**First-principles Study of Band Gap Tunability in Hydrogenated Graphene**

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There have been on-going efforts to tune the electronic structure of graphene through chemical modifications. Notable examples include *graphane*, a two dimensional analogue of diamond, obtained through complete hydrogenation of graphene. The hydrogen coverage undoubtly presents a experimentally accessible way to open the band gap of graphene. In this study, we present a systematic approach to instill hydrocarbon motifs in single-side hydrogenated graphene (SSHG) presumably in contact with substrate. Here, we employed electron counting rules, a well-established formalism for dangling bonds at semiconductor surfaces, in combination with first-principles calculations to identify the most probably SSHG structures and their corresponding electronic properties. Here, the bandgap opening can be atributed to quantum confinement of isolated aromatic hydrocarbon motifs based on benzene embedded in graphene through hydrogenation. In contrast, conducting polymer motif based on polyacetylene gives rise to robust metallic properties against Peierls distortion. Our results suggest an efficient way to prepare graphene-based devices with suitable band gap through controllable hydrogenation.