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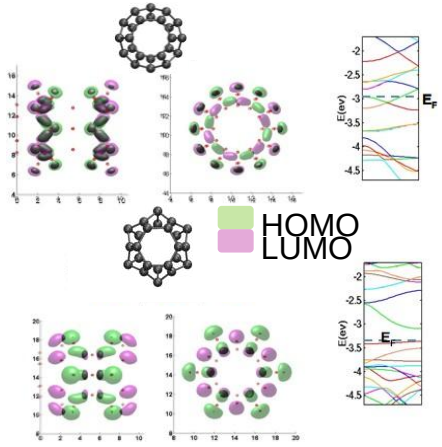
Surface and strain effects in nanostructures and nanodevices

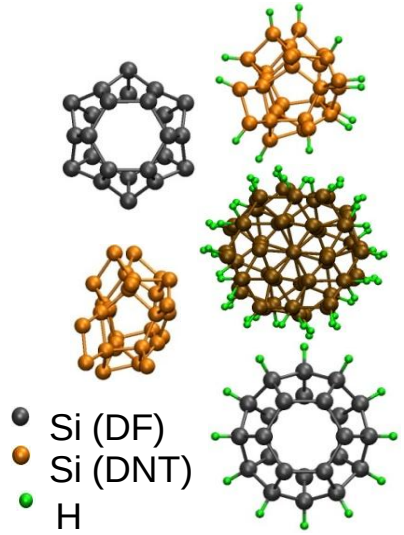
Methods employed/ developed: DFT, reactive FF MD, modified tight binding

~1nm dia silicon nanowires

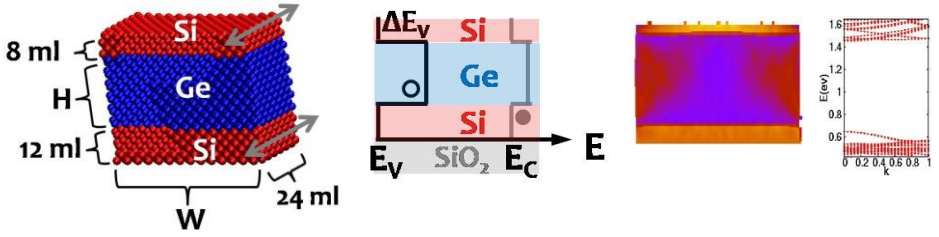
- *Goal:* exploration of new materials, photovoltaics, sensors, thermoelectrics, CMOS scaling, batteries

- **energetically most stable wires(**2 categories)
- tubelike: **non-bulk geometries**
- new bandgap ranges, **unique properties**
- surfaces => structural symmetry => properties



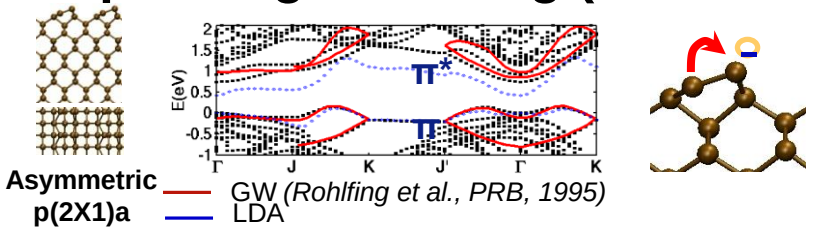


Electrical properties of Si-Ge-Si bars



- *Goal:* High performance electronics
- **inhomogeneous strain in Ge: reduced hole effective mass**
- bandgap between uniaxial and biaxial

Adaptive tight binding (Si surface)



- *Goal:* nanoelectronics (modified bonding), defects/ scattering in large systems
- modified TB parameters => good match with GW