Motivation:
Recently techniques for the production of junctions between different carbon nanotubes (CNT) have been developed. The experimental observation that these contacts exhibit nonlinear IV characteristics leads to their potential application as molecular nanoscale device components.

Objective:
Develop tube-diameter dependent models for the effective mass, doping, band offset, and dielectric constant of a CNT and then, using standard heterojunction physics, relate the physical properties of a y-junction array of CNTs (diameters) to its electrical properties (IV).

Effective mass averaged over indices (n,m)

\[ m^* = 1.3m(a_{cc}/d) \]

Electron mass \( m_e \), C bond length \( a_{cc} \), diameter \( d \)

Effective mass with varying \( d \) (gcd)

轩 (2018) \( \varepsilon \) = no. vertices / no. edges

Average effective mass

Upper valence bands of CNT

\[ \beta = 2.74 \quad N_2 = 3 \times 10^{28} \text{ cm}^{-3} \]

Unit cell

\[ \Delta E_v = \frac{1}{d_2} \left( \frac{1}{d_1} - 1 \right) \]

Linear response approximation gives dielectric constant:

\[ \epsilon \approx \left( \frac{dN_A}{m^*} \right) X \text{ (CNT number in array)} \]

Electron orbital hybridization gives acceptor density:

\[ N_A = \frac{N(a_{cc}/d)^3}{d} \]

Average bond energy method gives band offset:

Comparison with limited data available gives a donor level of about one in every 60 Carbon atoms in the CNT.

Conclusion:
- Theory for CNT diameter dependence of effective mass, doping, band offset, and dielectric constant useful in predicting electric properties of rectifying junctions.
- Comparison with limited data available gives a donor level of about one in every 60 Carbon atoms in the CNT.