

Abstract Submitted
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Electron-electron interaction effects on the optical excitations of single-walled carbon nanotubes¹ SUMIT MAZUMDAR, HONGBO ZHAO, University of Arizona — We report correlated-electron calculations of optically excited states in ten semiconducting single-walled carbon nanotubes (SWCNTs) with a wide range of diameters.² First, we show that optical excitation in SWCNTs occurs to excitons whose binding energies decrease with the increasing nanotube diameter, and are smaller than the binding energy of an isolated strand of poly-(paraphenylenevinylene), (PPV). Second, electron-electron interactions split the degeneracies characteristic of cylindrical geometries, and in all cases there occur forbidden excitons below the optical exciton. We ascribe the experimentally observed low quantum efficiency of the photoluminescence of SWCNTs to the presence of these forbidden states. Third, while within one-electron theory the transverse photo-excitations occur exactly halfway between the two lowest longitudinally polarized absorptions, they are shifted to considerably above the central region for nonzero electron-electron interactions. Finally, the ratio of the threshold energy of the second longitudinally polarized optical absorption to that of the lowest such transition in the widest SWCNTs is less than 2 within correlated-electron theory, in agreement with experiments.

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²Hongbo Zhao and Sumit Mazumdar, Phys. Rev. Lett. **93**, 157402 (2004)

Sumit Mazumdar
University of Arizona