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Effective One-Dimensional Electron-Hole Interaction in Single-Walled Carbon Nanotubes[1] JACK DESLIPPE, MARIO DIPOPPA, UC Berkeley and LBNL, DAVID PRENDERGAST, Molecular Foundry, LBNL, RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro, STEVEN LOUIE, UC Berkeley and LBNL — Using the results of ab initio GW-Bethe-Salpeter-Equation (GW-BSE) calculations on the excitonic effects in single-walled carbon nanotubes (SWCNTs), we derive a 1D quantum model for the electron-hole interaction in both semiconducting and metallic SWCNTs. The model includes the important effects of spatial dependent screening and reproduces the exciton binding energies and envelope wave functions of the complete GW-BSE solution of the electron-hole excited states. The inclusion of the spatial dependence in the dielectric function is essential to capture the positioning of the higher exciton states in the spectrum whose calculated energies differ dramatically from those obtained using previous models based on constant dielectric screening. The present effective interaction can be used to calculate the binding energies of exciton states in a range of SWCNTs, which would be impractical by ab initio study.

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Jack Deslippe
UC Berkeley and LBNL

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