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Highly Defective Graphene: The thinnest insulating membrane[1]
AURELIEN LHERBIER[2], UCL/IMCN/NAPS, STEPHAN ROCHE[3], CIN2/ICN-CSIC and Universitat Autonoma de Barcelona, OSCAR A. RESTREPO, UCL/IMCN/BSMA, YANN-MICHEL NIQUET, CEA-UJF/INAC/SP2M/L-Sim, ARNAUD DELCORTE, UCL/IMCN/BSMA, JEAN-CHRISTOPHE CHARLIER, UCL/IMCN/NAPS — The electronic structure and transport properties of two-dimensional highly defective sp2 graphene are investigated theoretically. Using classical molecular dynamics, large planes of highly defective graphene-based sheets are first generated. An accurate empirical tight-binding Hamiltonian is then elaborated, allowing the prediction of elastic mean free paths, conductivities, and charge mobilities using a real-space order-N Kubo-Greenwood method. In sharp contrast to pristine graphene, the highly defective sp2 carbon sheet displays high density of states close to the Dirac energy. However, the dynamics of the corresponding electronic wavepackets reveals extremely short mean free paths (below 1 nanometer) and quantum interferences, both yielding to particularly strong localization phenomena. Consequently, these highly defective graphene-based sheets, although exhibiting a metallic character through the density of states, are from an electronic transport perspective among the most insulating two-dimensional one-atom-thick membrane ever made.

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