Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Accurate effective model Hamiltonian for non-commensurate graphene on hexagonal boron nitride substrate[1] JEIL JUNG, ZHENHUA QIAO, ALLAN MACDONALD, The University of Texas at Austin — High quality hexagonal boron nitride (h-BN) crystals have emerged as a promising substrate and barrier-material for graphene nanoelectronic devices. The influence of the h-BN substrate on graphene's electronic properties is sometimes observable, but often extremely weak. We develop a theory of the h-BN graphene interaction that is based on first-principles electron tunneling amplitudes calculated as a function of horizontal displacement between commensurate honeycomb lattices. The effective Hamiltonian we derive is valid for arbitrary rotation angles between adjacent graphene and h-BN sheets.

[1]We acknowledge support from DOE Division of Materials Sciences and Engineering grant DE-FG03- 02ER45958

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Date submitted: 03 Dec 2012 Electronic form version 1.4