Topological Frustration in an Alkali-Graphene-Halogen System
YOUJIAN TANG, VINCENT CRESPI, Physics Department, Penn State University — We theoretically studied a system with alkali and halogen adsorbed to opposing sides of a graphene sheet, their mutual interactions then being modulated and constrained by the interposing presence of the sheet. Charge transfer from alkali to halogen generates a substantial dipole moment and large local electric field. Trends with respect to electron affinity, ionization energy, areal density, and the character of the bounding layer (i.e. BN versus graphene) will be discussed.

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