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The physics behind the family behavior of optical transition energies in single-wall carbon nanotubes GEORGII SAMSONIDZE, MIT, RIICHIRO SAITO, Tohoku University and CREST JST, Japan, JIE JIANG, Tohoku University and CREST JST, Japan, ALEXANDER GRÜNEIS, Leibniz Institute for Solid State and Material Research, Germany, ADO JORIO, UFMG, Brazil, SHIN GRACE CHOU, MIT, GENE DRESSELHAUS, MIT, MILDRED DRESSELHAUS, MIT — Experimental optical spectroscopy studies of single-wall carbon nanotubes (SWNTs) revealed $2n+m$=constant family patterns in the electronic transition energies. Meanwhile, the family behavior remained unexplained within the simple tight-binding approximation that has been commonly used for calculations of the SWNT band structure. We here present calculations for the optical transition energies in SWNTs using an extended tight- binding approximation which allows optimization of C-C bond lengths and bond angles along with the many-body corrections reported in the literature. Our calculations closely reproduce the experimentally observed family behavior, and find that the family behavior can be attributed to the collective effect of curvature-induced rehybridization, long-range atomic interactions, geometrical structure relaxation, and many-body interactions. Our calculations clarify controversial results concerning the magnitude of quasiparticle corrections and exciton binding energies in SWNTs.

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