

## Simulation of electronic transport in defective graphene. From point defects to amorphous structures

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Graphene, a one atom-thick membrane, 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 honeycomb lattice structure yielding both to the peculiar electronics of Dirac Fermions. 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 nanoelectronics. Graphene provide simultaneously is genuine playground for fundamental researches such as exploration of Anderson (anti-)localization phenomena in real two-dimensional systems.

In this presentation, simulations of electronic transport in defective graphene membranes are exposed. Employing tight-binding models validated by ab initio calculations, and using a real-space order-N Kubo-Greenwood transport method [1-2], the effect of structural defects disrupting the ideal honeycomb lattice is theoretically investigated. The case of various concentrations of “point defects” or single structural defects such as vacancies and Stone-Wales defects is first studied (Fig.1). Then, electronic and transport properties in the presence of a mixture of different structural defects is examined. Finally, using molecular dynamics simulations, highly defective graphene membranes presenting domains of amorphous graphene structure [3-5] are created (Fig.2), and their transport properties are carefully inspected. Structural defects are found to induce strong resonant scattering states at different energies depending on the nature and the concentration of defects [6-8]. These induced resonant scattering states can yield to extremely short mean free paths and low mobilities. At low temperatures, they also lead to an enhanced contribution of quantum interferences driving to localization phenomena in the quantum transport regime. In case of highly defective graphene membrane, the amorphization of the structure changes the system into a strong two-dimensional Anderson insulator material [9], which could be experimentally confirmed by the observation of a variable range hopping transport behavior at low temperatures.

### References

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## Figures

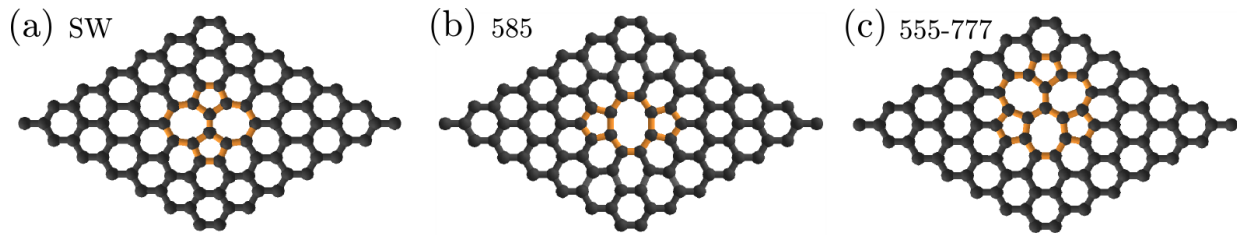


Figure 1: Three structural defects in graphene:  
 (a) Stone-Wales, (b) Divacancy 585, and (c) Divacancy 555-777

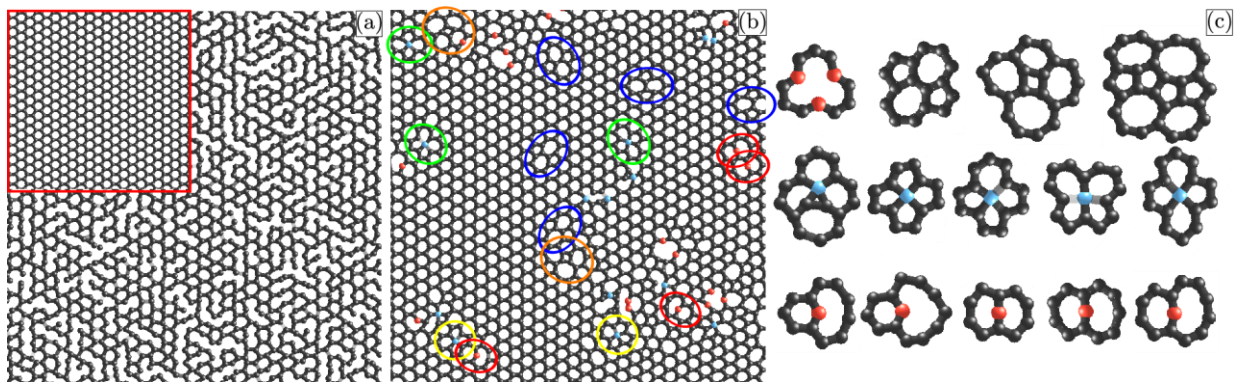


Figure 2: Highly defective graphene (HDG) membrane:  
 (a) Randomized graphene sample, (b) Structurally optimized model of HDG, (c) short list of frequently observed structural defects.