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Hofstadter butterfly and quantum transport in graphene on hexagonal boron nitride from multiscale lattice simulations NICOLAS LECONTE, University of Texas at Austin, US - Department of Physics, University of Seoul, Seoul 130-742, Korea, RAFAEL MARTINEZ-GORDILLO, Centre Interdisciplinaire de Nanoscience de Marseille, CINAM, CNRS and Aix Marseille University, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, ALLAN MACDONALD, University of Texas at Austin, US, JEIL JUNG, Department of Physics, University of Seoul, Seoul 130-742, Korea — Clear signatures of the Hofstadter butterfly have been experimentally observed in graphene on hexagonal boron nitride (G/BN), thanks to an appropriate balance between the length scale and the quality of the moir superlattices. During this talk, I will present a methodology to map the continuum moir pattern of incommensurable G/BN crystals obtained from ab initio calculations onto supercell lattice tight-binding Hamiltonians. Using efficient Lanczos recursion techniques for simulating large scale systems containing millions of atoms, the density of states and the dc conductivity are obtained as a function of energy or carrier density and magnetic field. The calculated Hofstadter butterflies and Landau fan diagrams show that the site potential variations, the mass, and substantial virtual strain contributions that appear even in the absence of real strains in the band Hamiltonian sensitively affect the electron-hole asymmetry, the gaps at the secondary Dirac points, as well as the tertiary features that appear at high-carrier densities.

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