Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab initio Mapping of Interlayer Coupling in Transition Metal Dichalcogenides and Graphene[1] SHIANG FANG, EFTHIMIOS KAXIRAS, Harvard University — Two-dimensional layered materials cover a wide variety of physics phenomena, such as topological phases, superconductivity, magnetism and charge density waves. Owing to the layered geometry and the van der Waals interactions in between, stacks of these van der Waals layered materials provide a venue to create a heterostructure with various physics properties. The interaction between different physics properties is particular interesting to engineer the material with the desired properties. One of the crucial ingredient in understanding the heterostructure is the interlayer coupling in between. In the literature, such kind of coupling has been proposed in various empirical forms. However, a true ab initio coupling model is still lacking. For the first time, here we have derived such interlayer coupling model from the first principle calculations based on the Wannier transformation of graphene stacks. We further investigate the Fermi velocity renormalization, van Hove singularities and the moire pattern for electron localization. Such microscopic understanding of the interlayer coupling would shed light on orbital hybridization and transport in multilayer stacks.

[1]This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, and by ARO MURI Award No. W911NF-14-0247.

Shiang Fang
Harvard University

Date submitted: 06 Nov 2015 Electronic form version 1.4