1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Research on electronic properties of moiré superlattices

1.1. Project goals

The project goals aim at understanding of electronic properties of various moiré superlattices obtained from twisted graphene layers and transition metal dichalcogenides heterostructures. We plan to utilize several multi-orbital tight-binding models for moiré unit cells containing up to several thousands of atoms, depending on moiré lattice constant. The effect of external magnetic field will be included using Peierls substitution. Both, perpendicular and parallel magnetic field to the crystal plane will be consider. The interaction effects will be included within mean-field Hartree-Fock method. The results will be confront with appropriate calculations using a reciprocal space model in plane wave basis (Bistritzer-MacDonald model). We aim to understand how the electronic properties vary with a moiré lattice constant, type of considered crystals and under external field – the effect of electric field will be also included. Our research will include studying the role of underlying lattice symmetry and disorder effects due to strain. Topological properties of moiré materials will be investigated, with characterization of topological edge states.

1.2. Outline

Moiré superlattices were shown to be a promising new platform for quantum simulators [1]. In particular the Hubbard model is one of the crucial models for understanding the essential many-body physics in condensed matter systems including Mott insulators and cuprate high-Tc superconductors. Recent experiments demonstrated antiferromagnetic Neel state at half-filling in WSe2/WS2 moiré superlattices [2]. For fractional fillings, generalized Wigner crystals have been identified [3–5]. While periodic moiré superlattices systems have been intensively studied in reciprocal space models, there are still many questions waiting to be answered [2, 6-8]. In particular, electronic properties of twisted bilayers, graphene and transition metal dichalcogenides heterostructures in the presence of the external magnetic field show new insulating phases [6]. Because the magnetic field breaks translation symmetry at least in one of two directions within a plane of the crystal (in Landau gauge), the problem is easier to investigate starting from the real space atomistic tight-binding models. A disadvantage is size of a unit cells containing up to several thousands of atoms. In this project, we will handle this problem using highly parallelized codes for multi-orbital tight-binding models. The results will be confronted with appropriate reciprocal space model calculations [1]. The effect of external fields and strain on electronic properties will be studied. Because flat bands around Fermi energy in twisted bilayer graphene reveal nontrivial topology, topological edge states will be characterized. Next, the effect of interactions will be included within a mean-field approximation, Hartree-Fock method. We will investigate the evolution of energy levels as a function of magnetic field strength and analyse formation of Landau levels. Insulating phases for

particular fillings of energy bands will be determined.
The project will be conducted in strong collaboration with NCN OPUS project "Twistronics - research on new quantum simulators", which is focused mainly on calculations in reciprocal space models. Therefore, apart from the doctoral school's regular salary, the Ph.D. candidate will be eligible to apply for an additional project-related scholarship.

1.3. Work plan

1. Development of tight-binding theoretical models aiming for the description of a broad family of moiré superlattices (graphene and transition metal dichalcogenides), including the effect of the magnetic field using Peierls substitution
2. Implementation of theoretical models as computer programs
3. Codes parallelization and initial large-scale calculations.
4. Implementation of Hartree-Fock method for mean-field calculations.
5. Moiré superlattice electronic properties calculations and analysis of results.
6. Writing scientific papers and PhD thesis; auxiliary calculations

1.4. Literature

[1] Wu, T. Lovorn, E. Tutuc, and A. H. MacDonald, Phys. Rev. Lett. 121, 026402 (2018).
[2] Y. Tang, L. Li, T. Li, Y. Xu, S. Liu, K. Barmak, K. Watanabe, T. Taniguchi, A. H. MacDonald, J. Shan, and K. F. Mak, Nature 579, 353 (2020).
[3] Y. Xu, S. Liu, D. A. Rhodes, K. Watanabe, T. Taniguchi, J. Hone, V. Elser, K. F. Mak, and J. Shan, Nature 587,214 (2020).
[4] C. Jin, Z. Tao, T. Li, Y. Xu, Y. Tang, J. Zhu, S. Liu, K. Watanabe, T. Taniguchi, J. C. Hone, L. Fu, J. Shan, and K. F. Mak, Nature Materials 10.1038/s41563-021-00959-8 (2021).
[5] X. Huang, T. Wang, S. Miao, C. Wang, Z. Li, Z. Lian,T. Taniguchi, K. Watanabe, S. Okamoto, D. Xiao, S.-F. Shi,and Y.-T. Cui, Nature Physics 10.1038/s41567-021-01171-w (2021).
[6] Petr Stepanov, Ming Xie, Takashi Taniguchi, Kenji Watanabe, Xiaobo Lu, Allan H. MacDonald, B. Andrei Bernevig, and Dmitri K. Efetov, Phys. Rev. Lett. 127, 197701 (2021).
[7] 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, and P. Jarillo-Herrero, Nature(London) 556, 80 (2018).
[8] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E.Kaxiras, and P. Jarillo-Herrero, Nature (London) 556, 43(2018).

1.5. Required initial knowledge and skills of the PhD candidate

- commitment and good motivation for work in science
- a degree in physics or similar
- ability to read scientific papers in English
- good computer programming skill

1.6. Expected development of the PhD candidate's knowledge and skills

- practical skills and expert knowledge in the field of nanostructure theory

- experience in high-performance computation
- practical understanding of machine learning algorithms and software
- ability to write scientific papers in English
- ability to present results of own research in a professional manner
- teamwork skills