Study of twisted bilayer Graphene: A Review

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ABSTRACT

There is not a controllable way to produce twisted bilayer graphene with a given angle, although some growth methods are more prone to yield twisted bilayers[1-2]. It was shown that graphene nanoribbons can be obtained by unzipping carbon nanotubes[3-4]. In this way twisted bilayer nanoribbons have been obtained by unzipping chiral multiwalled nanotubes[5]. Chiral graphene nanoribbons have edges with a mixture of armchair and zigzag components. It has been theoretically established that all edges, with the exception of the pure armchair, present zeroenergy localized states with a predominant weight at the edge atoms[6-7]. In pure zigzag nanoribbons, zeroenergy states are strongly localized at these atoms[8-9]. In chiral geometries edge states are also related to the presence of zigzag edge atoms, although they presented remarkable size effects. Indeed physical properties of chiral graphene nanoribbons and general edges can have a strong dependence on chirality[10-11]. The magnetic and electronic behaviour of graphene nanoribbons have been reported to be chirality dependent[12-16] but also their elastic and thermal characteristics[17-18]. Edge states of chiral graphene nanoribbon have been experimentally evidenced.

Introduction:

Recent experimental works point towards edge chirality control by means of electrical[19] or optical[20] tools, opening a novel way to engineer the properties of these systems. The intriguing dependence of the electronic properties of twisted bilayer graphene on these relative rotation angel between layers has attracted many theoretical[21-33] and experimental works[34-37]. If the rotation angle between the two graphene layers in large, i.e. from 10^0 to 30^0 with respect to the perfect AB stacking, the system behaves as if it were composed of the uncoupled layers[38], with a linear dispersion relation and the same Fermi velocity as monolayer graphene. For low rotation angles, a moire pattern in the density of states develops and distinct stacking regions can be observed[39]. Van Hove singularities revealed in density of states measurements by scanning tunnelling spectroscopy[40] and by an increase of the intensity of Raman modes measured in twisted bilayer graphene samples[41-42] Ming-Pei Lu[43] studied that charges trapped in the gate dielectricand acting as long range scatterers can wave a significant effect on carrier transport in graphene based nano devices. They theoretically investigated the charge capture kinetics of short distance channel defect interaction in graphene nanoribbon nano devices by employing the nonradiative multiphonon theory in conjunction with the coulomb energy ΔE . The peaks that emerged from the electron capture rate strongly correlated with the singularity characteristics of a one dimensional density of states. Moore's law has driven the evolution of semiconductor manufacture through shrinking of the dimensions of field effect transistors, there by improving the switching performance of electronic circuits and lowering the costs of commercial chips[44]. As

the dimensions of field effect transistors have decreased to become comparable with the screening length, a new issue has arisen, significant repulsive coulombic interactions between the channel carriers and the interface charged defects at short distance[45-47]. Several one dimensional nanomaterials have been proposed to act as channels in nano field effect transistors to increase the carrier mobility and improved the gate of bulk silicon MOSFETs[48-51]. Among those nanomaterials, graphene nanoribbons are particularly promising for use in high speed nanoelectronics and highly integrated nanochips, potentially replacing silicon in commercial nano field effect transistors, because of their extremely high carrier mobilites[52] and tuneable band gaps[53-54]. The effect of long range charge scattering arising from the charged centres during carrier transport in graphene based nanodevices has recently been high lighted[55-57]. Several groups have demonstrated experimentally that graphene and graphene nanoribbons nano field effect transistors covered with a thin top gate dielectric display improved switching characteristics[58-59], suggesting that the incorporation of top gate process into nano field effect transistor

fabrication be necessary to improve the performance of graphene based nano electronics. Alberto, Hector, Diego and Victor[60] studied the signatures of disorder in the production of orbital electron entanglement in quantum wires. Disordered entanglers suffers the effects of localization of the electron wave function and random fluctuations in entanglement production.They calculated the concurrence of distribution as a function of disorder strength within a random matrix approach. They also identified significant constraints on the entanglement production as a consequence of the breaking / preservation of time reversal symmetry. Quantum

entanglement has been identified as a key resource for emerging information technologies[61-62], especially in modern quantum electronics. Electron entanglement can be produced either by interacting mechanism[63-68] on noninteracting ones[69-75]. Electronic devices such as quantum dots and quantum wires have been proposed to produce entanglement of electrons without interactions[76-77]. The efficiency of these noninteracting entanglers depends on the scattering of electrons traveling through the system. Effectof quantum chaotic scattering on orbital entanglement production in quantum dots have been studied in past[78-83]. In essence, those works addressed the effect of the classically chaotic dynamics of the dot on entanglement production[84].

Dominik, and Lorenz[85] reported on hybrid Monte Carlo simulations of the tight binding model with long range coulomb interactionsfor the electronic properties of graphene. They investigated the spontaneous breaking of sub lattice symmetry corresponding to a transition from the semimetal to an antiferromagnetic insulating phase. Their short range interactions thereby include the partial screening due to electrons in higher energy states from ab initio calculation based on the constrained random phase approximation. From a theoretical perspective it has become clear that graphene can serve as a model system for a large number of concepts from high energy physics, ranging from topological phase transitions, chiral symmetry breaking and supersymmetry to quantum gravity[86-92]. Nguyen, Minoru and Susumu[93] studied the energetic and electronic structure of zigzag graphene nanoribbons with nanometer scale corners based on first principles total energy calculations. They found that the formation energy ofa short range with a 120^{o} corner was substantially smaller than that of a

straight zigzag edge with an infinite length. They also found that zigzag graphene ribbons with 120^o corners are semiconductors for which the band- gap decreased with increasing length between adjacent corners. The edge state was absent for zigzag graphene ribbons with short corner-corner distance, while the edge state energy for zigzag ribbon that have a corner-

corner distance greater than 1.5nm. The remarkable stability of the 120^0 corner of the short zigzag edges was in good agreement with the experimental observation of such corners of graphene edges. Graphene has stimulated intense interest because of its unique structural and electronic properties, a one atom thick sheet of hexagonally bonded sp^2 C provided with the ultimate two dimensional electron system comprising π electrons and resulted in two pairs of linear dispersion bands leading to a remarkable carrier mobility[94-95]. By verture of these properties, graphene holds a premier position not only in low dimensional sciences but also in nanoelectronic engineering[96-97]. The electron state is completely localized on atom with two fold coordination at the zone boundary, while it loses it

localized nature as the one dimensional wave number decreased[98-100]. It has been demonstrated that the spin polarization occurred at the edge atomic sites and that the polarised spins are ferromagnetically aligned along the edge[101]. Graphene of large are and excellent quality has been fabricated by chemical vapour deposition on metal surfaces[102]. Graphene frequently exhibited zigzag edges with corners with angle of 120^0 in transmission electron microscopy images[103-104]. Scanning tunnelling microscopy experiments showed that the corners occasionally consist of zigzag edges that are known to be energetically unstable edge conformations[105]. Early theoretical calculations showed that the edge formation energy of a zigzag

edge is larger by 0.2 eV per edge than that of an armchair edge[106] due to the emergence of the edge state Zhou and Wu[107] investigated quantum charge and spin pumping in armchair graphene nanoribbons under ac gate voltage connected with nonmagnetic / ferromagnetic leads via the non-equilibrium Green's function method. In the case of non-magnetic leads, where onlypart of the nanoribbon is subjected to an Ac voltage to break the left-right spatial symmetry, they showed that peaks of the charge pumping current appear that Fermi energies around the sub band edges in the field freeregion of the nonoribbon. In the case of ferromagnetic leads with the lead magnetizations being antiparallel to break the left-right symmetry, similar peaks appeared in the spin pumping current when the Fermi energies are around the edges of the majority spin sub bands in the ferromagnetic around the corresponding sub band edges. Tao et al[108] reported, graphene nano ribbon, a narrow strip of graphene has attracted intense interest for the fabrication of nanoscale devices because of its exotic electronic properties, such as edge states, size confined energy quantization[109-110] and magnetic order. Several approaches have been introduced to make graphene nanoribbons, including bottom up fabrication by chemical assembly[111], cutting graphene by lithography or plasma etching[112-113] and unzipping of carbon nanotubes by lithography[114], extensive oxidation, vapour expansion[115] or gas phase oxidation sonication[116]. Youpin et al[117] reported

on the electronic transport of graphene nanoribbon arrays fabricated by a chemical unzipping of well aligned single walled carbon nanotubes. The high quality of narrow graphene nanoribbons was implied by the existence of high field current saturation and the relatively low intensity of disorder peak in parallel

polarized Raman spectra. In a series of one dimensional systems such as single walled carbon nanoribbons[118-119], polymers[120] one dimensional semiconductor hetrojunction[121] and nanowires [122-123] interacting fermions exhibit collective excitation characteristics known as Luttinger liquid behaviour characterized by power law excitation spectra and thesuppressed density of states near Fermilevel[124-125].

Ihnatsenka and Kirezenow[126] presented numerical studies of conduction in graphene nanoribbons with reconstructed edges based on the standard tight binding model of the graphene and the extended Huckel model of the reconstructed defects. They performed atomic geometry relaxation of individual defects using density functional theory and then explicitly calculated the tight binding parameters used to model electron transport in graphene with reconstructed edge. The calculated conductance revealed strong back scattering and electron hole asymmetry depending on the edge and defect type. This is related to an additional defect induced band whose wave function is poorly matched to the propagating states of the pristine ribbon. They found a transport gap to open near the Dirac point and to scale inversely with the ribbon width, similarly to what has been observed in experiments. The transport gap measured experimentally in graphene nanoribbons exceed the theoretical electronic confinement gap[127]. This discrepancy is attributed to localized states induced by edge disorder[128-129]. Most theoretical studies of the electronic transport properties of graphene nanoribbons assumed simplified edge topologies[130]. Several experimental studies have characterized individual edge defects by means of Raman spectroscopy, scanning tunnelling microscopy or transmission electron [131-

[134] microscopy. The high degree of chemical reactivity of graphene edges favour edge reconstruction with different topologies, some of which were examined in abinito calculations[135-137]. Dubois et al[138] showed that realistic edge topologies strongly affect electron transport in the armchair graphene nanoribbons. Graphene has attracted a great deal of experimental and theoretical activity for its potential role as major future electronic materials. The peculiar band structure of electron in graphene predicted theoretically have been qualitatively confirmed by and angle resolved photoemission spectroscopy measurements[139-142]. In this measurements, a kink was observed[143] at about

200mev below the Fermi level $\in_F$. In order to explain this feature many

theories have been proposed[144-147]. Ming-Hao Liu and Kelans[148] studied the quantum transport formalism based on tight binding models is known to be powerful in dealing with a wide range of physical subject to external driving forces but is, at the same time limited by the memory requirement with the number of atomic sites in the scattering region. They demonstrated to achieve an accurate simulation of quantum transport feasible for experimentally sized bulk graphene hetero junctions at a strongly reduced computational cost. By solving the Dirac equation, perfect transmission at normal incidence across a potential step[149] as well as a potential barrier[150] was shown for monolayer graphene. This mimicks the Klein paradox in quantum electrodynamics[151] and was later referred to a Klein tunneling[152] which was attracted both experimental[153-160] and further theoretical[161-168] investigations. Ruseckas, Juzeliunas and Zozolenko[169] presented an analytical description of π electrons of a finite size bilayer graphene within

a frame work of the tight binding model. The bilayered structures considered were characterized by rectangular geometry and have a finitesize in one or both directions with armchair and zig-zag shaped edges.

They provided an exact analytical description of the spectrum of π electrons in the zig-zag and armchair bilayer graphene nanoribbons and nanotubes. They analysed the dispersion relations, the density of states and the conductance quantization. Graphene a single sheet of carbon atoms arranged in a honeycomb lattice, has attracted enormous attention because of its high unusual electronic and electronic properties, which are strikingly different from those of conventional semiconductor based two dimensional electronic systems[170-172]. The energy gap can be opened in a bilayer graphene by applying a gate voltage between the layers[173]. This gate induced band gap was demonstrated by Oostinga et al [174]and on/off current ration of around 100 at room temperature for a dual gate bilayer graphene field effect transistor was reported by IBM. Another way to introduce the gap is to form graphene into nanoribbons[175]. The conductance of graphene nanoribbons with lithographically etched edges indeed revealed the gap in the transport measurements[176]. This gap has been subsequently understood as the edge disorder induced transport gap[177] rather than the intrinsic energy gap expected in ideal graphene nanoribbons due to the confinement or electron interactions and edge effects. Controlled formation of edges by Joule heating, unzipping carbon nanotubes to form nanoribbons[178], a chemical route to produce nanoribbons with ultrasmooth edges[179] and automatically precise bottom up fabrication of graphene nanoribbons[180] analytic calculations for the electronic

structure of graphene nanoribbons have been reported [181-184]. The electronic structure of bilayer graphene was addressed by[185-190]. Where the analytical results were

presented Weizhe, Allan and Dimitrie[191] showed that conducting steady states of doped bilayer graphene have a nonzero sublattice pseudospin polarization. Electron-electron interaction renormalize this polarization even at zero temperature, when the phase space for electron-electron scattering vanishes they also presented that because of the strength of interlayer tunnelling, electron-electron interactions never the less have a negligible influence on the conductivity, which vanishes as the carrier number density goes to zero. The influence of interaction is qualitatively weaker than in the comparable cases of single layer graphene or topological insulators, because the momentum space layer pseudospin vorticity is 2 rather than 1. Their study relied on the quantum Liouville equation in the first born approximation with respect to the scattering potential with electron-electron interactions taken into account self consistently in the Hartree Fock approximation and screening in the random phase approximation.

In bilayer a band gap may be induced by a top gate[192-193] or by dual gates which can vary the carrier density in the two layers independently[194]. The theory of electronic transport in this unique and tuneable π band system has been investigated extensively[195-207]. Ting, Jian, Jinning and Yoshiuki[208] studied the electronic and magnetic properties of the zigzag edge graphene nanoribbon with a topological line defect under an external strain along ribbon axis by using first principle calculations. It was found that the applied strain induces the local magnetic moments on the line defect, whose coupling with those on the edges

leaded to turnover the spin polarization on one edge, making the line defect zigzag graphene nanoribbon become a ferromagnetic metal at a large enough strain. Graphene an important two dimensional carbon allotrope has been a hot topic due to its extraordinary mechanical electronic[209] optical and magnetic[210] properties. Both the graphene and the quasi-one-dimensional graphene nanoribbons have been extensively investigated in theoretical and experimental works[211-215]. The graphene nanoribbons magnetism has attracted great interest since its promising application in the design of nano scale magnetic and spintronics [216-217].

It has been shown that the graphene nanoribbons with zigzag edges are characterized with special localized edge states, showing a ferromagnetic order in the same edge but antiferromagnetic order between two opposite edges [218-220]. Ting Zhang, Rolf Heid, Kalus, Ping and Chan[221] reported a first principle study of the lattice dynamics of small graphene nanoribbons with zigzag edges. Their investigation was based on spin polarized density functional calculations. Nesting properties in the electronic band structure are very different for nanoribbons with unpolarised ferromagnetic and antiferromagnetic configurations. As a result, the phonon spectrum and nesting related softening in phonon frequencies differ in these cases. The unpolarised and ferromagnetic structures showed nesting related phonon softening and considerable electron phonon line width; while for the antiferromagnetic structure, a band gap at the Fermi energy eliminates these effects. Saturating the nanoribbon edge with hydrogen has negligible effect on the phonon spectra for the magnetic structures while for the unpolarised configuration all structures without hydrogen are unstable due to soft phonon modes.

1.2 Conclusion :

We have studied the band structure, density of states and spatial localization of edge statics in twisted bilayer graphene nanoribbon. Due to the spatially in homogeneous interlayer coupling, edge states stemming from region with stacking are closer to the energy of the Dirac point, where as those arising from stacked states are split in energy due to stronger interlayer coupling.

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