Abstract Submitted
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The 2D Frenkel-Kontorova model of graphene on hexagonal boron nitride[1] JEIL JUNG, Department of Physics, University of Seoul, Seoul 02504, Korea, ASHLEY DASILVA, Department of Physics, University of Texas at Austin, Texas 78712, USA, SHAFFIQUE ADAM, Department of Physics, National University of Singapore, and Yale-NUS College, 6 College Avenue East, 138614, Singapore, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin, Texas 78712, USA — Graphene on hexagonal boron nitride (G/BN) constitutes a 2D realization of the coupled Frenkel-Kontorova model where the lattices of graphene tend to align with the commensuration potential generated by the substrate. We analize the map of free energies in G/BN as a function of lattice constant expansion in graphene and twist angle, and propose that the thermal annealing process will favor an equilibrium configuration with zero twist angle and expanded lattice constant of graphene. The twist-angle dependent energy map suggests that substantial sample rotation will take place during device annealing and that the moire period can expand beyond the 15 nm set by the lattice constant mismatch between graphene and BN. The delicate balance of the energetics involved in the adhesion free energy minimization of graphene on hexagonal boron nitride suggests the possibility of using anisotropic strains or curvatures as control knobs to tailor the moire pattern dependent band gap, carrier transport and optical response properties.

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