Designing programmable simulators of strongly correlated electron systems in 2D materials

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Synthetic correlated electron systems offer the possibilty to design topological quantum matter with properties vastly different from its consituents, with superconductivity, ferromagnetism and incompressible liquids of the fractional quantum Hall effect as good examples. Electronic correlations and associated with it entanglement originate from electron-electron interactions in a flat band, degenerate electronic shell of single electron levels. Recently, two systems allowing the design of degenerate electronic shells were proposed: magic angle twisted bilayer graphene (MATBG) [1-3] and triangular graphene quantum dots with zig-zag edges (triangulenes) [4-6].

In MATBG, 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].

In this work, we present a Hofstadter's butterfly spectrum for the MATBG obtained using an *ab initio* based multi-million atom tight-binding model [7]. We incorporate a hexagonal boron nitride substrate and out-of-plane atomic relaxation. The effects of a magnetic field are introduced via the Peierls modification of the long-range tight-binding matrix elements and the Zeeman spin splitting effects. A nanoribbon geometry is studied, and the quantum size effects for the sample widths up to 1μ are analyzed both for a large energy window and for the flatband around the Fermi level. For sufficiently wide ribbons, where the role of the finite geometry is minimized, we obtain and plot the Hofstadter spectrum and identify the in-gap Chern numbers by counting the total number of chiral edge states crossing these gaps. Subsequently, we examine the Wannier diagrams to identify the insulating states at charge neutrality.

In the case of triangulenes obtained by on-surface synthesis [8], one electron energy levels collapse at the Dirac point and a degenerate electronic shell arises. At half-filling the shell is spin polarised but the polarisation is a non trivial function of the shell filling due to e-e interactions as in the lowest Landau level. By combining DFT and configuration interaction methods, we are able to manipulate the many-body spectrum of mono-, bi-layer and twisted bilayer triangulenes.

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Bio: Alina Wania Rodrigues obtained her B.Sc. and M.Sc. in Quantum Engineering at the Wroclaw University of Science and Technology in Poland. The focus of her thesis was designing electronic properties of twisted graphene heterostructures. Currently, she is a PhD student in the Quantum Theory group at the University of Ottawa, working with synthetic topological quantum matter in nanostructured 2D materials for quantum information processing. She is particularly interested in the electronic and optical properties of strongly correlated 2D systems, such as moiré materials.