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

Prof. Peter Bermel

March 8, 2013

Recap from Wednesday

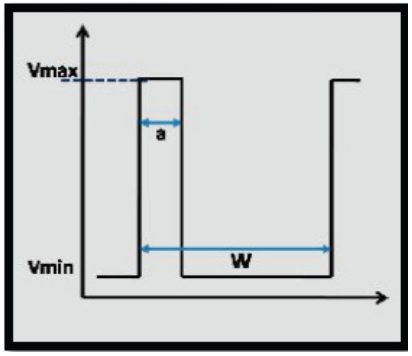
- Electronic bandstructure lab
  - Basic principles
  - Input Interface
  - Exemplary Outputs
- Density functional theory (DFT)
- DFT in Quantum ESPRESSO

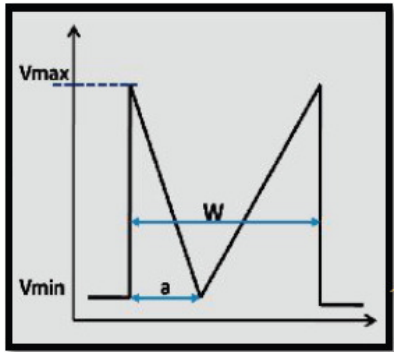
Outline

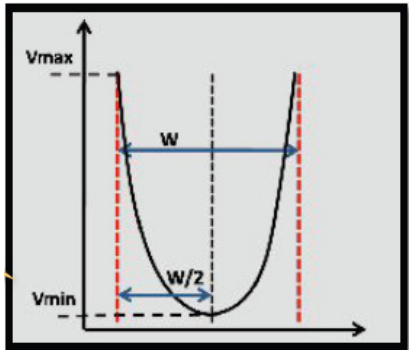
- Recap from Wednesday
- Periodic Potential Lab
  - Basic principles
  - Input Interface
  - Exemplary Outputs
- CNTbands
  - Basic principles
  - Input Interface
  - Exemplary Outputs

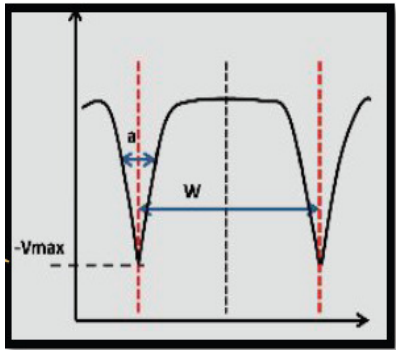
Periodic Potential Lab

- Solves single-electron Schrodinger equation in simple periodic potentials
- Calculates:
  - Energy bands
  - Electron wavefunctions
  - Effective masses
  - Bandgaps







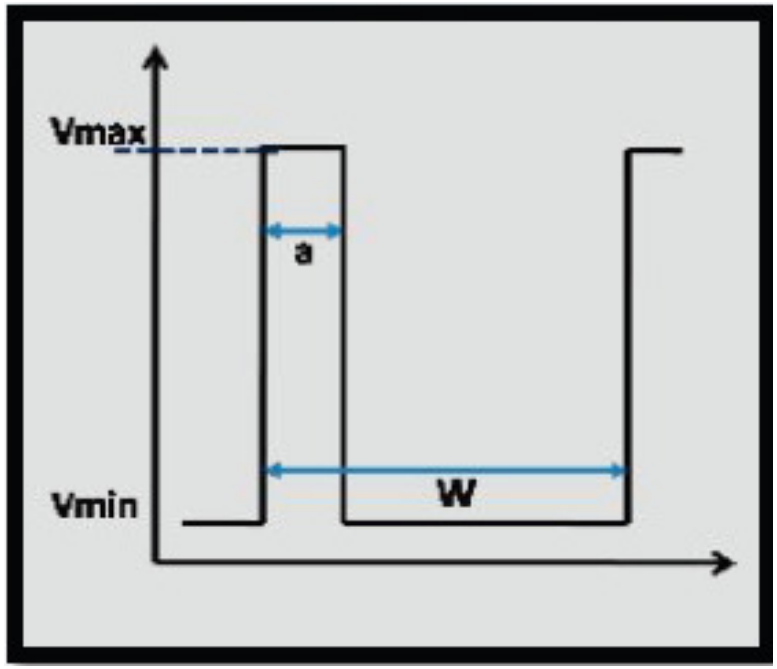


Available on nanoHUB at:
http://nanohub.org/tools/kronig_penney

Abhijeet Paul & Gerhard Klimeck, "Periodic Potential Lab User Guide" (2011).

Periodic Potential Lab

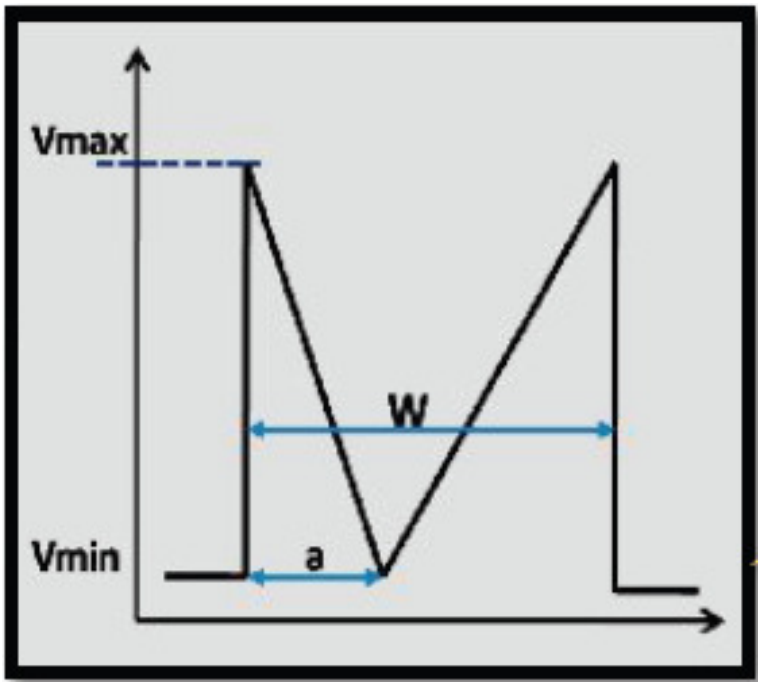
- Input for step well (Kronig-Penney problem):
  - Max energy V_{max}
  - Min energy V_{min}
  - Energy over barrier ΔE
  - Period W
  - Barrier width a
  - Particle mass m_o



Abhijeet Paul & Gerhard Klimeck, "Periodic Potential Lab User Guide" (2011).

Periodic Potential Lab

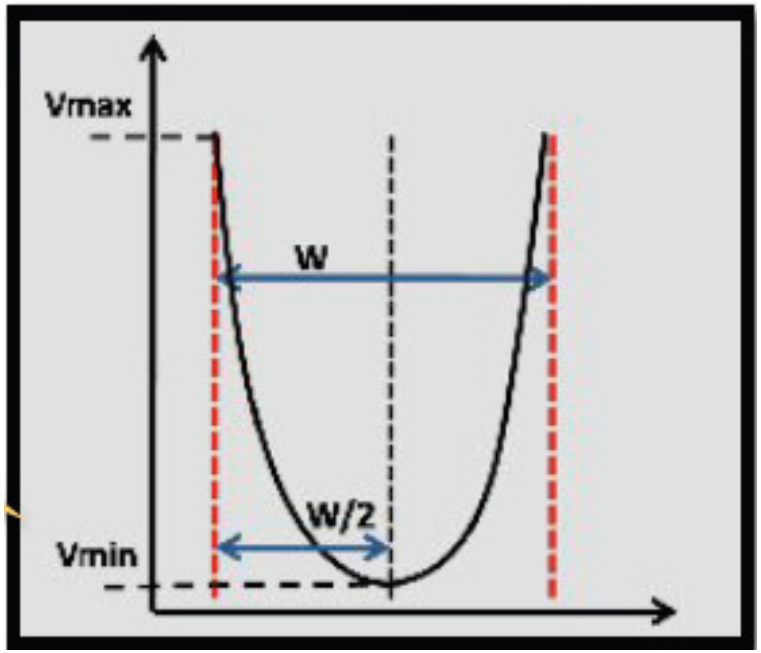
- Input for triangular well:
  - Left branch width *a*



Abhijeet Paul & Gerhard Klimeck, “Periodic Potential Lab User Guide” (2011).

Periodic Potential Lab

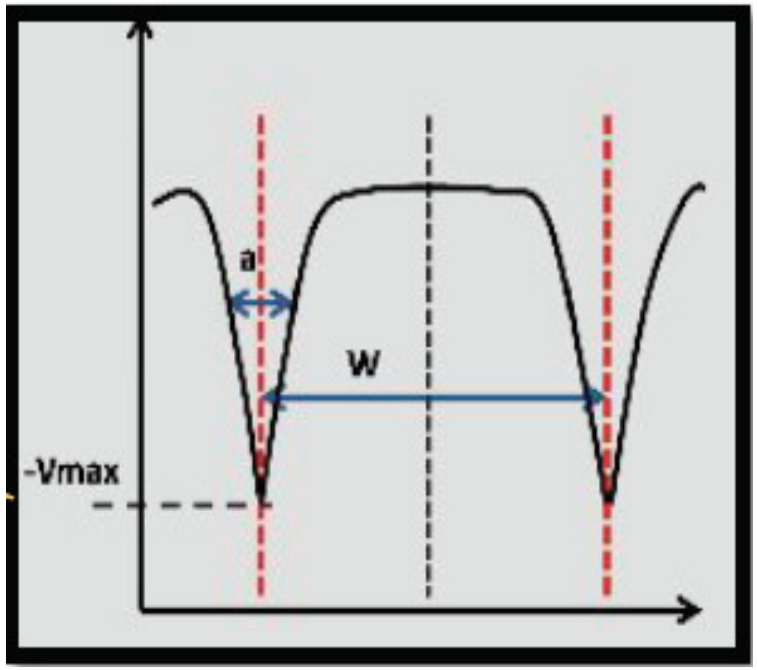
- Input for parabolic well:
  - Left branch $a=W/2$



Abhijeet Paul & Gerhard Klimeck, "Periodic Potential Lab User Guide" (2011).

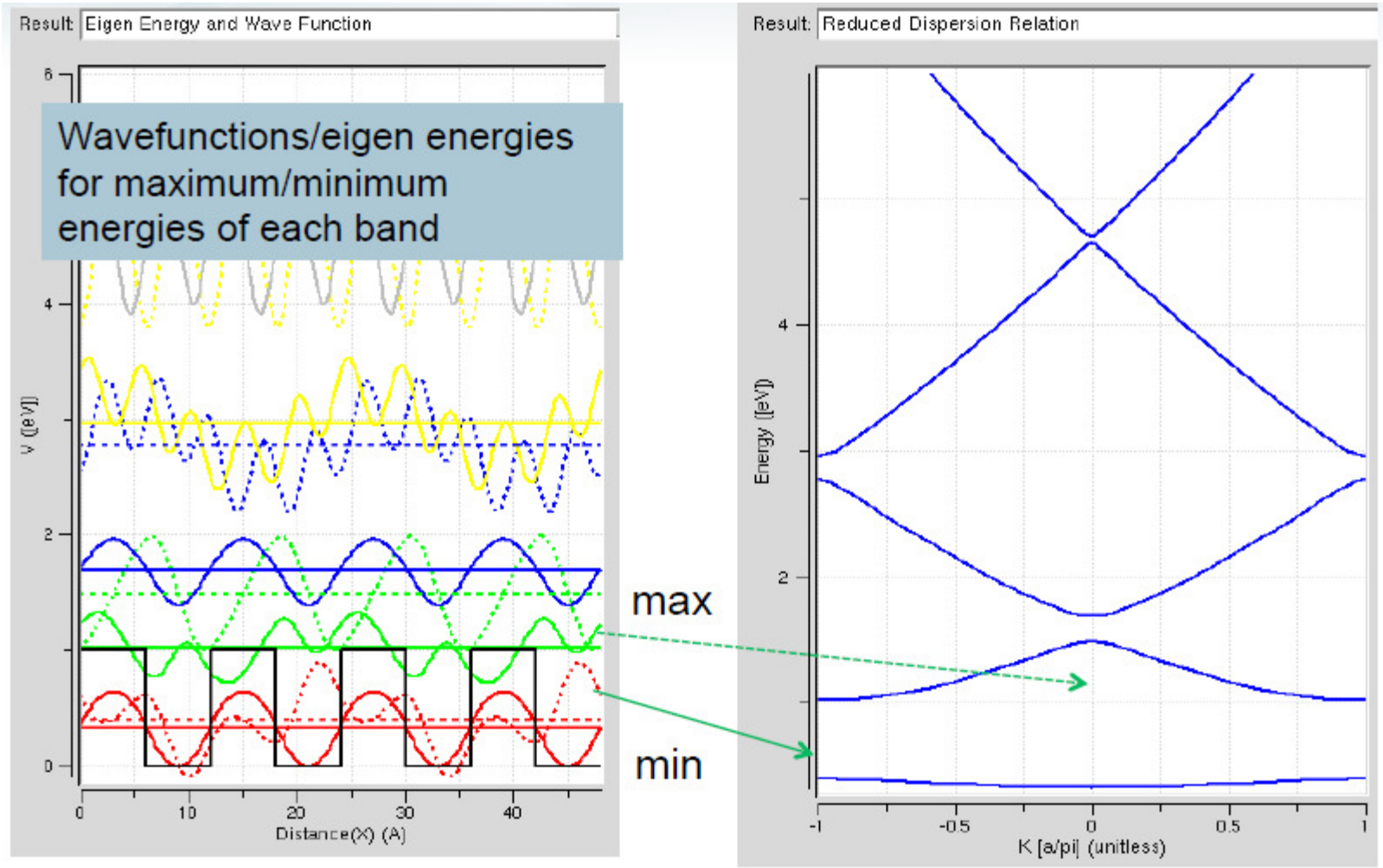
Periodic Potential Lab

- Input for Coulombic well:
  - Well width *a*



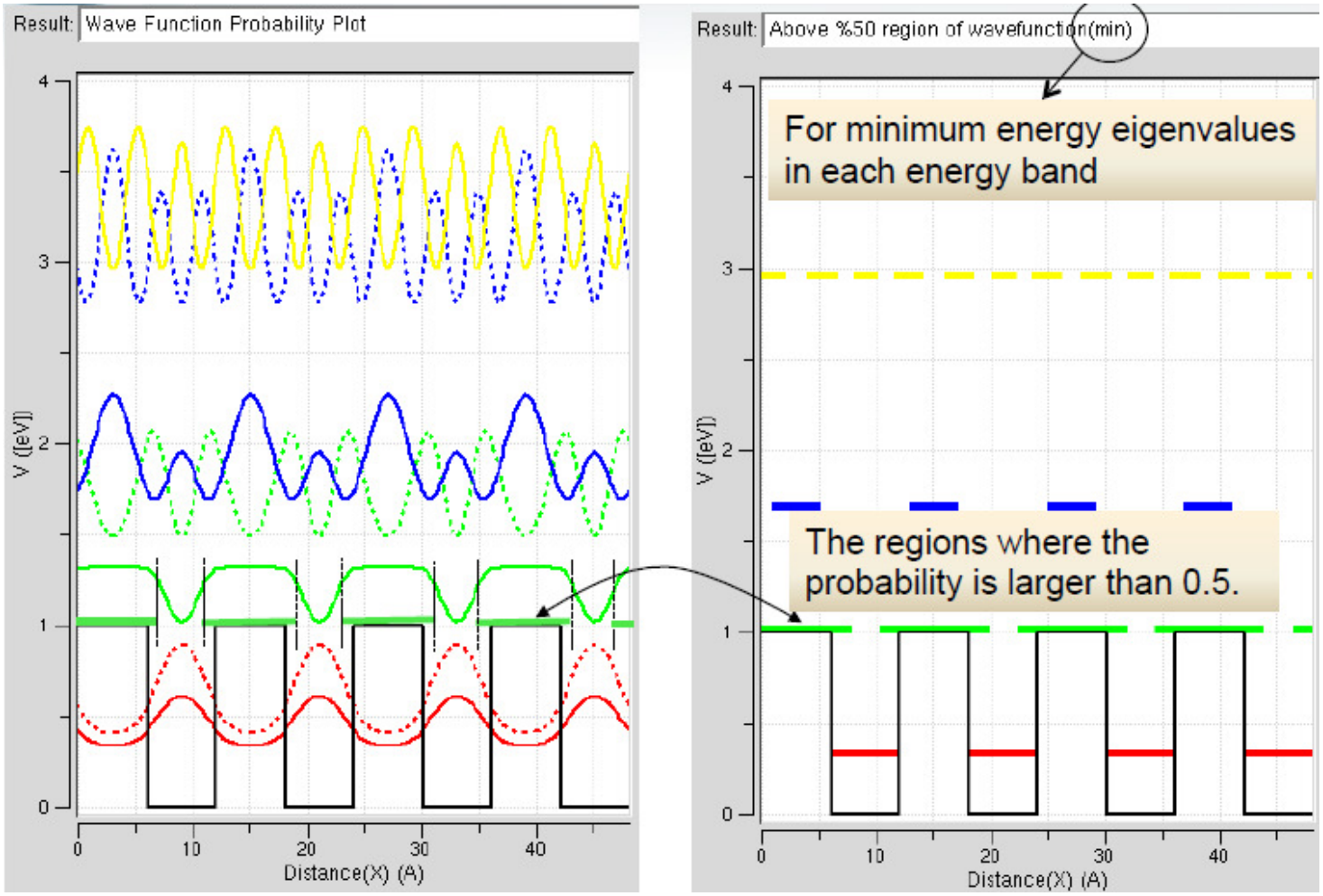
Abhijeet Paul & Gerhard Klimeck, "Periodic Potential Lab User Guide" (2011).

Periodic Potential Lab: Output



Abhijeet Paul & Gerhard Klimeck, "Periodic Potential Lab User Guide" (2011).

Periodic Potential Lab: Output



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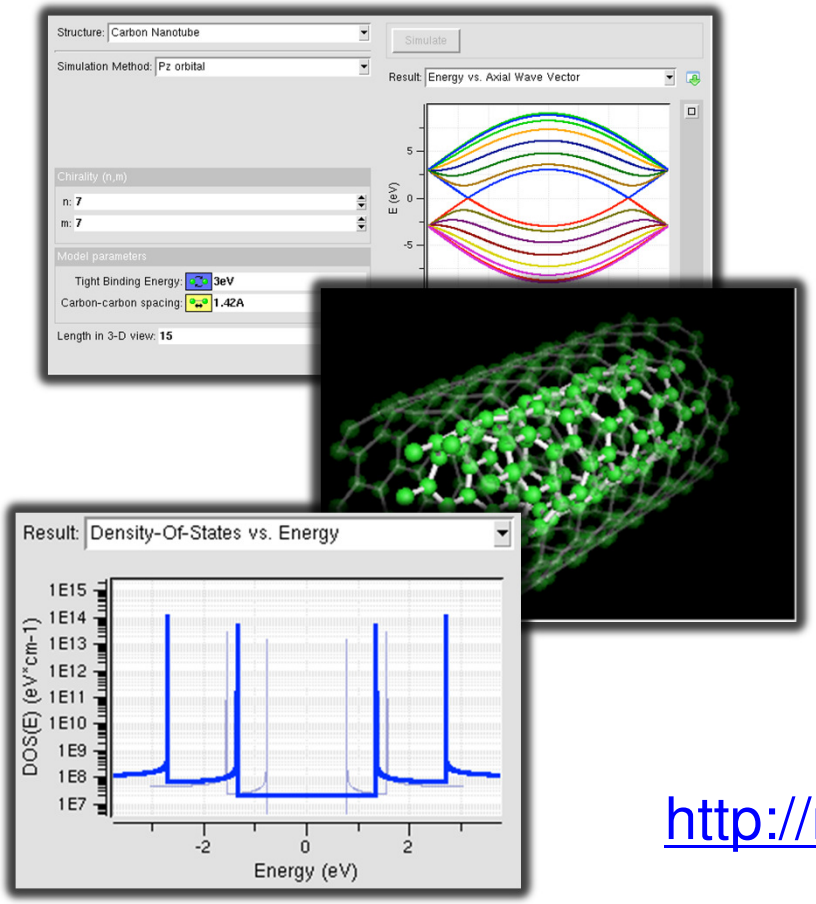
CNTbands



- **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.

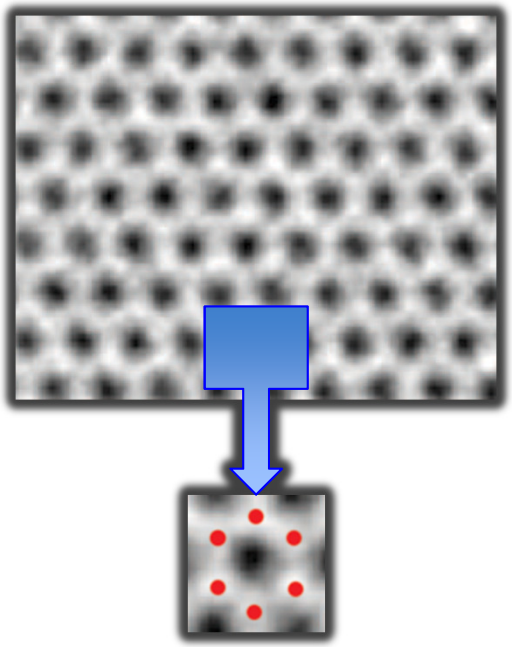
Available on nanoHUB at:

http://nanohub.org/resources/cntbands-ext

Xufeng Wang and Youngki Yoon, "CNTbands first-time user guide" (2011).

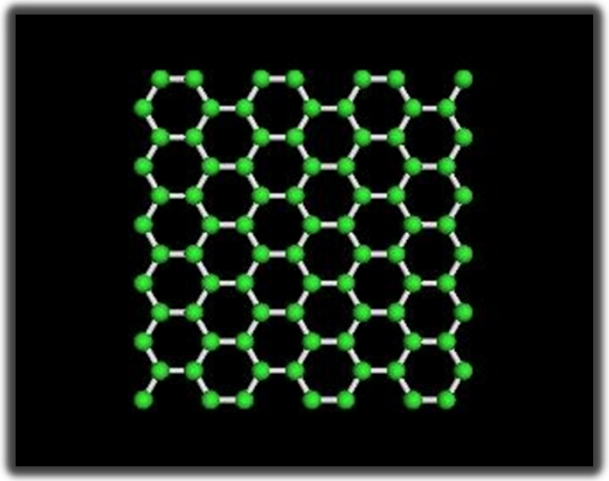
CNTbands

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

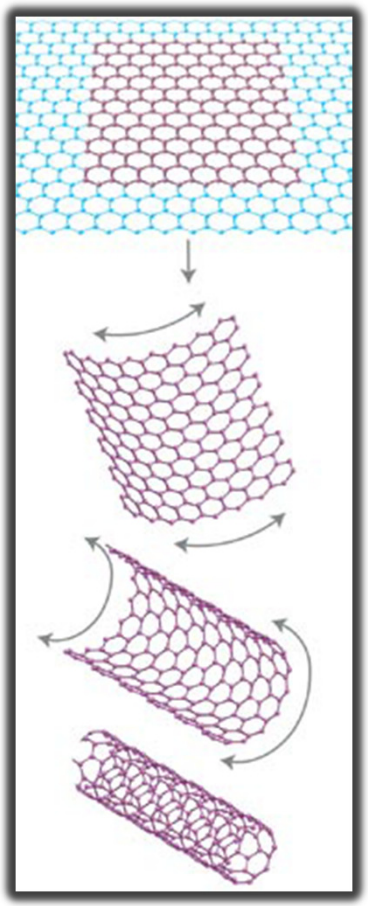


Direct image of a single-layer graphene membrane (Red dots denote carbon atoms)
J.C.Meyer et al., “Direct imaging of lattice atoms and topological defects in graphene membranes”, Nano Lett., 8, 3582-3586 (2008).

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).



CNTbands

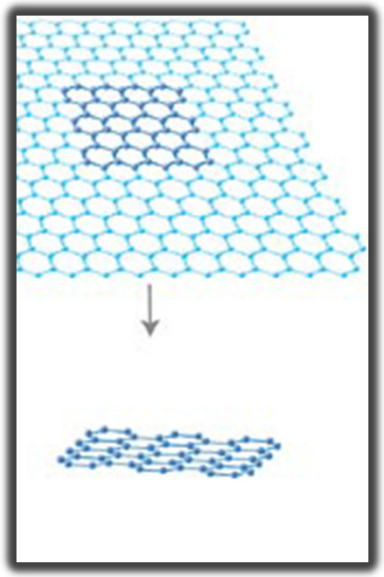


Rolling of a Carbon nanotube (CNT) from a graphene sheet

- 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



Cutting of a graphene nanoribbon (GNR) from a sheet of graphene

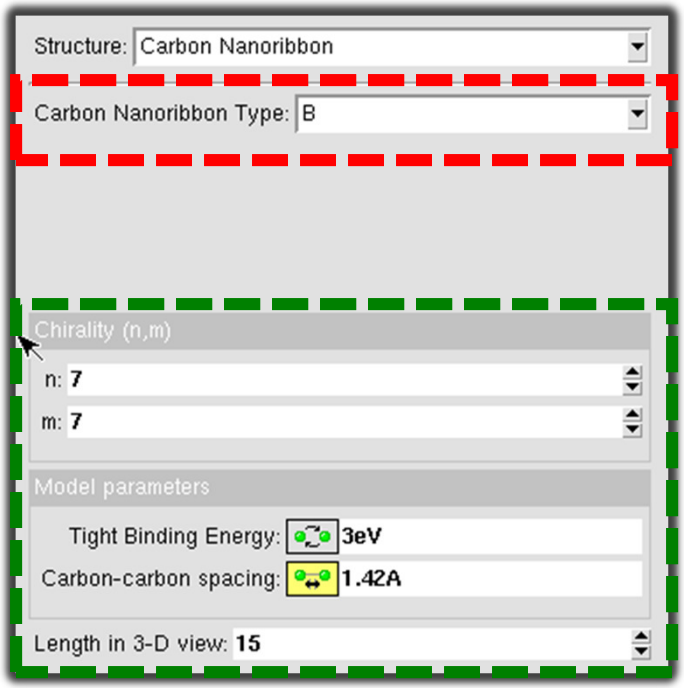
- Graphene Nanoribbons are thin strips of graphene.
- The electronic property of GNR largely depends on its edge structure.
- Since GNRs are “strips,” its length is defined via chirality as well.
- Its width, or the “thinness” of strip, is usually defined using how wide it is in nanometers or angstroms.
- 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

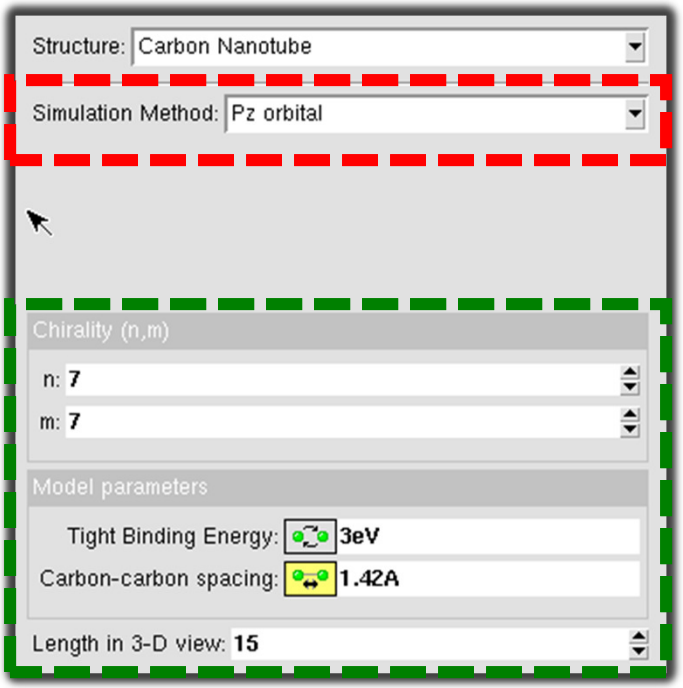
For GNR



Structure specific

Common for both CNT and GNR

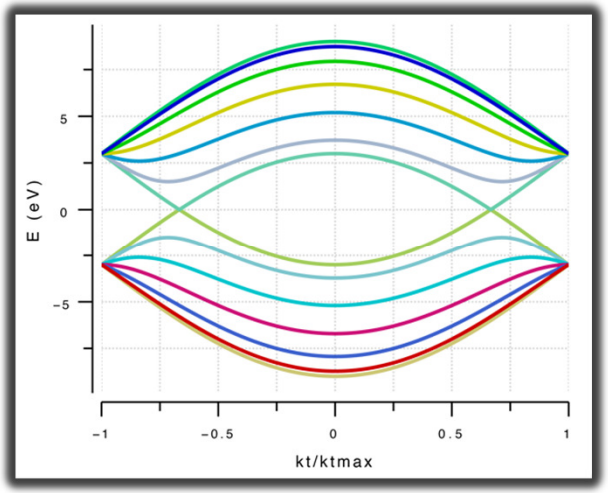
For CNT



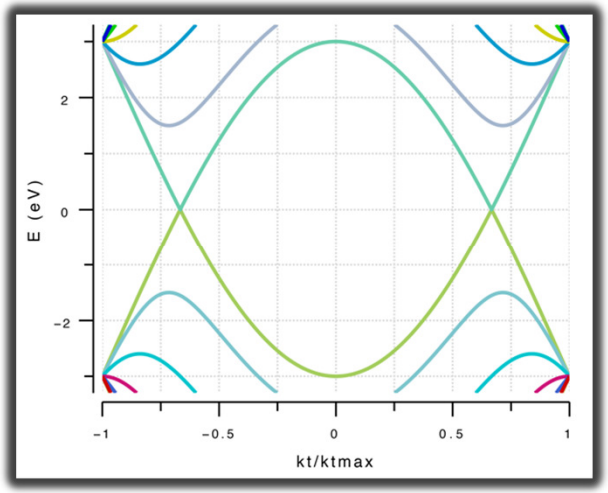
Xufeng Wang and Youngki Yoon, "CNTbands first-time user guide" (2011).

CNTbands

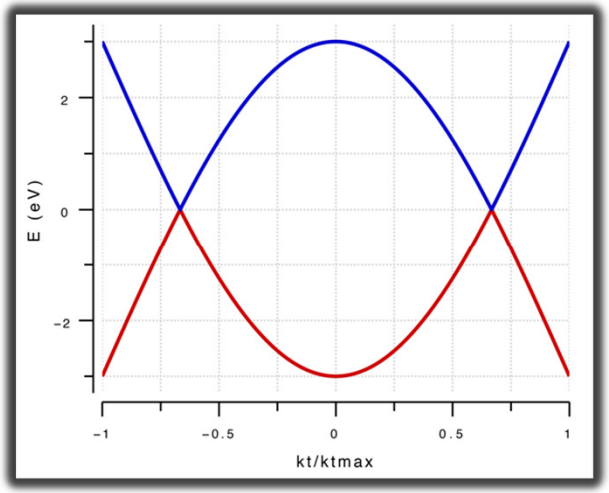
- The E-k diagram describes the energy-wave momentum relationship for carriers within the first Brillouin zone.
- Each continued line is an allowed level of energy for carriers, or a subband. The E-k diagram thus describes the "bandstructure" of the studied material.
- Subbands closest to the equilibrium 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".



E-k diagram



Zoomed in E-k diagram



Lowest subbands

Xufeng Wang and Youngki Yoon, "CNTbands first-time user guide" (2011).

Next Class

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