Role of Defects in Carbon Nanotubes

Objective:

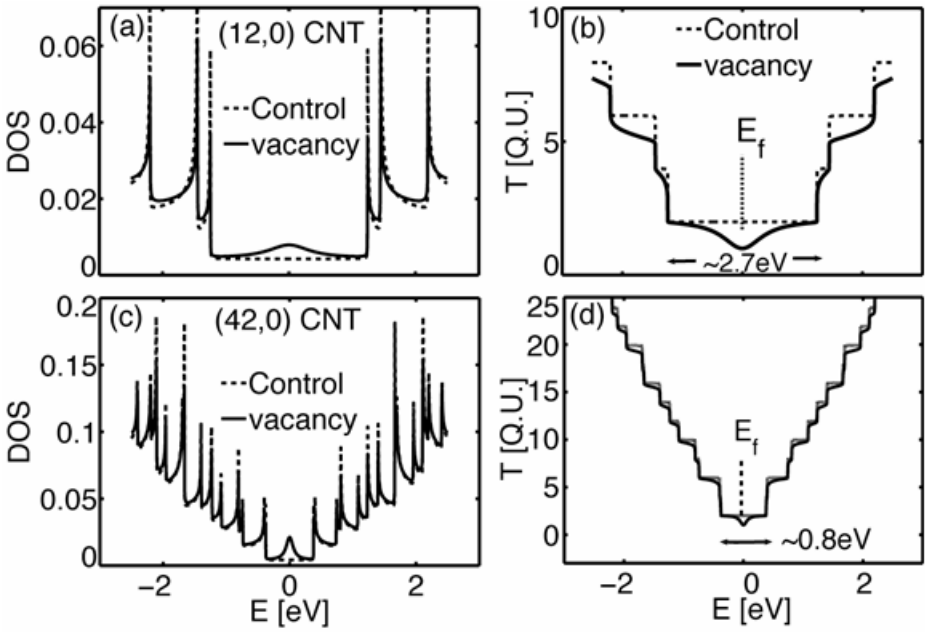
- Simulations of I-V characteristics of metallic carbon nanotubes under the influence of atomistic vacancy defects.

Approach:

- Nonequilibrium Green's function (NEGF) transport solver self-consistently coupled with a three-dimensional (3D) atomistic FEM Poisson kernel. A nearest neighbor tight binding model based on a single pz orbital is used to describe the device Hamiltonian.

Impact:

- CNTs used in analog applications must be defect free
- Impurities and/or defects in CNTs used in interconnects can have deleterious impact in signal transmission.



Result:

- A single vacancy defect in the channel of a small diameter metallic carbon nanotube can decrease its conductance by a factor of two.
- More than one vacancy in the channel can further drastically decrease the conductance.
- Larger diameter nanotubes suffer less from the presence of vacancy defects.