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The Interdependent Atomic and Electronic Structures of Graphene on Hexagonal Boron Nitride¹ JEIL JUNG, Department of Physics, National University of Singapore, ASHLEY DASILVA, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin, SHAFFIQUE ADAM, Yale-NUS college, Graphene Research Centre and Department of Physics, National University of Singapore — Recent progress in preparing well controlled 2D van der Waals heterojunctions has opened up a new frontier in materials physics. I will address the intriguing energy gaps that are sometimes observed when a graphene (G) sheet is placed on a hexagonal boron nitride (hBN) substrate, demonstrating that they are produced by an interesting interplay between structural and electronic properties, including electronic many-body exchange interactions. Our theory is able to explain the observed gap behavior by accounting first for the structural relaxation of graphene's carbon atoms when placed on a hBN substrate and then for the influence of the substrate on low-energy π -electrons located at relaxed carbon atom sites. All three contributions of the moire pattern pseudospin Hamiltonian play a role in defining the features of the moire bands including the degeneracy of the mini-Dirac cones and the particle-hole asymmetry. We find that the effective anisotropic strains arising from virtual hopping are associated with effective magnetic fields on the order of ~ 10 T and they dominate over the pseudomagnetic vector potentials generated by the moire strains due to partial commensuration.

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