PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to de published online)

Project title:

1.1. Project goals

The primary scientific objective is to characterize and explore methods for controlling boundary modes arising at the junction between two systems in different topological phases. Specifically, the project aims to:

- Develop a formal framework to classify and describe boundary conditions in graphene-based 2D crystals, focusing on how atomic arrangements and adatoms influence topological robustness.
- Investigate the stability of multilayer graphene stackings (e.g., Bernal vs. rhombohedral) under external conditions like strain and substrate effects.
- Identify stable lattice geometries that maintain topological protection at their interfaces, paving the way for electronics governed by topological order.

1.2. Outline

Topological materials host robust conducting surface states protected by global symmetries, yet these states are inherently sensitive to the specific physical implementation of the boundary. The bulk-edge correspondence—a fundamental principle of topological physics—provides a framework to determine the number of topological modes based on global bulk properties. However, their actual existence and behavior remain contingent upon the microscopic realization of the interface. The project focuses on the interplay between symmetry, structure, and topological properties at the junctions of 2D heterostructures. By employing atomistic models and ab initio calculations, we will investigate how varying parameters—such as layer number, stacking configurations, and specific junction implementations—can be used to tune electronic transport.

1.3. Work plan

The 4-year PhD project is divided into two main research lines: (A) Junctions and (B) Stacking stability:

- Year 1: Preliminary training in solid-state theory and numerical tools. Modeling basic junction realizations in graphene and hexagonal boron nitride (hBN) using tight-binding (TB) methods.
- Year 2: Implementation of additional degrees of freedom (spin, orbitals) and analysis of symmetry preservation at interfaces. Developing the general formalism for interface state control.
- Year 3: Transition to ab initio (DFT) calculations. Investigating the electronic properties and stability of multilayer graphene, specifically focusing on substrate influence and stacking changes under strain.
- Year 4: Analyzing the stability of specific edges and interfaces identified as topologically interesting. Generalizing findings to other 2D lattices and finalizing the doctoral thesis.

1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

M. Z. Hasan et al., Reviews of Modern Physics 82, 3045 (2010).
C.-K. Chiu et al., Reviews of Modern Physics 88, 3 (2016).
W. Jaskólski, M. Pelc, et al., Nanoscale 8, 6079 (2016).
M. Pelc et al., Physical Review B 92, 8 (2015).

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W. Jaskólski, M. Pelc, et al., 2D Materials 5, 2 (2018).
R. Guerrero-Avilés, M. Pelc, et al., Nanoscale 14, 16295 (2022).
F. R. Geisenhof, M. Pelc, et al., ACS Applied Nano Materials 2, 6067 (2019).

1.5. Required initial knowledge and skills of the PhD candidate

- Master's degree in Physics or a closely related field.
- Strong foundation in condensed matter physics and mathematical physics.
- Basic skills in computer programming (e.g., MATLAB, Mathematica, or Python).
- Proficiency in English for scientific communication.

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

- Expertise in topological band theory and the physics of 2D materials.
- Advanced skills in numerical modeling techniques: Tight-Binding (TB) and Density Functional Theory (DFT) using packages like SIESTA or VASP.
- Skills in code development and running large-scale simulations on high-performance computing clusters.
- Experience in international collaboration and disseminating research through high-impact journals and conferences.

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