Atomistic Calculations of Filling Dependent Electronic States in Magic Angle Twisted Bilayer and Trilayer Graphene

A. Wania Rodrigues[1], M. Bieniek[2], D. Miravet[1], M. Korkusiński[3], P. Potasz[4] and P. Hawrylak[1]

[1]*Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada*
[2]*Institute of Theoretical Physics, Wroclaw University of Science and Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland*
[3]*National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada*
[4]*Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudzi-adzka 5, 87-100 Torun, Poland*

a.waniaro@uottawa.ca

Moiré materials offer a promising platform for designing tunable simulators of 1D and 2D strongly correlated, topologically nontrivial, systems. In magic angle twisted bilayer graphene, the moiré lattice potential leads to the formation of flat bands at the Fermi level, which host a variety of strongly correlated phases [1]. The bands can be populated by up to eight electrons per moiré unit cell, due to four flavours (two spins and two valleys) per two energy bands. Insulating states at integer fillings, and superconductivity between them, were already observed [2-3]. Similar phenomena have been seen in mirror-symmetric magic angle twisted trilayer graphene, which has better tunability of its electronic structure and superconducting properties [4].

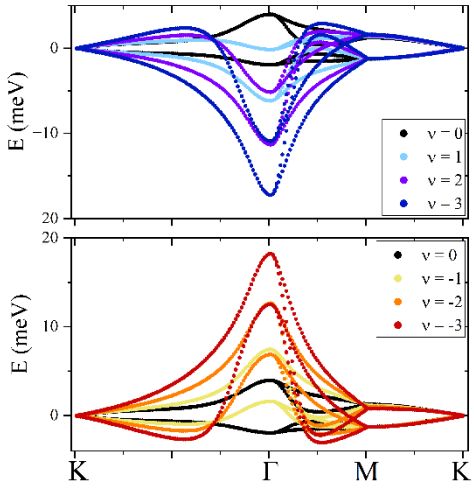

Fig.1. Band structure of magic angle twisted bilayer graphene for different fillings ν after the inclusion of the Hartree correction.

In this work we determine the electronic properties of both platforms using an *ab initio* based, multi-million atomistic p_z tight-binding model [5]. We account for the effects of electron/hole asymmetry by including a long-range hopping up to the 6th nearest neighbor. We include the relaxation effects that modulate the interlayer distance based on the stacking configuration. We also simulate the presence of an hBN substrate by including a staggered potential on the bottom layer of our system. Using all-bands and projected Hartree-Fock methods, we determine the evolution of the ground state as a function of the filling factor, including spin occupancy. We analyze the role of the long- and short-range Coulomb interactions and their influence on the band structure of the twisted bi- and tri-layers. We elaborate on the different types of the competing ground states, focusing on their topological properties. We determine the phase diagram dependence on the details of models of electron-electron interaction and on screening. We also determine the topological aspects of bands, focusing on the quantum geometry and the potential in realizing integer and fractional Chern insulator states.

References:

[1] E. Bistritzer and Allan H. MacDonald, PNAS **108**, 12233 (2011)
[2] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, R. C. Ashoori & P. Jarillo-Herrero, Nature **556**, 80 (2018)
[3] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras & P. Jarillo-Herrero, Nature **556**, 43 (2018)
[4] J. M. Park, Y. Cao, K. Watanabe, T. Taniguchi, P. Jarillo-Herrero, Nature **590**, 249–255 (2021)
[5] A. Wania Rodrigues, M. Bieniek, P. Potasz, D. Miravet, R. Thomale, M. Korkusiński, P. Hawrylak, PRB **109**, 7 (2024)