

Abstract Submitted
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Positive lithiation potential on functionalized Graphene sheets¹

RAJIV KUMAR CHOUHAN, PUSHPA RAGHANI, Boise State University, Boise, ID 83725, USA — Designing lithium batteries with high capacities is major challenge in the field of energy storage. As an alternative to the conventional graphitic anode with a capacity of $\sim 372mAhg^{-1}$, we look at the adsorption of lithium on 2D graphene oxide (GO) sheets. We have included van-der-waal's interaction in our calculation and compared with literature showing its importance in Li binding on Graphene sheets. In comparison to the negative lithiation potential in pristine graphene sheets, we were able to get positive lithiation potential by introducing functional groups such as epoxy(-O-) and hydroxyl(-OH) on graphene. Also the non-stoichiometric nature of GO provides better potential to increase the lithiation potential in compare to the defects induced graphene 2D sheet. Dramatic charge redistribution within the sheet due to presence of highly electronegative oxygen plays an important role in increasing the capacity.

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