Theory of Electronic Structure and Optical Properties of Graphene Nanodisks

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Graphene is a material with fascinating transport properties, but with a limited scope for opto-electronic applications because of its gapless nature. One way to overcome this hurdle is to work with nanostructures of graphene such as graphene nanoribbons or graphene nanodisks many of which are gapped because of their reduced dimensions, and resultant quantum confinement. However, in order to realize the full potential of graphene nanostructures in opto-electronic applications, it is essential to obtain a deep understanding of their electronic structure and optical properties. In this talk we will discuss the theory of electronic structure and optical properties of graphene nanodisks, within a Pariser-Parr-Pople (PPP) model Hamiltonian based correlated electron approach, developed recently in our group. We will present results of theoretical calculations of the optical absorption spectra of graphene nanodisks of different shapes and sizes. In addition to the linear optical absorption spectra, results on the nonlinear optical process of two-photon absorption will also be presented. Large-scale multi-configuration interaction methodology employed in this work ensures that our calculations include electron correlation effects to a high order.

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