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Li Storage Properties of Disordered Single- and Bi-Layer Graphene H. YILDIRIM, Purdue University School of Chemical Engineering , ALPER KINACI, Argonne National Laboratory, ZHI-JIAN ZHAO, Purdue University School of Chemical Engineering , MARIA CHAN, Argonne National Laboratory, JEFFREY P. GREELEY, Purdue University School of Chemical Engineering — Due to the limited capacity of the traditional intercalation-type graphite materials (373 mAh/g, LiC_6), much effort has been made to explore new anode materials to meet the increasing demand for batteries of high energy density. Among them, graphene has much attracted attention as an ideal platform for higher Li storage capacity, and for obtaining fundamental understanding of Li-C interaction. In this respect, we performed extensive first-principles calculations to model Li adsorption and intercalation in single- and bi-layer graphene, which are activated by defects for Li adsorption. For a wide range of Li coverages, the calculations predict that defect-free single layer graphene is not thermodynamically favorable compared to bulk metallic Li. However, graphene activated by defects are generally found to bind Li more strongly, and the interaction strength is sensitive to both the nature of defects and their densities. A rigorous thermodynamic analysis establishes the theoretical Li storage capacities of the defected graphene, and in some cases, these capacities are found to approach, although not exceed, those of bulk graphite. We will provide a performance comparison between defected single- and bi-layer graphene and bulk-graphite for Li storage capacities. A detailed analysis of the effect of the van der Walls (vdW) interactions will also be presented.

H. Yildirim
Purdue University School of Chemical Engineering

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