Electronic properties of graphene-hBN giga-sandwich

In recent years 2D materials have become one of the most studied systems within physics due to a whole array of exotic properties that these materials exhibit. Graphene is the first and most prominent of these materials, consisting of a hexagonal honeycomb lattice made of carbon atoms.

A material with a similar lattice is hexagonal boron-nitride (hBN), being a hexagonal honeycomb lattice, but now consisting of alternating boron and nitrogen atoms instead of carbon and a slightly larger lattice constant of ~1.8%. When graphene is placed on an hBN substrate, a van der Waals heterostructure is created in which a moiré pattern emerges [1,2]. This pattern occurs because of the lattice mismatch between graphene and hBN, drastically increasing the size of the unit cell and inducing an effective 2D potential on the graphene layer.

By making an encapsulation of bilayer graphene (BLG) surrounded by hBN layers, we can create a moiré pattern separately on the top and bottom graphene layer so that we can now make combinations of moiré patterns as we please. The combining of moiré patterns can significantly modify the electronic properties of the BLG such as inducing strong localization of the charge carriers and strongly correlated electron states such as superconductivity. It is also known that stacking layers of graphene quickly leads to the dilution of the graphene properties until graphite is effectively obtained [3]. By alternating between BLG and hBN we might effectively overcome this as the hBN would largely shield the BLGs from each other, creating what is effectively a giga-sandwich. A bulk material can thus be created with the properties of BLG that can be tuned by changing the precise stacking of the hBN layers in between. Among possible properties are the emergence of highly correlated electron states such as Mott insulation and superconductivity. One could also tune the localization within the graphene layers to match vertically, perhaps changing the transport properties in the vertical direction.

For this project you will first have to create the structure by defining the position of all the individual atoms within the structure. This can be done by using *Pybinding* [4] (a Python package). Next you will have to create your very own tight-binding model and solve it by using both Pybinding and KITE [5] from which we can determine the electronic properties. In reality however, crystalline structures tend to strain and buckle as the lattice tries to achieve the configuration with the minimal interaction energy. This process is called relaxation and can be simulated by using semi-classical molecular dynamics for which you will use LAMMPS [6].

[1] P. Moon and M. Koshino, *Phys. Rev. B* **90**, 155406

[2] M. Yankowitz, *J. Phys. Condens. Matter* **26,** 303201

[3] B. Partoens and F. M. Peeters, *Phys. Rev. B* **74**, 075404

[4] https://docs.pybinding.site/en/stable/

[5] https://quantum-kite.com

[6] https://www.lammps.org