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Photophysics of Nanostructures: Tubes, Sheets, and Ribbons¹

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The restricted geometry of nanostructures often gives rise to novel, unexpected properties and phenomena. In particular, symmetry and many-electron effects can play a vital role in determining the behaviors of these systems. In this talk, I discuss some recent work on using first-principles theory and computation (employing the GW-BSE approach) to understand and predict the electronic structure and optical response of carbon nanostructures including nanotubes, graphene and graphene nanoribbons. We show that, owing to reduced dimensionality, many-electron interaction (self-energy and excitonic) effects change qualitatively the nature of the photo-excited states in both semiconducting and metallic carbon nanotubes. Exciton states with extraordinarily large binding energies and an unusual spectrum (arising from an “anti-screening” phenomenon) are predicted for the semiconducting tubes. Moreover, unlike bulk systems, we discover that excitons also exist in the metallic carbon nanotubes. Similar studies show that excitonic effects are equally dominant in the optical spectra of the graphene nanoribbons, although the characters of the exciton states are quite different. Other quasi-1D systems, such as the boron-nitride nanotubes and semiconductor nanowires, exhibit similar behavior. We discuss the physics behind these phenomena and present comparison of our theoretical predictions to recent measurements.

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