**Time-Dependent Density Functional Methods for Real Scale Systems**

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Abstract

The ab-initio framework of Time-Dependent Density Functional Theory [1] is reviewed in light of the recent synthesis of atomically precise, graphene based or beyond graphene materials, being promising prototypes for high-performance, ultra-compact and ultra-low power devices [2–5]. The basic features of real space and reciprocal space methods are discussed, with emphasis on radiation damage, charge transport, and light-matter coupling dynamics at sub-wavelength resolution, i.e., below the diffraction limit in the optical band [6, 7]. A particular focus is devoted to few-atom-width nanoribbon and nanoribbon hetherostructures, where the signature of such a coupling are two peculiar charge-density oscillations, generated at the interface of the nanoribbons with the external dielectric environment [8]. These fundamental resonances, quantised as an edge and a surface plasmons, are here scrutinised by looking at the frequency-dependent permittivity and conductivity of graphene nanoribbons- being 5 to 29 carbon atoms wide- over the far-infrared to the near-ultraviolet range. A specifically developed adjustment on the random phase approximation is presented, which allows to distinguish the electromagnetic response of isolated (purely one-dimensional) nanoribbons from correlated (two-dimensional) nanoribbon arrays. A split-operator correction is further applied to account for band gap changes due to mechanical deformation or many-body GW-effects. A specific exchange correlation kernel is presented to improve the knowledge of electron correlations on isolated graphene nanoribbons. Finally, an effective ready-to-use model is derived from the ab initio framework, which is able to catch the main aspect of the two-plasmon structure at reasonably small momentum transfers.

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