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Structural and Electronic Properties of Single-Walled Carbon Nanotube Heterojunctions[1] JOYDEEP BHATTACHARJEE, Molecular Foundry, LBNL., YOUNG WOO SON, Dept. of Physics, Konkuk Univ., Seoul, Korea., BHUPESH CHANDRA, JAMES HONE, Dept. of Mech. Eng., Columbia Univ., JEFFREY B. NEATON, Molecular Foundry, LBNL. — Inspired by recent experiments[1], we present a systematic approach to construct structural models of mostly linear single walled carbon nanotube (SWCNT) heterojunctions. A minimum number of 5-7 defects is found to be required to join two SWCNTs of differing chiralities. Using nearest-neighbor tight-binding and first-principles density functional theory, we explore the sensitivity of the heterojunction electronic structure and transport properties to different arrangements of the interfacial 5-7 defects, and discuss their implications for future experiments and nanoelectronic applications.

References

[1] B. Chandra, J. Hone, *Unpublished*.

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