

Abstract Submitted  
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**Alkali and halogen adsorption on graphene using ab initio calculation** CHENGIN CHIA, VINCENT CRESPI, Department of Physics, Pennsylvania State University, University Park — A seamless sp<sup>2</sup> graphene sheet prevents the penetration of atoms through the sheet, yet allows the penetration of electrons. Thus, a suspended single sheet graphene forms a geometrical constraint by separating the surrounding vacuum into upper half and lower half spaces. Alkali and halogen atoms, each constrained to one of the spaces, are forced to interact electrostatically via charge transfer through the sheet. We have found that under this constraint, a K atom can break the Cl-Cl bond of a chlorine molecule and form a new class of inter-atomic interaction, with strong long-ranged Coulomb effects on the band-structure. This investigation has now been extended to other alkali atoms (Na, Rb) and halogens (Br, I) to determine the generality of these new physical effects.

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