

Porphyrin Functionalised Graphene Nanoribbons

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Pristine graphene does not have an electronic band gap, but its electronic properties can be engineered by forming graphene nanoribbons (GNR) through molecular self-assembly or top-down fabrication methods [1,2]. Chemical modification of GNRs is also an effective method to engineer their band gaps. Functionalisation strategies for modifying the electronic and chemical properties of GNRs have typically followed the same methodologies developed for graphene and have focused on edge site functionalisation; the introduction of defects or non-covalent functionalization. However, for the fabrication of functional multicomponent nano-systems the covalent bonding of organic molecules within the GNR is desirable. In this work we have developed an on-surface synthesis method for functionalization of armchair nanoribbons with porphyrin molecules. These novel nanostructures, termed porphyrin-functionalised graphene-nanoribbons (Py-fGNRs), are expected to exhibit significantly different electronic, chemical, transport and optical properties than the GNR or Py. Developing electronic devices using Py-GNRs has the potential for enhanced and emergent functionality in nanoscale devices. In particular, the versatile chemical functionality of the different transition metals within the integrated-porphyrin macrocycle (TM-Py), determines much of these electronic, optical, and chemical properties, as well as defining the exciting transport and spin-transport properties. Here we report the on-surface synthesis of Py-fGNRs and their characterisation. With STM we determine the possible distinct configurations that occur when the porphyrin couples to the GNR. These configurations are explored by DFT calculations which reveal a large reduction in the HOMO-LUMO band-gap on the porphyrin molecule.

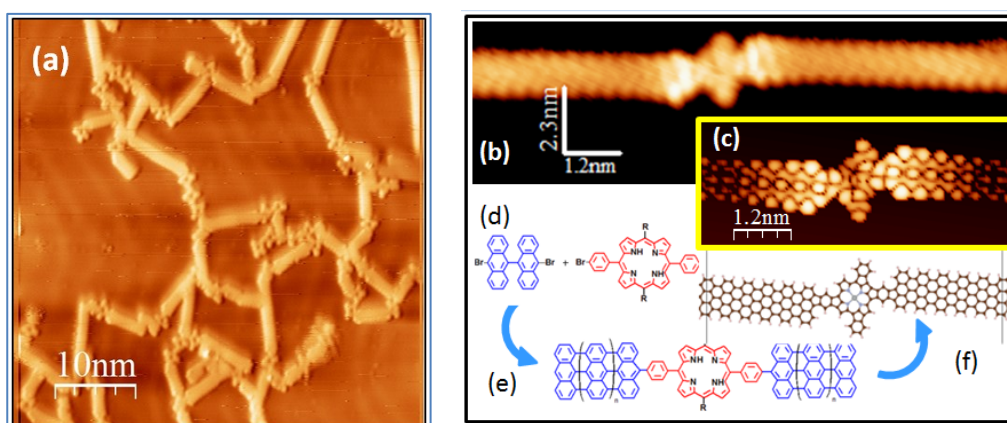


Figure : (a) STM image of porphyrin functionalised GNRs on Au(111) (b) STM image of individual Ni-Py-fGNR on Au(111); (c) simulation of HOMO orbitals of Ni-Py-fGNR via density functional theory calculation; (d) di-bromo-di-anthracene and di-bromo-tetra-phenyl-porphyrin precursors used for Ni-Py-fGNR formation; (e) physical structure of Ni-Py-fGNR following fusion; (f) structure determined by DFT.

References:

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