Electronic and transport properties of (un)strained graphene with structural defects: Numerical calculations

The study deals with modelling electronic and transport properties of unstrained and uniaxially deformed graphene with structural imperfections: zero-dimensional (point) and one-dimensional (extended) defects. Point defects are modelled as resonant (neutral) adsorbed atoms or molecules, vacancies, charged impurities, and local distortions. Extended (line) defects are attributed to atomic steps and terraces in epitaxially-grown graphene, and grain boundaries, quasi-periodic nanoripples or wrinkles in polycrystalline (chemically vapor-deposited) graphene. Results are obtained numerically using the quantum-mechanical Kubo–Greenwood formalism along with tight-binding approach. Calculated behaviours of electronic density of states and conductivity indicate that deviations from perfection can be useful: they make possible tailoring graphene's electrotransport properties for achievement of new functionalities.