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Structural and metal adsorption properties of graphene and graphene derivatives

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Two dimensional materials are those layered structures in which the interaction between layers is sufficiently weak as to permit the easy exfoliation of the individual layers. Graphene is perhaps the most widely known member of this family, as it is commonly used in a variety of technologically important applications. The properties of graphene can be engineered for specific applications by creating defects, adding functional groups, reducing its dimensionality, and by substitutional doping or a combination of the above modifications. The dimensionality of graphene can be reduced to a quasi-one-dimension giving raise to edges, namely, armchair and zigzag. The presence of these edges produces a variety of electronic behaviors and affects not only the reactivity of the carbon material toward the adsorption of adatoms, such as Li or Na, but also their diffusion characteristics. Furthermore, upon oxidation and subsequent reduction, some of these properties are altered and can be optimized for particular applications. However, the question remains on whether these properties can be successfully controlled for the targeted uses. Here, I will briefly discuss the generalities of the theoretical framework employed in the calculations and present our numerical results for metal adsorption on graphene-based systems as well as our experimental results on graphene oxide derivatives. I will further discuss the effects of substitutional doping on the intercalation properties to show the effect of electron deficient species on these properties. In particular, I will present our results for a graphene-like material with high boron content and I will show its structural properties as well as its voltage characteristics with respect to metal ion intercalation.

Keywords: graphene; intercalation; calculations