Abstract Submitted
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Coulomb effect and nonlinear optical properties of single-walled carbon nanotubes[1] HONGBO ZHAO, University of Arizona, SUMIT MAZUMDAR, University of Arizona — We investigated theoretically nonlinear optical properties of ten single-walled carbon nanotubes (SWCNTs) with a wide range of diameters, within a semiempirical Pariser-Parr-Pople model with a long- range Coulomb interaction. The excited states are calculated within Single Configuration Interaction (SCI) scheme. In our previous work [2] we have shown that there occur dark exciton states below the first optically allowed exciton, and that this is the reason for low photoluminescence quantum efficiency. In the present work we report calculations of photoinduced absorption (PA) from both dark and optically allowed lowest excitons for a mixture of SWCNTs, and compare our result with experimental ultrafast PA spectra. As with π-conjugated polymers, the lowest PA energies give lower bounds to the exciton binding energies. Our SCI calculations do not take into account double excitations, and hence we are unable to describe the high energy PA in SWCNTs. We speculate that the origin of the high energy PA is the same as in PPV. [3]

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[2]Hongbo Zhao and Sumit Mazumdar, Phys. Rev. Lett. **93**, 157402 (2004)
[3]A. Shukla, H. Ghosh and S. Mazumdar, Phys. Rev. B **67**, 245203 (2003)

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