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Electronic-structure and quantum conductance of pristine and defective graphene layers and ribbons GIOVANNI CANTELE, Coherentia CNR-INFM and Università di Napoli "Federico II", YOUNG-SU LEE, MIT, DOMENICO NINNO, Coherentia CNR-INFM and Università di Napoli "Federico II", NICOLA MARZARI, MIT — Graphene has recently emerged as a fascinating alternative to carbon nanotubes as a subject both of fundamental research and of promising technological applications. In this work, we study the electronic structure and the transport properties of graphene layers and of graphene ribbons in the presence of several defects - from vacancies to topological defects to substitutional impurities. Very large systems with random distributions of defects are treated fully from first-principles and with chemical accuracy thanks to a formulation that combines density-functional theory and maximally-localized Wannier functions [1]. Our results are also compared with previous tight-binding calculations, when available.

[1]Young-Su Lee et al, Phys. Rev. Lett. 95, 076804 (2005)

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