Curvature-induced optical transitions in graphene

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Graphene is a two-dimensional hexagonal crystal with an atomic thickness and its isolation has opened new frontiers for the researches. Recent observations showed that suspended graphene sheets are not perfectly flat showing corrugations that have been detected from electron microscopy and diffraction. Besides the intrinsic corrugation, the structure of graphene supported on substrate was found to be dedicated by the substrate roughness. Establishment of relationship between properties and geometrical configuration of graphene may add to the design of electronic and optical graphene-based devices.

We have performed ab initio calculations using plane-wave self-consistent field formalism to investigate the electronic and optical properties of rippled graphene. Armchair-edged graphene models were constructed using a cylindrical arrangement of carbon atoms. Dielectric function calculation was performed in the framework of the random-phase approximation.

We found that corrugation of graphene results in appearance of additional peaks in the imaginary components of the dielectric function and shift of main resonances typical for flat graphene for certain light polarization. Analysis of interband transitions demonstrated a contribution of electron transitions being forbidden for the flat graphene ($\pi \to \sigma^*$ and $\sigma \to \pi^*$ transitions for $E \perp c$ and $\pi \to \pi^*$ and $\sigma \to \sigma^*$ transitions for $E \| c$) in the in-plane and out-of-plane components of dielectric function of rippled graphene. Thereby, we conclude that positions and shape of peaks in optical absorption spectra are very sensitive to the geometry of rippled models. Stressing the graphene mechanically or placing the layer on an artificial substrate one could control the graphene rippling constructing a material with optical properties adjusted for a certain application. Particularly, bending of graphene can tune optical transparency window of the material.