Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Self-consistent perturbation theory for two dimensional twisted bilayers SHARMILA N. SHIRODKAR, GEORGIOS A. TRITSARIS, EFTHIMIOS KAXIRAS[1], John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA — Theoretical modeling and ab-initio simulations of two dimensional heterostructures with arbitrary angles of rotation between layers involve unrealistically large and expensive calculations. To overcome this shortcoming, we develop a methodology for weakly interacting heterostructures that treats the effect of one layer on the other as perturbation, and restricts the calculations to their primitive cells [2]. Thus, avoiding computationally expensive supercells. We start by approximating the interaction potential between the twisted bilayers to that of a hypothetical configuration (viz. ideally stacked untwisted layers), which produces band structures in reasonable agreement with full-scale ab-initio calculations for commensurate and twisted bilayers of graphene (Gr) and Gr/hexagonal boron nitride (h-BN) heterostructures. We then self-consistently calculate the charge density and hence, interaction potential of the heterostructures. In this work, we test our model for bilayers of various combinations of Gr, h-BN and transition metal dichalcogenides, and discuss the advantages and shortcomings of the self-consistently calculated interaction potential.

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[2]Georgios A. Tritsaris *et. al.*, Perturbation theory for weakly coupled two-dimensional layers, **under review.**

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Date submitted: 04 Nov 2015 Electronic form version 1.4