Excitons in Carbon based quasi-1D systems: an ab-initio study of nanotubes and graphene ribbons

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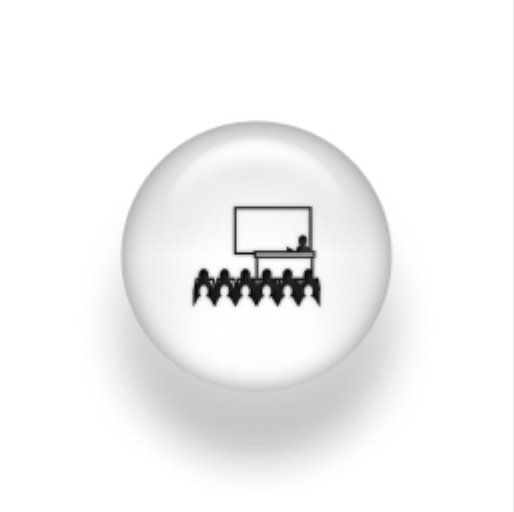
Dr. Deborah Prezzi



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We discuss the main characteristics of optical excitations in C semiconductor nanotubes and nanoribbons, as obtained from ab-initio many-body calculations. Our theoretical approach includes both self-energy corrections and excitonic effects through the GW-BSE formalism, providing full understanding of excited-state properties.
Electron-hole interaction is found to suppress the van Hove singularities -as known for other 1D systems- and introduces strongly bound excitonic peaks.
For C nanotubes, we show that exciton binding energy must thus be extracted from two-photon optical spectra and is of the order of several tenths of eV. A complete symmetry analysis of the excitonic states allows to understand the luminescence features observed in experiments [1]. In graphene ribbons we analyse different geometries and show that strong exciton binding is accompanied by relevant effects of the ribbon termination [2]. Based on simple prototype structures, we also discuss the possibility to obtain strong 0D confinement in graphene dots and antidots [3].
[1] Maultzsch et al., Phys. Rev. B 72, 241402(R) (2005) [2] D. Prezzi et al., arXiv:0706.0916v1 (2007) [3] D. Prezzi et al., in preparation (2007).