Center for Nanostructured Graphene - Highlights in 2019

Nano-porous Graphene: Covalent carbon circuitry for quantum transport

In a 2018 SCIENCE paper (Fig. 1a) "bottom-up" fabrication and electronic function of so-called "Nano-porous Graphene" (NPG) was demonstrated for the first time. The NPG can be viewed as parallel graphene nanoribbons connected by molecular bridges. In principle it is possible to change the molecular precursor builing-blocks and thereby tune the electronic structure and functionality of the two-dimensional covalent framework.
Following this work we have employed density functional theory (DFT) calculations to investigate how the electronic properties of similar NPG's may be tuned by varying the molecular bridges. In particular, we have found that a slight structural change of the bridge can change its electronic "transparancy", and there by the inter-ribbon coupling. Subsequently we have employed our in-house multi-scale transport method to study the electron flow on the 100 nm length scale. As a main result, we have shown how NPG's consisting of sections of less(meta) and more(para) transparent bridges may, together with electronic gating, be used to control the electronic current flow injectred from a point source (Fig. 1b). In this way we may envision to build 2D covalent carbon circuitry and harness quantum interference effects.
Some of these predictions are currently being investigated by the experimental groups.

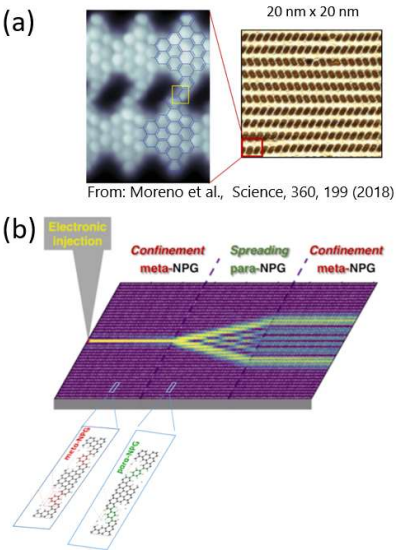

Figure 1. Multi-scale quantum transport simulation of point-injected electronic current in a NPG structure consisting of different molecular precursor building blocks (meta/para). It is demonstrated how the current flow displays quantum interference patterns which may be designed by the molecular structure and controlled with electronic gating.

G. Calogero, I. Alcón, N. Papior, A.-P. Jauho, M. Brandbyge (2019*) Quantum interference engineering of nanoporous graphene for carbon nanocircuitry*, J. Am. Chem. Soc. **141**, 33, 13081, doi: 10.1021/jacs.9b04649

Bandgap engineering of graphene using 10 nm patterning

The theoretical prediction that patterning of graphene with a high resolution could modify the bandstructure, was the initial motivation for establishing CNG. Researchers from CNG have been competing with top groups worldwide for a decade to be first in overcoming this surprisingly hard challenge. The problem is that disorder at the edges of the antidots, consistently ruins the subtle quantum transport properties. In 2019 we showed that by taking full advantage of the world-class lithography facilities at DTU and carefully tuning the etching process, graphene can be patterned on a 10 nm scale without destroying the transport properties. We find that the unique changes in the quantum transport properties are in very close agreement with numerical and analytical predictions (see Fig. 2), and that the carrier mobility is nearly 3 orders of magnitude better than previous results by us and others. We also found that the subtle Moire-minibands, a much-hyped consequence of the superlattice generated by two 2D crystals on top of each other with a slight twist-angle, can survive nanopatterning even on this small scale. Our discovery shows that contrary to the last 10 years disappointments, graphene can indeed be patterned on a very fine scale, which allows high-quality nano-scale circuits and devices to be fabricated, and that even the most subtle quantum transport features need not be destroyed in the process. The work was published in Nature Nanotechnology, and was by many media quoted as a breakthrough for graphene nanoelectronics.

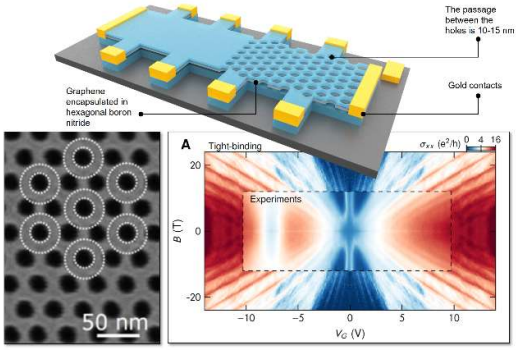

Figure 2. Graphene encapsulated in high quality hexagonal boron nitride, and patterned with 25 nm holes (10 nm spacing). The conductivity as a function of gate voltage and magnetic field shows an energy bandgap and a wealth of subtle features, in quantitative agreement with numerical and analytical predictions.

B. Jessen, L. Gammelgaard, M. R. Thomsen, D. M. A. Mackenzie, J. D. Thomsen, E. Duegaard, K. Watanabe, T. Taniguchi, T. J. Booth, T. G. Pedersen, Antti-Pekka Jauho, P. Bøggild, Nat. Nanotech, 14 (2019) 340-346 *Lithographic band structure engineering of graphene*