Simulation of Electronic Transport in Quasi-Amorphous Graphene.

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Abstract

Graphene, a one atom-thick layer of carbon arranged in a honeycomb lattice, has sparked out intense research activities from both experimental and theoretical sides since almost a decade now. The striking properties of graphene in various fields, such as mechanical, thermal, or electronic transport properties, are intrinsically related to its two-dimensional aspect and to its bipartite honeycomb lattice structure yielding both to the peculiar electronics of Dirac Fermions and pseudo-spin symmetry. From the electronic transport point of view, clean graphene samples exhibit particularly long coherence length and high electronic mobility both interesting for devices applications in nanoelecronics. Graphene provide simultaneously a genuine playground for fundamental researches such as exploration of Anderson (anti-)localization phenomena in two-dimensional systems.

In this presentation, simulations of electronic transport in quasi-amorphous graphene structures will be exposed. Employing tight-binding models, and using a real-space order-N Kubo-Greenwood method [1-2], the transport properties of quasi-amorphous graphene structures are computed. The impact of a huge amount of various structural defects disrupting the ideal honeycomb lattice is thus investigated. Starting from a randomized graphene plane, molecular dynamics simulations are conducted to obtain highly defective graphene structures exhibiting both domains of amorphous graphene [3-5] and reconstructed pristine graphene areas (Fig.1). A careful analysis of the transport properties is performed through the Kubo-Greenwood formalism. Structural defects are found to induce strong resonant scattering states at different energies depending on their nature [6-8], inducing extremely short mean free paths and low mobilities. At low temperatures and in the coherent transport regime, large contributions of quantum interferences driving to localization phenomena are predicted. Actually, in regards to the results obtained, such quasi-amorphous graphene structures are predicted to behave as a strong two-dimensional Anderson insulator material [9], which could be experimentally confirmed by the magneto transport measurements at low temperatures for instance.

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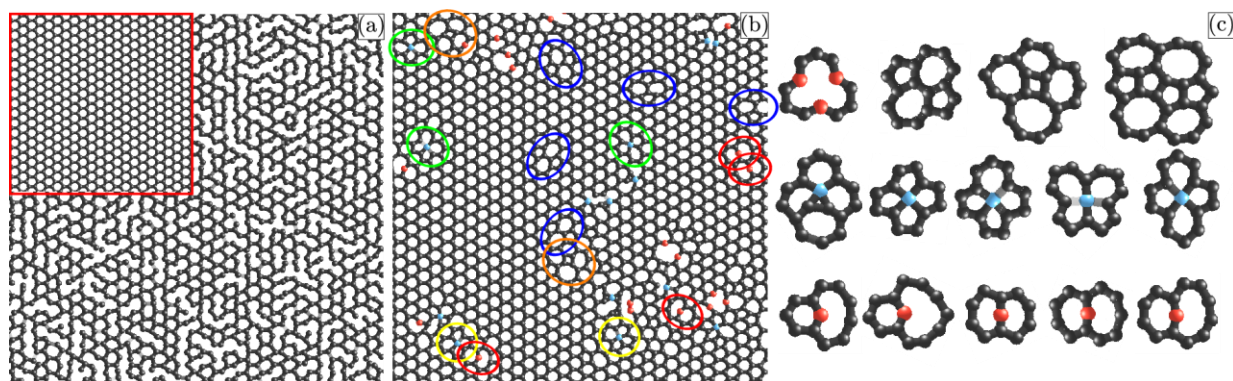
Figures

Figure 1: Highly defective graphene (HDG) structure: (a) Randomized graphene sample, (b) Structurally optimized model of HDG, (c) short list of structural defects observed.