Transport in Biphenylene ribbons

*Biphenylene (BP), **Fig. 1**, is the last member of the 2D carbon allotropes family which has been reported very recently [Fan et al., Science 372, 852–856 (2021)]. It is made of a combination of 4-, 6- and 8-membered rings. BP has been characterized as a 2D metal, due to the closing of the band gap upon increasing the width of BP ribbons via scanning tunnelling spectroscopy (STS). In this project we consider transport in BP and nanostructures based on BP (nanoribbons, nanomesh).*

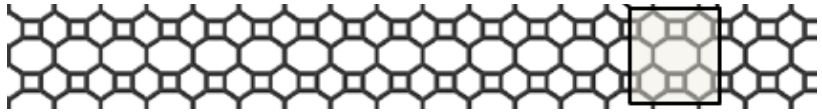


Fig. 1

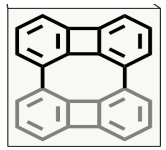


Fig. 2a

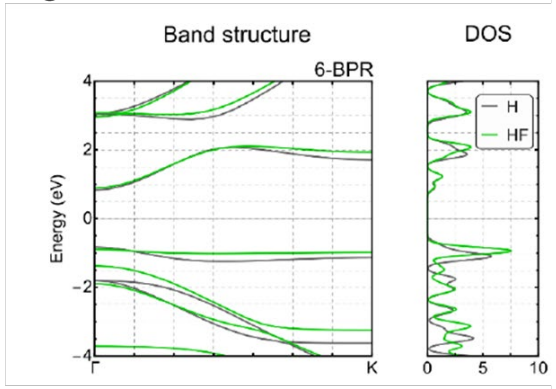
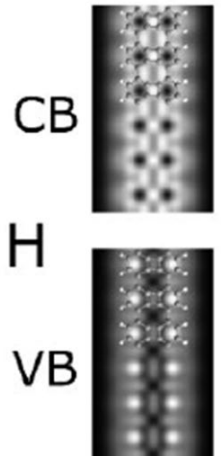


Fig. 2b



Plan

1. Calculate the bandstructure for a BP-nanoribbon of width 6 cells with the simple tight-binding model (see suppl. Mat. Of Science 372, 852–856 (2021)), **Fig. 1, 2a.**

2. Compare the LDOS maps in valence and conduction band with the STM Pictures, see Fig**. 2b**.

3. Calculate the transmission through the perfect ribbon and compare to the 1D bands.

4. Create defected structures (remove atoms in the middle or at the edge) or add an adsorbate atom and calculate the transmission.

5. Calculate bond-currents and see how they change with the defects.

Transport in a Biphenylene 2D network

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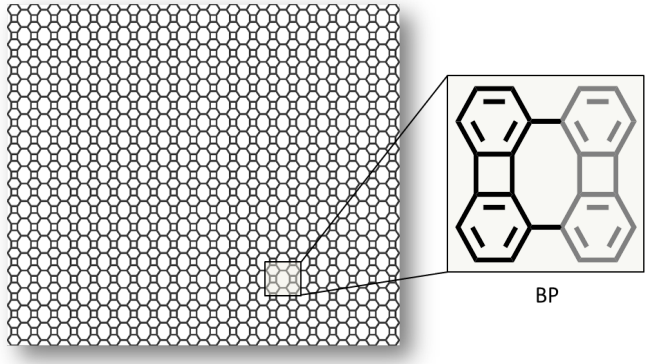


Fig. 1

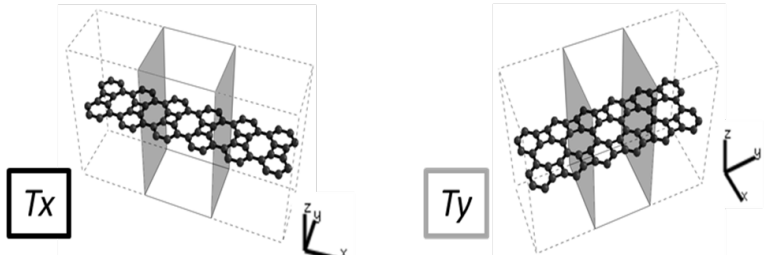
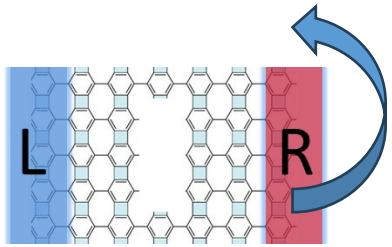


Fig. 2



Periodic boundary conditions

Plan

1. Calculate the bandstructure for BP (2D) with the simple tight-binding model.
2. Implement transverse k-point sampling in your transport code.
3. Calculate the transmission in the x and y directions as a function of transverse k, see **Fig. 1**. Make 3D or contour-plots of T(k,E), and plot k-averaged transmission.
4. Create structures with holes, **Fig 2**. Calculate bandstructure for periodic holes. Calculate transport through a periodic line of holes.
5. Consider holes along x or along y and vary distance.

Transport through molecular bridges in NPG

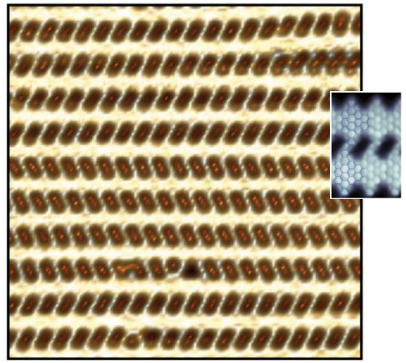


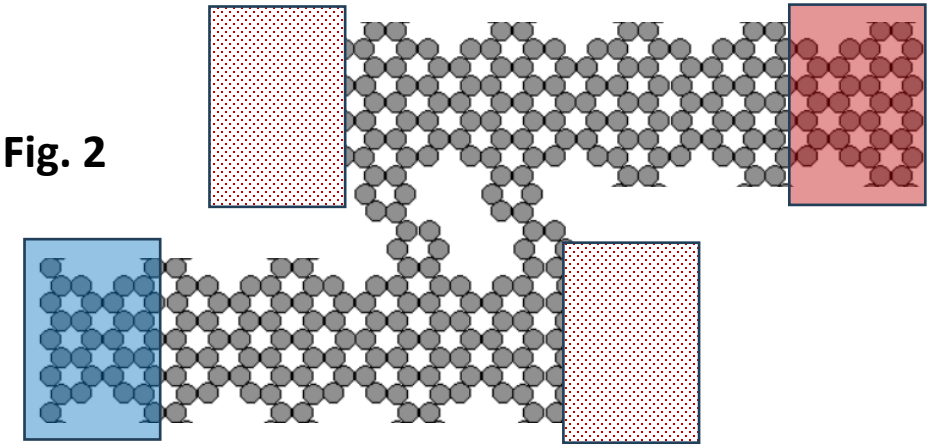
Fig. 1 *César Moreno et al. Science 2018;360:199-203*

Nanoporous graphene (NPG) ***Fig. 1*** *can be considered as carbon nanoribbons connected by molecular bridges. By changing the bridges one may change the electronic coupling between the nanoribbons. In this project we will consider just two ribbons coupled by one or a few molecular bridges (Fig. 2) and study how the transmission/coupling may be changed by changing the structure of the bridges.*

Plan

1. Calculate the 1D bandstructure for the pristine ribbon which will work as electrode using the simple tight-binding model.

Fig. 2



2. For the structure in Fig. 2 and calculate the transmission for 1 and 2 bridge molecules: Consider the case where the dotted region is an abrupt cut in the structure.
3. Calculate and visualize the bond-currents.
4. Try to replace the dotted region with self-energies to avoid the cut.
5. Change the bridge molecule from para to meta connected benzene rings (Fig. 3) and observe the change in transmission.
6. Try to change the bridges (play!) and calculate the transmission.

Fig. 3