Integrating simulations and experiments to study graphene nanoribbons and their derivatives

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Known carbon nanostructures span all four spatial dimensionalities and display properties intimately related to different expressions of quantum spatial confinement. The discovery of fullerenes (0D),[1] carbon nanotubes (1D),[2] and the more recent experimental isolation of graphene sheets (2D)[3] have complemented the family album long occupied by the centuries-old 3D forms of carbon (e.g. graphite and diamond). The discoveries made over the past 30 years have unveiled a number of emerging phenomena and paved the way to the possibility of devising a spectrum of diverse carbon nanostructures where elementary low-dimensional building blocks are assembled into systems with ever-increasing complexity. For instance, the most recent isolation of graphene from graphite has triggered an unprecedented material science research activity in the study of a wide variety of graphene derivatives, such as graphitic nanoribbons (GNRs).

First, I will present results obtained using a variety of theoretical methods, ranging from Density Functional Theory to Tight-Binding approach, to study the structural, electronic, and transport properties of carbon based nanostructures. Emphasis will be placed on structures relevant to experiments, as well as on proposed device assemblies displaying emerging properties absent in the constituent building blocks. The effect of local chemistry, structural defects, molecular absorption, and substrate influence will be presented for a number of problems.

Second, I will provide a short overview of the properties of carbon nanotubes and the transport properties at their interfaces and how these properties can be controlled and exploited for applications.[4] The second part of the talk will be focused to our recent works devoted to GNRs, and their assembly into useful nano-assemblies such as networks[5] and regularly curved nanosystems[6]. A number of case studies where DFT modeling was instrumental in rationalizing experimental observations will be presented, including recent STM imaging of edge defects in GNRs as well as how GNRs can be obtained by thermally shocked N_2-filled MWNTs.[7]

Throughout the talk, insight on growth, assembly, interactions with interfaces, and transport properties will be provided on the basis o large-scale first-principles modelling combined with a variety of experimental studies.

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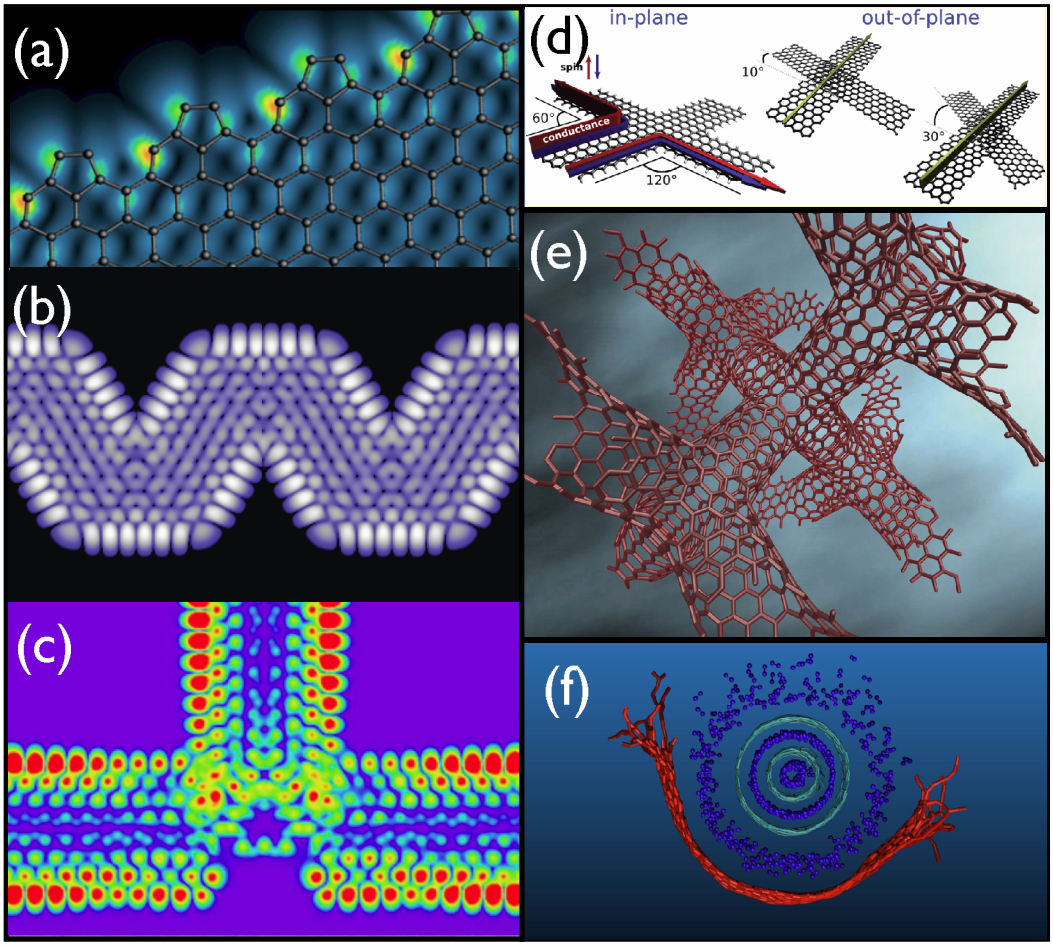

Fig. 1. Selected schematics of computational modeling of graphene based systems for nanoscience and nanotechnology studies. (a) STM image simulation of edge reconstruction in a GNR.;[7] (b) Charge density of a graphitic nanowiggle, obtained by self-assembly of small organic precursors;[6] (c) Charge density plot of a three-terminal nano-transistor sandwiching a small molecule used as an quantum interferometer;[8]; (d) Examples of multi-terminal GNR-based networks assembled using covalent (left) and non-covalent (right) interactions;[5] (e) Example of a nanonetwork made up of seamlessly connected carbon nanotubes (note the presence of octagons at the junctions, needed to account for high-genus differential surface);[4] (f) Classical molecular-dynamics snapshot representing the creation of a single-layered GNR induced by the thermally-shocked N_2-filled carbon nanotube (work in press).