Dirac electrons and holes in artificial 2-D lattices and in real materials

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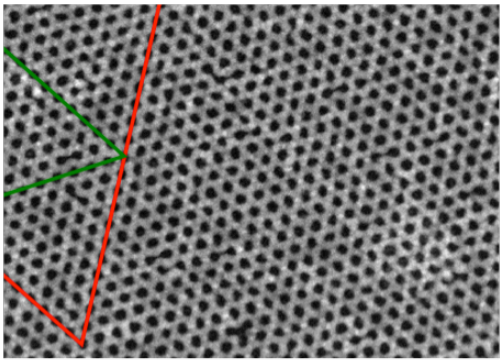
In the last decade, it has been realised that geometry in two-dimensions is a key factor in the development of new electronic materials that show deep-going physics, and novel electronic properties that may find applications in opto-electronics[1-4]. This revolution was in first instance initiated by the isolation of single layers of graphene. The ensuing electronic characterisation of this material showed for the first time the existence of carriers (massless Dirac Fermions) with a linear relationship between kinetic energy and momentum, a direct consequence of the honeycomb geometry. It was soon realized that this type of band structure could also be implemented in all-day 2-D semiconductors such as many II-VI and III-V compounds, provided that the electrons can be forced into a honeycomb lattice with a periodicity in the nm range. In addition, it has been predicted theoretically that other lattice geometries (graphynes, kagome and Lieb) also feature massless Dirac carriers and topological non-trivial bands. The consequences of a Dirac band structure are, among others: (1) high carrier mobility, (2) smaller influence of electrostatic defects, (3) the existence of new electronic phases such as the quantum spin Hall effect and carriers with zero kinetic energy (flat bands), (4) novel types of electron-hole excitons. In this lecture, I will present the attempts of us and others to prepare 2-D semiconductors with a honeycomb geometry, which are based on (i) fabrication of 2-D honeycomb semiconductors by lithography[5], (ii) using the spontaneous 2-d assembly and atomic bonding of colloidal nanocrystals[6-8].

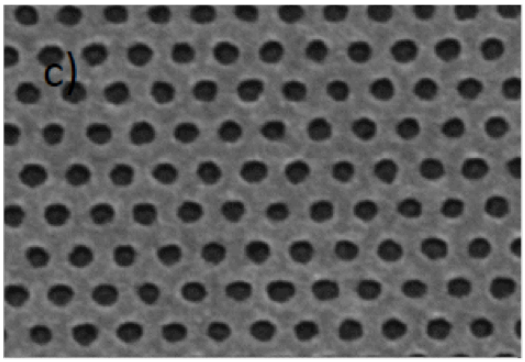
Awaiting these novel semiconductor materials, it is of high interest to test the theoretical predictions of the effects of geometry using ultra-clean artificial lattices that are easier to make and act as quantum simulators of real materials, under complete microscopic control. The group of Manoharan showed the potential of this approach by patterning the Cu(111) surface with CO molecules to force the surface electrons into a honeycomb pattern. The CO molecules were positioned on the Cu(111) surface by manipulation in an ultra-high vacuum cryogenic STM. The same apparatus was used to measure the density of states, demonstrating the Dirac cones of the honeycomb lattice. In an ensuing effort, we describe how we pattern a square-depleted Lieb lattice by manipulation of CO molecules on a Cu (111) surface. This is far from trivial, since the Cu surface atoms are arranged in a hexagonal geometry, while the Lieb lattice has square symmetry. We measure the density of states and wave function amplitude maps on the specific sites of the lattice. The results show a Dirac cone, crossed by a flat band. These results are reproduced using both muffin-tin and tight-binding based calculations. The results are highly distinctive, and

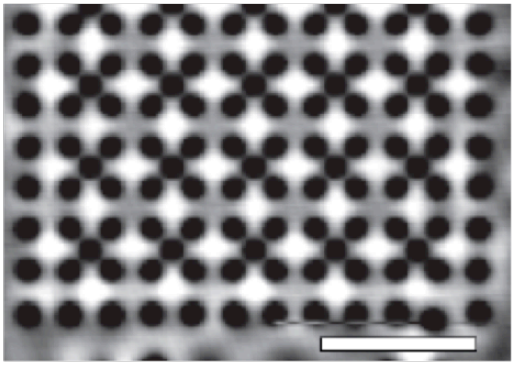
allowed us to derive the tight-binding parameters, such as nearest-neighbour hopping, besides showing that next-nearest neighbour hopping cannot be neglected. The novelty of our work in a broader sense is that we demonstrate how to make electronic lattices of arbitrary geometry that are directly accessible for a deep electronic characterization by tunneling spectroscopy. In this sense, our work shows tremendous potential to attack the compelling questions in the currently central era of solid state physics, i.e. topological electronic systems, as we can prepare lattices of nearly all geometries and implement in them controlled disorder, spin-orbit coupling and Cooper pairs.

PbSe honeycomb, 5 nm period

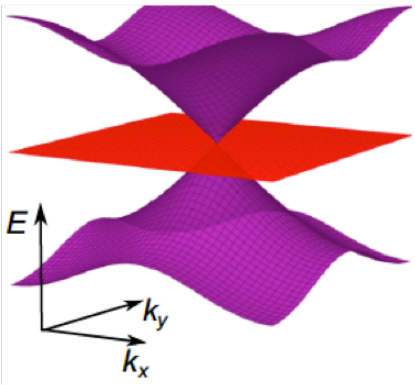


GaAs honeycomb, 50 nm period





Wave function map of a Lieb lattice, 1 nm period, formed by CO (black) on Cu(111)



Dirac - and flat band of the Lieb lattice

1 Nadvornik, L. *et al.* From laterally modulated two-dimensional electron gas towards artificial graphene. *New Journal of Physics* **14**, 053002 (2012).

2 Park, C.-H. & Louie, S. G. Making Massless Dirac Fermions from a Patterned Two-Dimensional Electron Gas. *Nano Lett.* **9**, 1793-1797 (2009).

3 **Kalesaki, E. *et al.* Dirac Cones, Topological Edge States, and Nontrivial Flat Bands in Two-Dimensional Semiconductors with a Honeycomb Nanogeometry. *Phys. Rev. X* 4, 011010 (2014).**

4 **Beugeling, W. *et al.* Topological states in multi-orbital HgTe honeycomb lattices. *Nat. Commun.* 6, 7316 (2015).**

5 Tadjine, A., Allan, G. & Delerue, C. From lattice Hamiltonians to tunable band structures by lithographic design. *Phys. Rev. B* **94**, 075441 (2016).

6 **Boneschanscher, M. P. *et al.* Long-range orientation and atomic attachment of nanocrystals in 2D honeycomb superlattices. *Science* 344, 1377-1380 (2014).**

7 **Vanmaekelbergh, D. Superlattice substitution. *Nature* 524, 418-419 (2015).**

8 **Geuchies, J. J. *et al.* In situ study of the formation mechanism of two-dimensional superlattices from PbSe nanocrystals. *Nat. Mater.* 15, 1248-1254 (2016).**