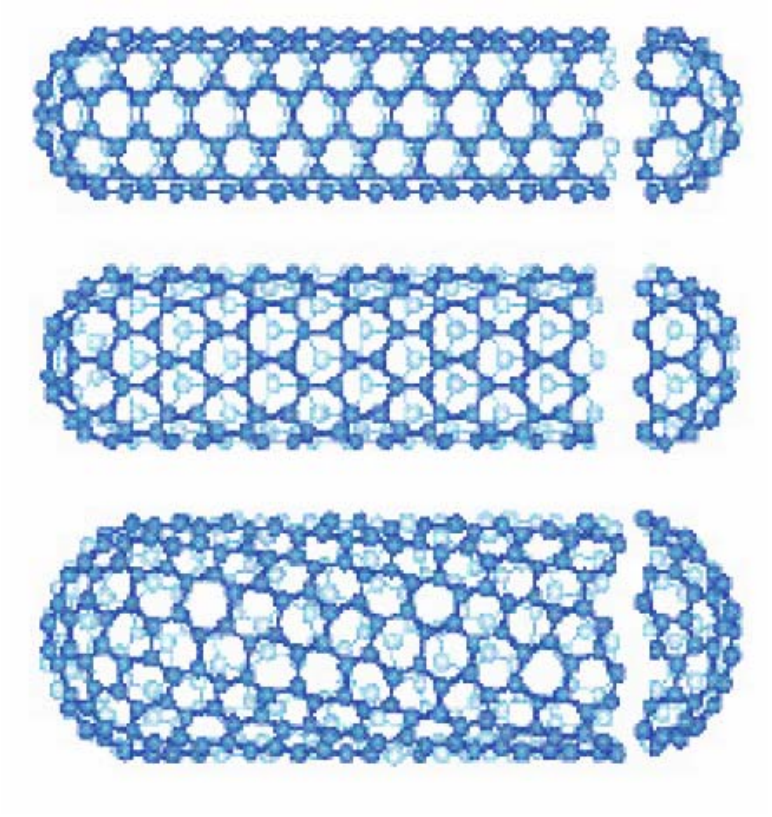
Carbon nanotubes

Carbon nanotubes - rolled up graphene



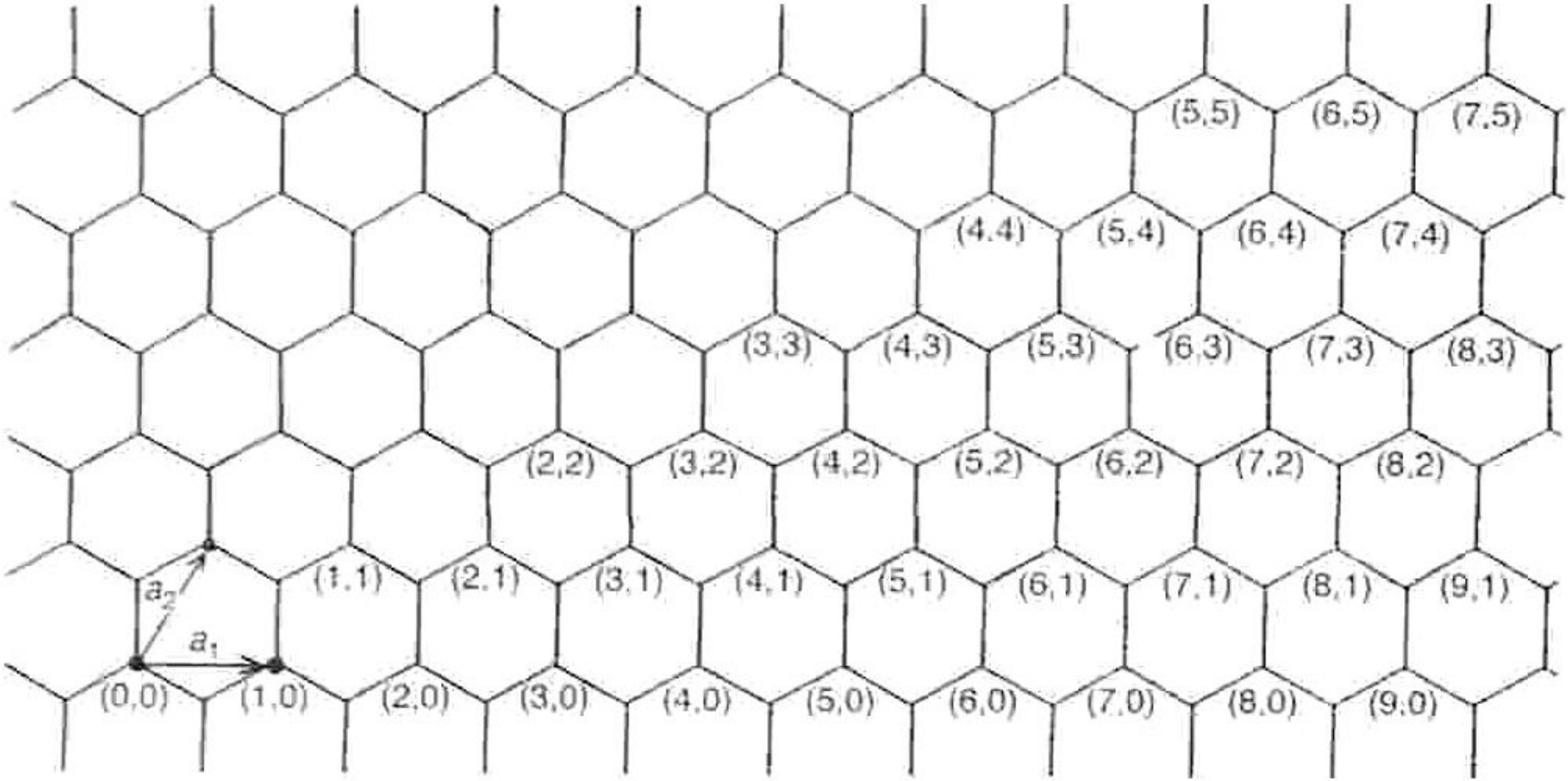
armchair

zig-zag

chiral

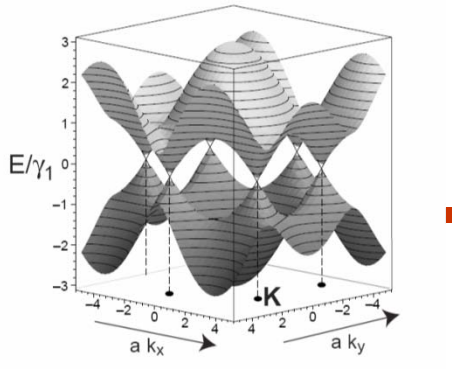
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

(*m*,*n*) notation

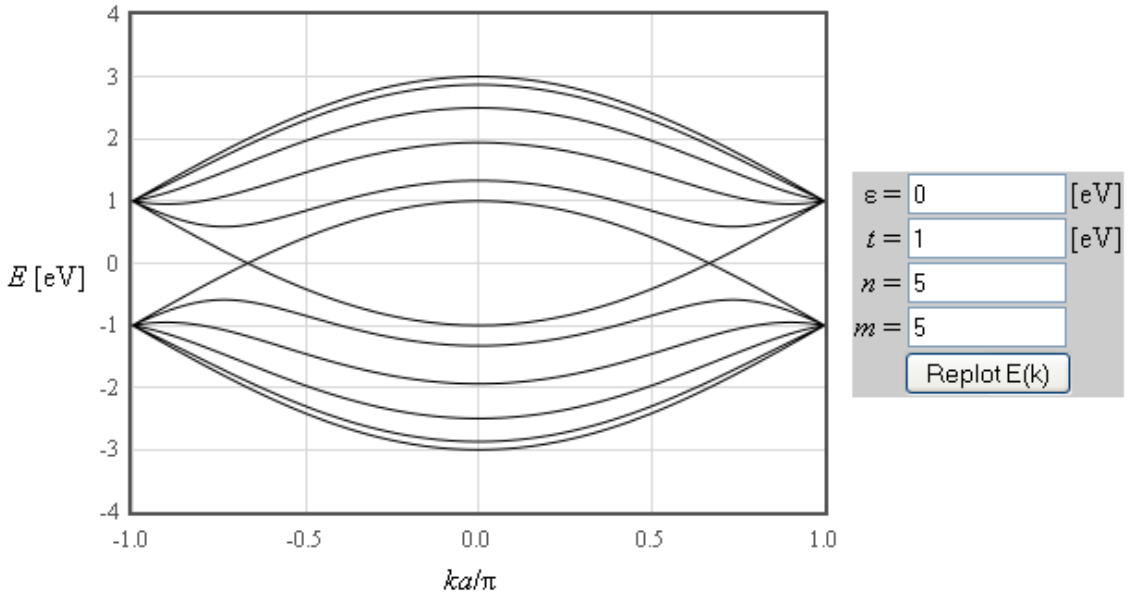


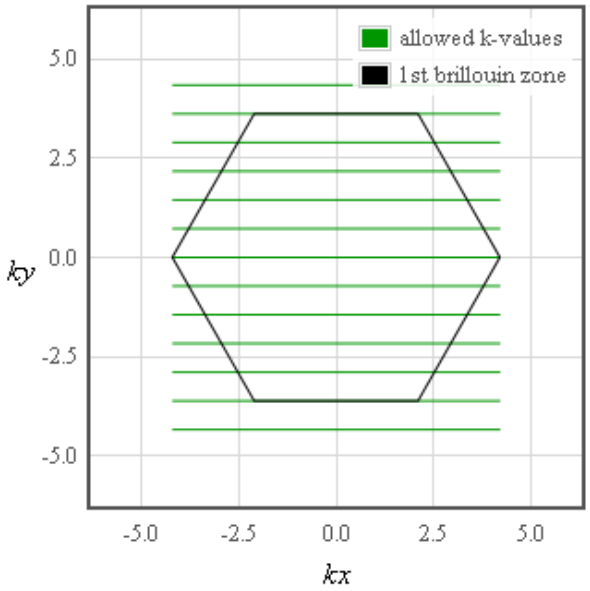
http://www.personal.rdg.ac.uk/~scsharip/tubes.htm

Carbon nanotubes



$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$

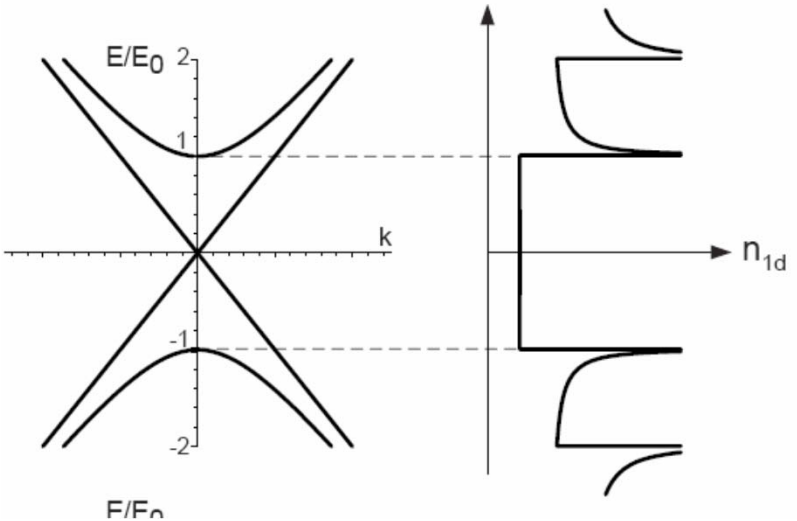


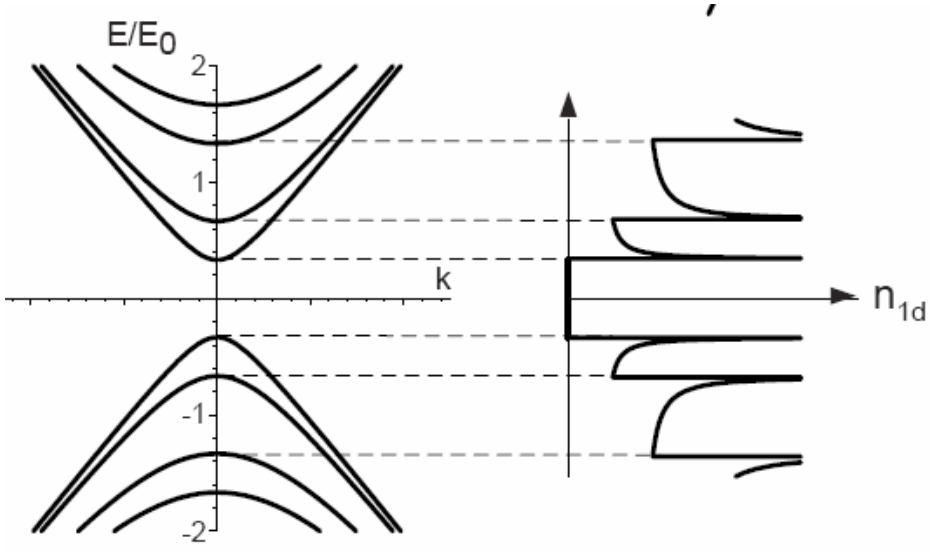


metallic (5,5) armchair tube

http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/CNTs.html

Carbon nanotubes



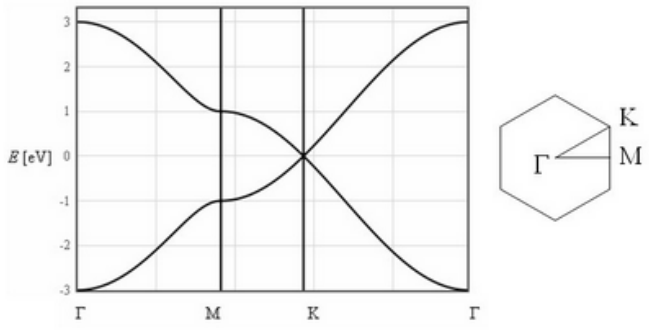
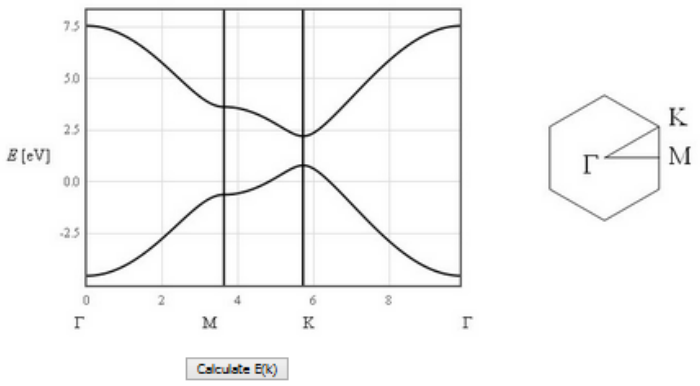
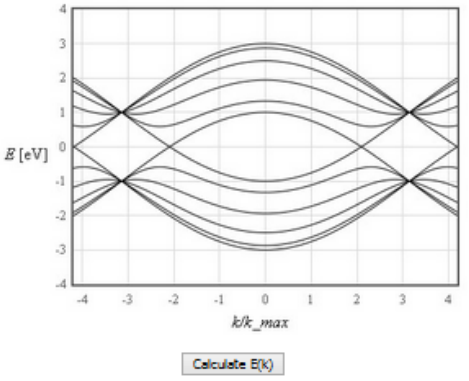
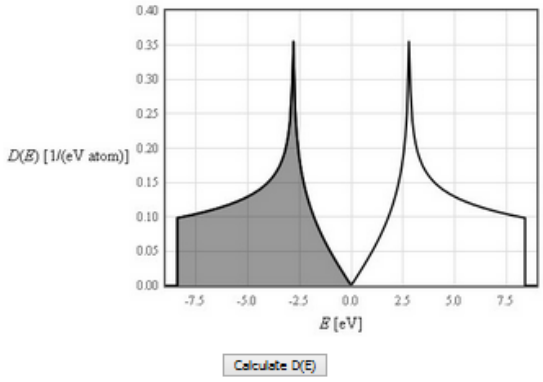
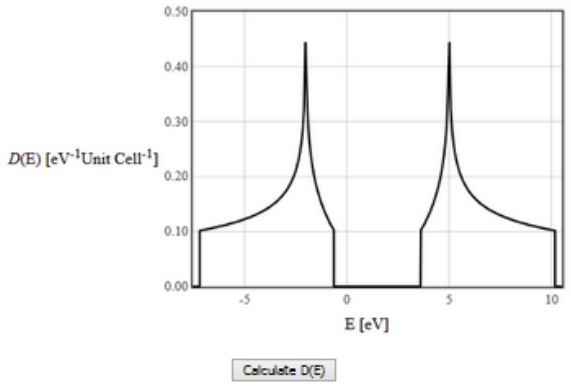
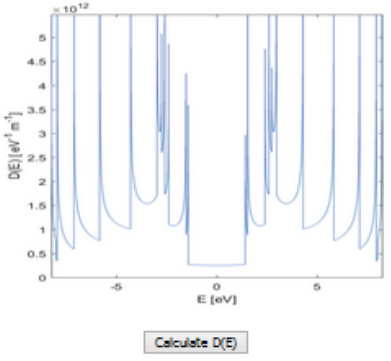


metallic $m - n = 3Z$

semiconducting

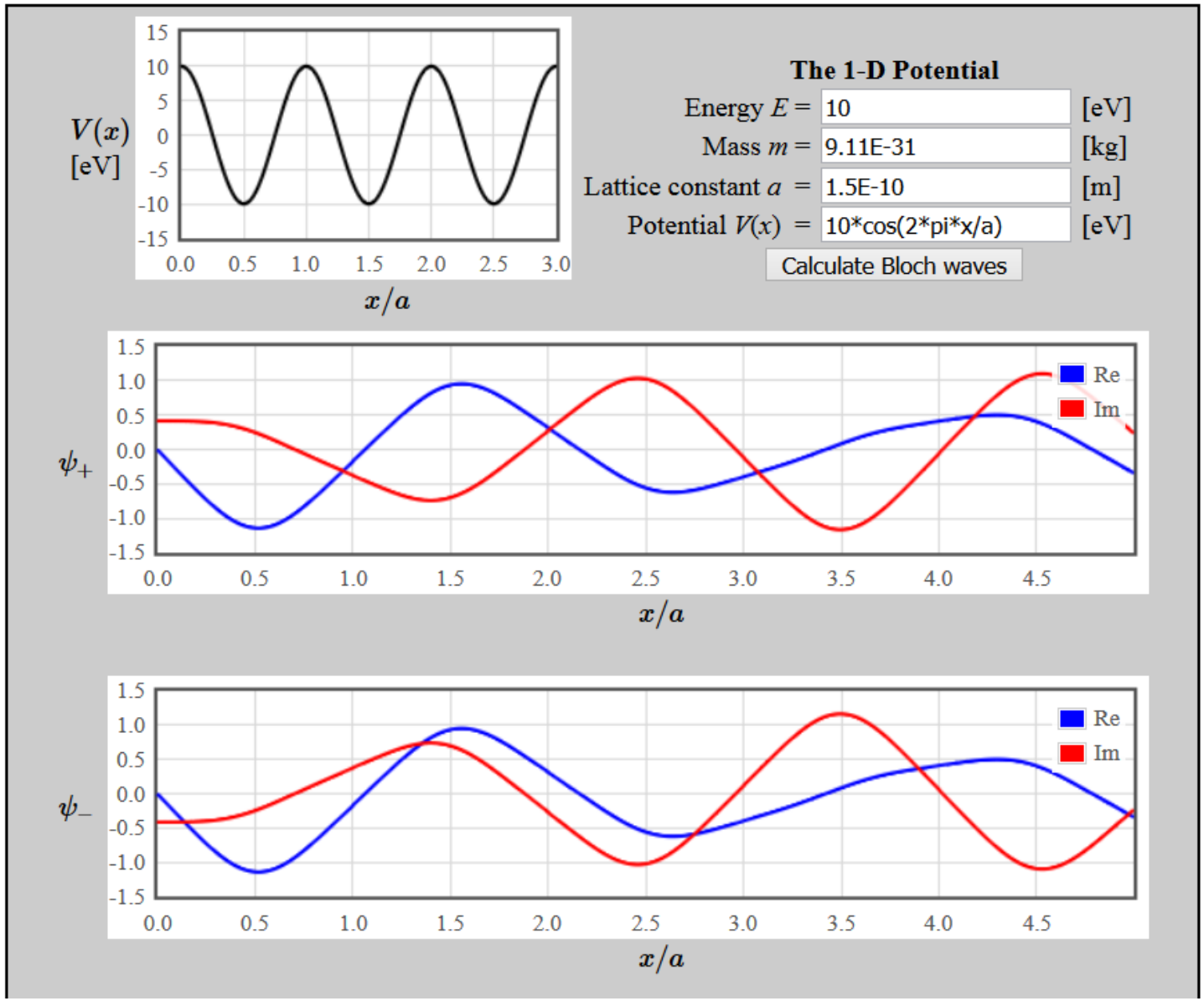
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

Table of tight-binding calculations

Graphene	2-D boron nitride	Carbon nanotubes
$E = \varepsilon \pm t\sqrt{1+4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_y a}{2}\right)}$	$E = \frac{\varepsilon_1+\varepsilon_2}{2} \pm \sqrt{\frac{(\varepsilon_1-\varepsilon_2)^2}{2}+4t^2\left(\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+\cos^2\left(\frac{k_y a}{2}\right)+\frac{1}{4}\right)}$	
		
$D(k) = \frac{k}{\pi}$ m^{-1}	$D(k) = \frac{k}{\pi}$ m^{-1}	$D(k) = \frac{2}{\pi}$
		

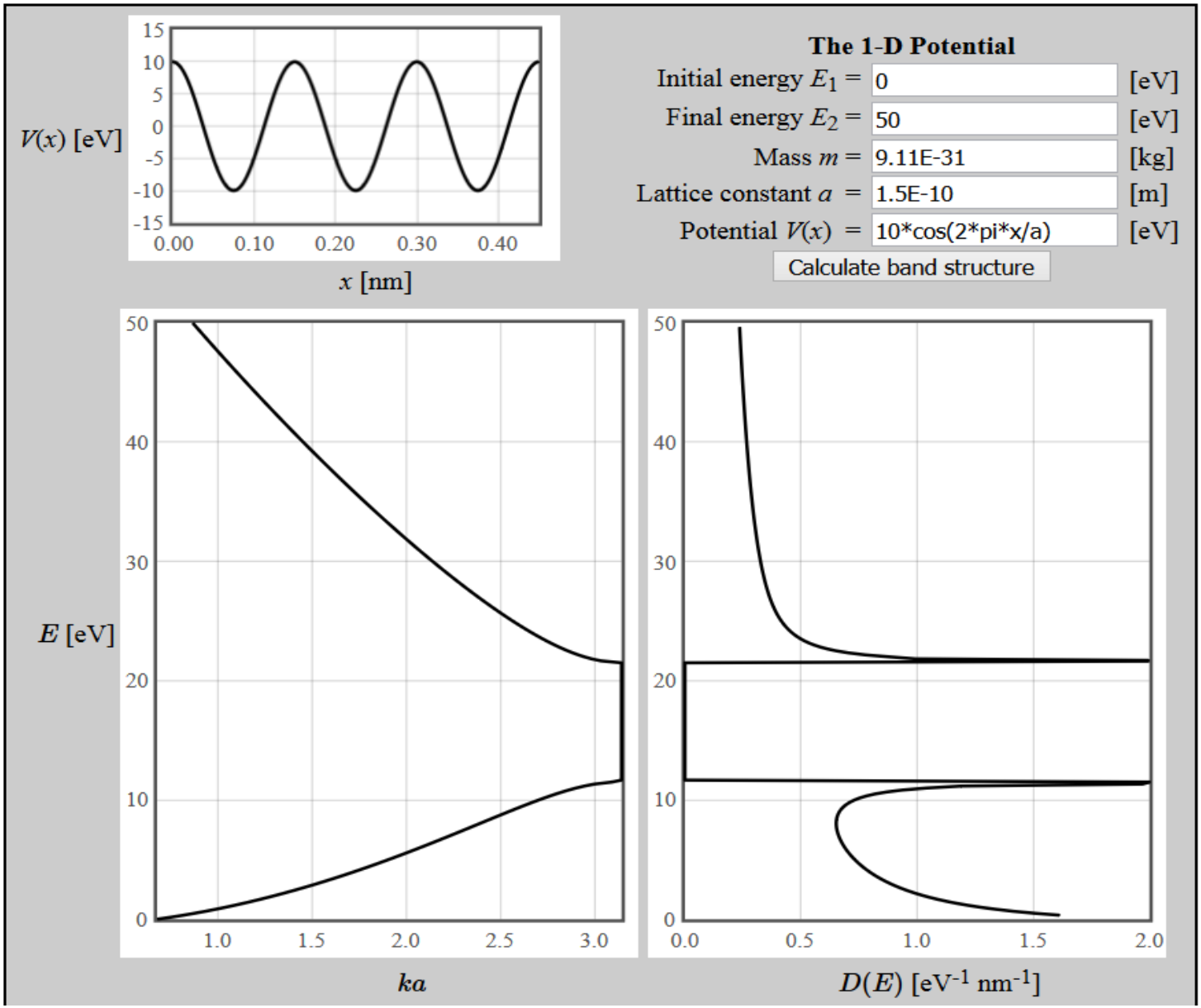
http://lampx.tugraz.at/~hadley/ss1/bands/tbtable/tbtable.html

Bloch waves in one dimension



http://lampx.tugraz.at/~hadley/ss1/bloch/bloch.php

Band Structure in one dimension



http://lampx.tugraz.at/~hadley/ss1/bloch/bloch.php

- Band structure calculations: GaN, 6H SiC, GaAs, GaP, Ge, InAs
- Calculated electron density of states
  - Al fcc, Au fcc, Cu fcc, Na bcc, Pt fcc, W bcc, Si diamond, Fe bcc, Ni fcc, Co fcc, Mn bcc, bcc, Gd hcp, Pd fcc, Pd_3Cr, Pd_3Mn, PdCr, PdMn , GaN, 6H SiC, GaAs, GaP, Ge, InAs

Bandstructure of hexagonal gallium nitride (GaN)

The bandstructure calculation for gallium nitride was calculated using the program Quantum Espresso (version 5.2.1) and the pseudopotentials for Ga and N.