2 and lithium intercalation in Al2O3 is studied both theoretically and experimentally. Lithium interacts with these two types of oxides in distinctly different behaviors. Reversible insertion/extraction of lithium in SiO2 up to a Li density of 2/3 Li per Si are demonstrated experimentally. Densityfunctional-theory (DFT) calculation shows that neither free interstitial Li atoms (no reduction) nor formation of a local Li2O cluster plus a Si-Si bond (full reduction) is energetically favorable. However, two Li atoms can effectively break a Si-O bond and be stabilized between the Si and O atoms. Such a defect, representing a state of partial reduction of SiO2, is energetically favorable. DFT simulation shows that intercalation of SiO2 at high Li density through partial reduction results in crystalline compounds LixSiO2 (x < 2/3) with tunable band-gaps in the range of 2-3.4 eV. In sharp contrast, Al2O3 is very stable against lithiation through any form of reduction. However, good conductivity of Li ions is shown in porous Al2O3.

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