ECE 595, Section 10
Numerical Simulations
Lecture 25: Further Bandstructure Simulation Tools

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Recap from Wednesday

• Electronic bandstructure lab
  – Basic principles
  – Input Interface
  – Exemplary Outputs

• Density functional theory (DFT)

• DFT in Quantum ESPRESSO
Outline

• Recap from Wednesday

• Periodic Potential Lab
  – Basic principles
  – Input Interface
  – Exemplary Outputs

• CNTbands
  – Basic principles
  – Input Interface
  – Exemplary Outputs
Periodic Potential Lab

• Solves single-electron Schrodinger equation in simple periodic potentials

• Calculates:
  – Energy bands
  – Electron wavefunctions
  – Effective masses
  – Bandgaps

Available on nanoHUB at:
http://nanohub.org/tools/kronig_penney

Periodic Potential Lab

• Input for step well (Kronig-Penney problem):
  – Max energy $V_{\text{max}}$
  – Min energy $V_{\text{min}}$
  – Energy over barrier $\Delta E$
  – Period $W$
  – Barrier width $a$
  – Particle mass $m_o$

Periodic Potential Lab

• Input for triangular well:
  – Left branch width $a$

Periodic Potential Lab

• Input for parabolic well:
  – Left branch $a=W/2$

Periodic Potential Lab

• Input for Coulombic well:
  – Well width $a$

Periodic Potential Lab: Output

Wavefunctions/eigen energies for maximum/minimum energies of each band

Periodic Potential Lab: Output

For minimum energy eigenvalues in each energy band.

The regions where the probability is larger than 0.5.

CNTbands

- **CNTbands v2.2** can simulate electronic band structure and density-of-states for carbon nanotubes (CNTs) and graphene nanoribbons (GNRs).
- It also computes some basic parameters: nanotube diameter, primitive basis, bandgap, etc.

Available on nanoHUB at: [http://nanohub.org/resources/cntbands-ext](http://nanohub.org/resources/cntbands-ext)

Graphene is a one-atom-thick planar sheet of carbon atoms that is densely packed in a honeycomb crystal lattice.

Direct image of a single-layer graphene membrane (Red dots denote carbon atoms)

Computer generated graphene visual showing the honeycomb lattice structure
Youngki Yoon; James K Fodor; Jing Guo; Akira Matsudaira; Diego Kienle; Gengchiau Liang; Gerhard Klimeck; Mark Lundstrom, "CNTbands" (2006).
Carbon nanotubes (CNT) are basically graphene sheets rolled up in a certain direction. “Chiral vector” or “chirality” describes how a graphene sheet is rolled up to form CNT. CNT might be metallic or semiconducting, depending on its chirality. The chirality is denoted by (m,n).

Xufeng Wang and Youngki Yoon, “CNTbands first-time user guide” (2011)
CNTbands

- Graphene Nanoribbons are thin strips of graphene.
- The electronic property of GNR largely depends on its edge structure.
- Since GNRs are “strips,” its length is defined via chirality as well.
- Its width, or the “thinness” of strip, is usually defined using how wide it is in nanometers or angstroms.
- GNRs’ chirality is defined slightly different from that of CNT. We will explain this later in detail.

Xufeng Wang and Youngki Yoon, “CNTbands first-time user guide” (2011)
CNTbands

Two possible input interfaces

For GNR

Structure specific

For CNT

Common for both CNT and GNR

• The E-k diagram describes the energy-wave momentum relationship for carriers within the first Brillouin zone.

• Each continued line is an allowed level of energy for carriers, or a subband. The E-k diagram thus describes the “bandstructure” of the studied material.

• Subbands closest to the equilibrium Fermi level (denoted E = 0 here) are of particular interest, since they are usually the levels giving rise to current. In CNTbands, these subbands are extracted and outputted as “Lowest subbands.”

Next Class

- Is on Monday, March 18 – enjoy Spring Break!
- Please submit the HW assignment today if possible