Abstract Submitted
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Strain-induced chiral symmetry breaking leads to Dirac cone opening in graphene heterostructure[1] ENRIQUE MUNOZ, Pontif Univ Catolica de Chile, DEYA DAS, SWASTIBRATA BHATTACHARYYA, ABHISHEK SINGH, Materials Research Centre, Indian Institute of Science, Bangalore — Using first-principles calculations, we report [1] a large band-gap opening in the van der Waals heterostructure of graphene and graphane (hydrogenated graphene) under normal compressive (NC) strain. In the presence of graphane, interlayer charge transfer from graphene to graphane triggers the intralayer charge redistribution in graphene, breaking the equivalence of the two sublattices. The application of the NC strain enhances the inter- and intralayer charge transfer leading to a splitting of the Dirac cone, reflected as a redshift of the G peak in Raman spectra. We further present an analytical theory, based on the Dirac approximation, that provides a simple explanation of this effect within a general framework that suggests the same mechanism for band gap opening can be observed in other graphene based heterostructures. References [1] D. Das, S. Bhattacharyya, E. Munoz and A. K. Singh, Phys. Rev. B 94, 115438 (2016)

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Enrique Munoz
Pontif Univ Catolica de Chile

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