

## Thematic area: Nanoscale physics

### Effects of external magnetic field, uniaxial strain, and impurities on electronic states in graphene sheet

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We study magnetoelectronic properties of uniaxially stressed graphene with impurities in a perpendicular magnetic field applying the Peierls tight-binding model. To calculate electron density of states (DOS), we implement numerical algorithm (where the total computational effort linearly scales with number of atoms in the system) using Green's functions, continued fraction technique and tridiagonalization for Hamiltonian matrix. To take into account in electronic properties the effect of external stress applied to graphene lattice, we follow idea that strain ( $\varepsilon$ ) induces changes in bond lengths between sites and leads to changing hopping integrals, thus affects resulting electronic structure.

In case of absence of external magnetic field, the presence of randomly distributed impurities in a strained graphene counteract the band-gap opening and even can suppress the gap occurs when they are absent. However, impurity ordering contributes to the band gap appearance and thereby re-opens the gap being suppressed by random dopants in graphene stretched along zigzag-edge direction. The band gap is found to be non-monotonic with strain in case of mutual action of impurity ordering and zigzag deformation. Herewith, the minimal tensile strain required for the band-gap opening ( $\approx 12.5\%$ ) is smaller than that for defect-free graphene ( $\approx 23\%$ ), and band gap energy reaches the value predicted for maximal nondestructive strains in the pristine graphene. Effective manipulating the band gap in graphene requires balanced content of ordered dopants: their concentration should be sufficient for a significant sublattice asymmetry effect, but not so much that they may suppress the band gap or transform it into the “quasi- (or pseudo-) gap”.

A perpendicular magnetic field ( $B$ ) results in discrete Landau energy levels broadening as field  $B$  increases. Disordered and small content of ordered impurities smear and suppress Landau levels except the peak at a zero energy  $E$ . However, Landau levels re-appear on DOS curves for high concentrations of ordered impurities.