A 3D Atomistic Quantum Simulator for Realistic Carbon Nanotube (CNT) Structures

nanoHUB online simulation and more — an NCN project

Objective:

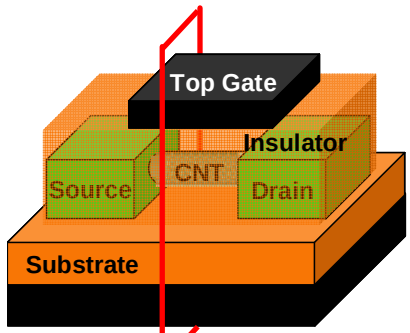
- Investigate the electrostatic effect of the 3D environment on 1D channels
- Investigate atomistic quantum transport in CNT devices

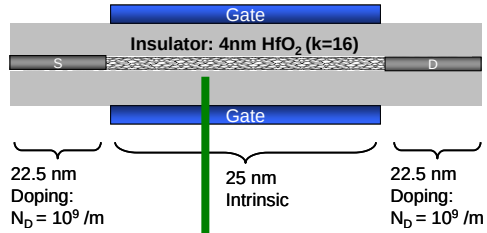
Approach:

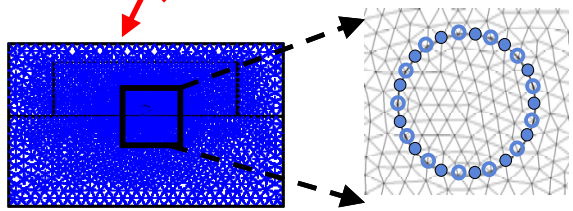
- A 3D simulation domain based on the FEM for treatment of the electrostatics
- Details involved:
  - Merge of the cylindrical CNT geometry to the rectangular device environment
  - Atomistic description of the CNT
  - Finite extent of the contacts (3D objects) to account for parasitic fringing fields
- Quantum transport based on NEGF

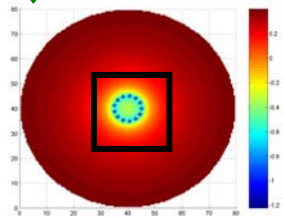
Impact:

- Insight on the electrostatics of 1D channel transport devices
- Quantum mechanical investigation of the effects of atomistic defects in 1D transport









Results:

- Electrostatics of 1D channels:
  - Sensitive to the oxide thickness
  - Not sensitive to the size of the contacts (except very near the contact point)
- Single atomistic defects can degrade the performance by ~30%.
- Exponential increase in channel resistance as the number of defects increases (in small diameter CNTs)

Publications:

- Tool online at nanoHUB.org CNTFET
- J. Comp Electr [J76], APL [J83], IWCE [P70]

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