**Structural relaxation, electronic structure, and electron-phonon coupling in magic-angle twisted bilayer graphene**

Young Woo Choi,1 and Hyoung Joon Choi1,\*

*1 Department of Physics, Yonsei University, Seoul 03722, Korea*

\* E-mail: h.j.choi@yonsei.ac.kr

Interplay between the interlayer coupling and the rotational mismatch between two graphene layers results in flattening of Dirac cones at certain special twist angles , called magic angles. Recently, correlated insulator behavior and superconductivity were experimentally observed near the first magic angle , demonstrating rich physics induced by the presence of the flat bands. In this regard, more detailed characterizations for the magic-angle twisted bilayer graphene (MA-TBG) are being done. In this poster, we investigate structural relaxations, electronic structure, electron-phonon coupling in MA-TBG at the atomistic level. First, equilibrium atomic positions are determined by minimizing the total energy of the system, consisting of the in-plane strain energy and the interlayer binding energy. Then, we calculate the electronic structure and phonon spectrum using the tight-binding approach and the force constants, respectively. The electron-phonon matrix elements are then obtained from the modulation of hopping parameters due to atomic displacements of phonon modes. We present the electron-phonon coupling strength in MA-TBG with as a function of doping level, and discuss implications for superconductivity in this system. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2017-C3-0079). Y.W.C. acknowledges support from NRF of Korea (Global Ph.D. Fellowship Program NRF-2017H1A2A1042152).

