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Geometrical constraint on alkali and halogen adsorption on graphene CHENGING CHIA, Department of Physics, Penn State University — A seamless sp2 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 constrained background 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. A new type of chemical interaction is formed under this constraint, which we call topologically frustration bonding. We have calculated the interaction of a K atom on the upper surface with a halogen atom on the lower surface of a pure-carbon graphene sheet using density functional theory. The system becomes ferroelectric under this new geometrical constraint.

ChengIng Chia
Department of Physics, Penn State University

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