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Nearly quantitative fitting of exciton energies and exciton binding energies of semiconducting single-walled carbon nanotubes (S-SWCNTs) within a π-electron model[1] ZHENDONG WANG, University of Arizona, SUMIT MAZUMDAR, University of Arizona — We use to Pariser-Parr-Pople π-electron Hamiltonian, which has been widely used to understand the excitonic energy spectra of π-conjugated polymers, to determine the energy spectra of S-SWCNTs. For the Coulomb interaction parameters, we use the screened Ohno parameters that were successfully used before for the quantitative fitting of the excitonic energy spectrum of poly-(paraphenylenevinylene) [2]. In order to take into account of the curvature effects, we use a π-electron nearest neighbor hopping integral that is substantially smaller than the standard 2.4 eV. With these modified parameters we are able to fit the lowest two exciton energies of a very large number of S-SWCNTs. We make detailed comparisons between the calculated and experimental [3]. We also obtain a binding energy of $\sim$ 0.4 eV for the lowest exciton of S-SWCNTs with diameters $\sim$ 0.8 nm, in agreement with experiments.

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[2]M. Chandross and S. Mazumdar, Phys. Rev. B **55**, 1497 (1997)
[3]R.B. Weisman and S.M. Bachilo, Nano Lett. **3**, 1235 (2003)

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