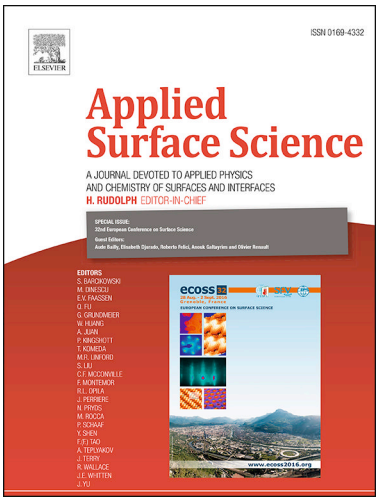
Accepted Manuscript



Short Communication

Lithium and Sodium adsorption properties of two-dimensional aluminum nitride

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PII: S0169-4332(18)31262-5
DOI: https://doi.org/10.1016/j.apsusc.2018.04.264
Reference: APSUSC 39263

To appear in: *Applied Surface Science*

Received Date: 9 February 2018
Revised Date: 20 April 2018
Accepted Date: 29 April 2018

Please cite this article as: A. Sengupta, Lithium and Sodium adsorption properties of two-dimensional aluminum nitride, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.04.264

Lithium and Sodium adsorption properties of two-dimensional aluminum nitride

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Abstract: *In this work the lithiation and sodiation properties of 2-dimensional (2D) AlN sheets are studied from density functional theory (DFT) simulations. 2D AlN showed theoretical specific capacity of 500.8 and 385.3 mAhg-1, maximum open circuit voltage of 1.49 and 1.86V and diffusion barriers 0.40 and 0.15eV, for Li and Na adsorption respectively. The calculations show 2D AlN as a possible alternative as anode material in Li-ion and Na-ion batteries. Further the high specific capacity and small diffusion barriers for Na atoms can make 2D AlN useful in supercapacitors. The change in carrier transport properties due to Li/Na adsorption on monolayer AlN can also be useful in chemical/bio-sensors and nanoelectronics devices.*

Keywords: Li-ion battery, Na-ion battery, 2D materials, DFT

I. Introduction:

With the ongoing search for superior anode materials for Li and Na-ion batteries, the vast potential of 2-dimensional (2D) materials is yet to be fully explored. [1]-[3] In recent years, there have been a number of reports on 2D sheets as silicene, germanene, black phosphorous, MoS_2, VS_2, MnO_2, Mo_2C, borophene etc. for their theoretical performance as potential electrodes in Li-ion/ Na-ion batteries (LIB/SIBs). [1]-[20]

With high research interest in mechanical/chemical exfoliation of layered materials and also advances in layer deposition techniques, the library of 2D crystals is only expanding. Thus impetus has been provided to study the lithiation or sodiation characteristics of various nanosheets, ribbons and nanotubes. 2D AlN, which has received significant attention [17,18,21]-[30] of-late owing to its electronic, optical and magnetic properties, could be another material of interest for ion-battery and other applications such as chemical sensors. In recent reports, one dimensional structures, as nanotubes of AlN have been explored for their possible application in gas sensors [18, 28], hydrogen storage [29] and LIBs. [17,30] In this context, 2D sheets can offer a rather different prospect for atom/ion adsorption than nanotubes, which has not yet been studied as extensively. The change in dimension from 1D nanotubes to 2D sheet is expected to significantly alter the adsorption behavior in terms of the binding energies and the number of available sites, and also influence the electrostatics of the system. Further the issue of Li/Na diffusion on planar AlN has not been addressed in the earlier works. [30] These factors draw us to investigate the case of Li/Na adsorption on 2D AlN sheets.