PhD Project Description

Title: Electronic phenomena in van der Waals heterostructures of two-dimensional crystals
Supervisor: Marcin Mucha-Kruczynski

Two-dimensional crystals are a new class of materials, with the first and most well-known representative being graphene, a single layer of carbon atoms arranged in hexagons [1]. They can be obtained by exfoliation of the “parent” layered bulk material like graphite (which is built of many graphene layers stacked on top of each other) or molybdenum disulphide. Because of the reduced dimensionality, properties of two-dimensional crystals often differ from those of their bulk counterparts. For the same reason, many of those properties are sensitive to the environment, e.g. presence and type of the substrate, and can be modified via chemical functionalization.

A recent idea is to use two-dimensional crystals as building blocks and by stacking those in a desired sequence arrive with new artificial materials [2]. The large choice of physical properties represented by the initial materials – e.g. semiconducting, insulating, metallic or superconducting (at low enough temperatures) – allows investigating completely new or previously inaccessible physical phenomena. The first such heterostructures, made of graphene and hexagonal boron nitride, were for example used to demonstrate for the first time the fractal spectrum of electrons in two dimensions exposed to external magnetic field and a periodic potential [3].

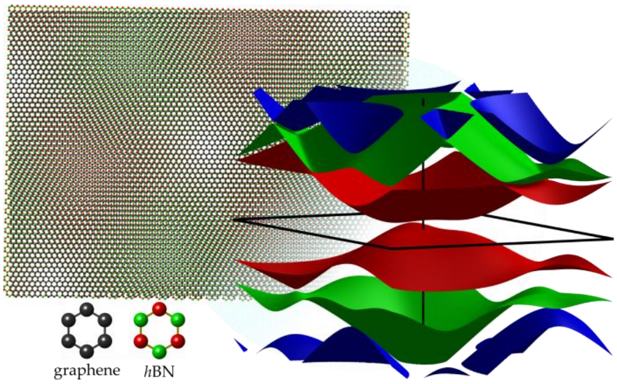

Figure 1 Moiré pattern of graphene on hexagonal boron nitride (*h*BN) and the electronic miniband structure of bilayer graphene on *h*BN [4].

During this project, realised within the group led by Dr Marcin Mucha-Kruczynski, the student will conduct theoretical investigations of the electronic band structure and transport properties of the heterostructures of various two-dimensional crystals, both in the absence and presence of external magnetic fields. The student will also explore the avenues to modify their electronic properties, for example by strain or chemical functionalization. The theoretical problems will be motivated by and closely related to experimental developments, and often pursued in collaboration with other groups in the UK and abroad (recent collaborations include theorists at Lancaster University and Nordita and experimentalists at ETH Zurich and University of Manchester). Examples of the theoretical questions tackled by the group members include investigation of the electronic band structure of graphene on hexagonal boron nitride [3,4] and tuning of the Lifshitz transition in bilayer graphene [5]. Because of the problem-oriented approach within the group, the student will, over the course of their project, learn to apply a mixture of analytical and numerical methods to physical problems.

For more detailed information on the research, please visit http://people.bath.ac.uk/mlmk20/

The successful candidate should hold, or expect to receive, a first class or good 2.1 Master’s degree (or equivalent) in Physics (Theoretical Physics preferred) or Theoretical/Quantum Chemistry (or other closely related field). A keen interest in theoretical condensed matter physics and a strong work ethic are essential. Also required is basic programming experience as well as some knowledge of Matlab/Mathematica.

Potential sources of funding include an EPSRC Centre for Doctoral Training (UK/EU citizens) or individual EPSRC/University of Bath scholarships. Candidates are encouraged to contact Dr Marcin Mucha-Kruczynski (m.mucha-kruczynski@bath.ac.uk) with informal enquiries.

References:
[1] A. K. Geim, *Graphene: Status and Prospects*, Science **324**, 1530 (2009).
[2] A. K. Geim and I. V. Grigorieva, *Van der Waals heterostructures*, Nature **499**, 419 (2013).
[3] L. A. Ponomarenko, R. V. Gorbachev, G. L. Yu, D. C. Elias, R. Jalil, A. A. Patel, A. Mishchenko, A. S. Mayorov, C. R.Woods, J. R.Wallbank, M. Mucha-Kruczynski, B. A. Piot, M. Potemski, I. V. Grigorieva, K. S. Novoselov, F. Guinea, V. I. Fal’ko, and A. K. Geim, *Cloning of Dirac fermions in graphene superlattices*, Nature **497**, 594 (2013).
[4] M. Mucha-Kruczynski, J. R. Wallbank, and V. I. Fal’ko, *Heterostructures of bilayer graphene and h-BN: Interplay between misalignment, interlayer asymmetry, and trigonal warping*, Physical Review B **88**, 205418 (2013).
[5] A. Varlet, D. Bischoff, P. Simonet, K. Watanabe, T. Taniguchi, T. Ihn, K. Ensslin, M. Mucha-Kruczynski, and V. I. Fal’ko, *Anomalous Sequence of Quantum Hall Liquids Revealing a Tunable Lifshitz Transition in Bilayer Graphene*, Physical Review Letters **113**, 116602 (2014).