
04 MODELISATION AND SIMULATION

HIGHLIGHT 1

Quantum dots embedded in graphene nanoribbons by chemical substitution

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The effect of boron dopants at low concentration on the electronic and transport properties of armchair graphene nanoribbons (aGNRs) with seven dimer lines across their width (7-aGNR) has been studied by a collaboration between the Modelization and Simulation group at CFM and the Nanoimaging group at NanoGUNE. Our study is based on a combination of scanning tunneling spectroscopy (STS) and large-scale density functional calculations using non-equilibrium Green's functions techniques.

Using on-surface synthesis strategies it is possible to grow 7-aGNRs substitutionally doped with diboron (2B) moieties at the centre of the ribbon. In our study we focus on regions where the 2B centres are separated by several nanometers. Besides impurity levels localized around the 2B centres, in the pristine regions between two 2B centres, we find clear signatures of the quantization of some of the 7-aGNR bands. Theoretical calculations have been instrumental to understand the origin of the quantized levels in detail.

Figure a shows a scheme of one of the studied systems, composed by 2B defects situated 6.5 nm apart. Figure

e shows the corresponding STS results. Besides the 2B-defect levels at ~ -0.5 eV and ~ -1.8 eV, one can see resonances at well-defined energies extending over the whole pristine region between the defects. They were tentatively assigned to quantum well states (QWSs) coming from the bands of the pristine 7-aGNR. Figure c shows the corresponding projected density of states (PDOS) from density functional calculations. Except for small energy shifts of the levels, the favourable comparison between theory and experiment is evident. The calculations confirm the number and approximate energy location of the localized 2B-defect levels, as well as the presence of QWSs.

Figure b shows the computed electron transport characteristics. These results show the enhanced transport at the energies corresponding to each QWS. This effect is similar to that of Fabry-Perot resonances in optics. Figure b clearly indicates that the QWSs are derived from the valence band (VB) of the 7-aGNR. In contrast, the lower valence minus one (VB-1) band is almost immune to scattering at the 2B impurities. This is further confirmed by the inspection of the transmission eigenchannel wavefunctions in Figure d. The different behaviour can be traced back to the different symmetry of both bands. The VB has even symmetry across the ribbon and interacts strongly with the 2B-derived defect states appearing at higher energies. In contrast, the VB-1 presents a node in the centre of the ribbon and is only weakly affected by the 2B defects. Similar differences take place between the conduction (CB) and CB+1 bands.

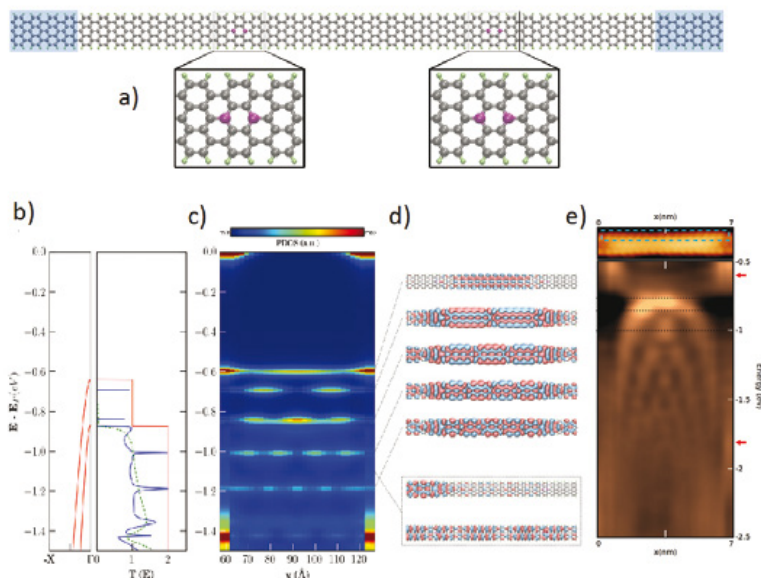


Figure: a) Model of the studied system formed by a pristine 7-aGNR region enclosed by two 2B-defects 6.5 nm apart. b) Dispersion of the VB and VB-1 bands of a pristine 7-aGNR, (left) and transmission function (right) for a pristine ribbon (red), a single boron pair (dashed green) and for the confined system formed by two boron pairs (blue). c) Projected density of states for the pristine segment. Quantized levels up to $n=5$ are clearly observed between the boron localized states. d) Real part of the eigenchannel functions taken at the energies corresponding to the $n=2, 3, 4$ and 5 QW levels. In the dashed panel are presented the real part of the eigenchannel functions taken at $E-E_F=-1.10$ eV, i.e. between quantized levels. The eigenchannel corresponding to the VB shows no transmission through the boron segments, while VB-1 fully transmits through. e) Experimental results obtained using scanning tunneling spectroscopy.

HIGHLIGHT 2

Electric-field-driven direct desulfurization

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A collaboration with the experimental group of Prof. Klaus Kern at the Max Planck Institut in Stuttgart has permitted us to explore chemical reactions implying the dissociation of carbon-sulfur bonds, which are fundamental for understanding the carbon and sulfur cycles in nature. Additionally, desulfuration reactions are of industrial significance in processes aimed at cleaning natural fuels. However, a clear

understanding of desulfuration reaction at the sub-molecular level, including the identification of the reaction paths, is a challenging problem.

In this work, we track the chemical pathway of an irreversible direct desulfuration reaction of tetra-ceno thiophene adsorbed on the Cu(111) closed-packed surface at the submolecular level. Using