



Example 4

Graphene & nanotubes



Graphene & nanotubes

- Calculate the band-structure of graphene.
- Compare that to the bands of the 4 nanotubes:
 - zigzag: (12,0) & (13,0)
 - armchairs: (3,3) & (6,6).
- Notice that armchairs are metallic, but the effect of small diameter is clearly seen near the K-point.



Graphene & nanotubes

- Use Xcrysden to visualize the “HOMO”.
 - In the input flag, check the LDOS block
 - The range of energies used, should be that of the HOMO. Use the .EIG file to check if that is the case.
 - What can you say of the character of the state?
- You can also repeat the calculation for different energy ranges (LUMO, for example).



Graphene & nanotubes

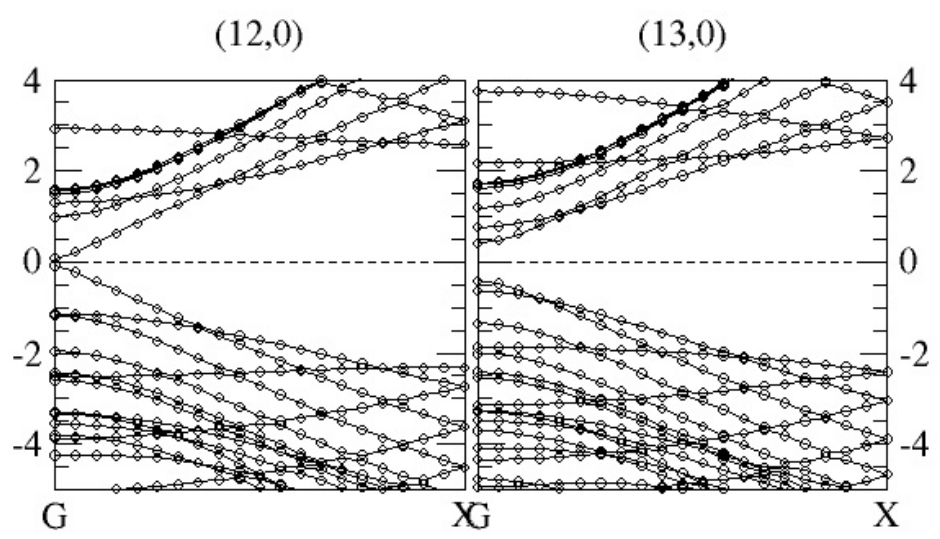
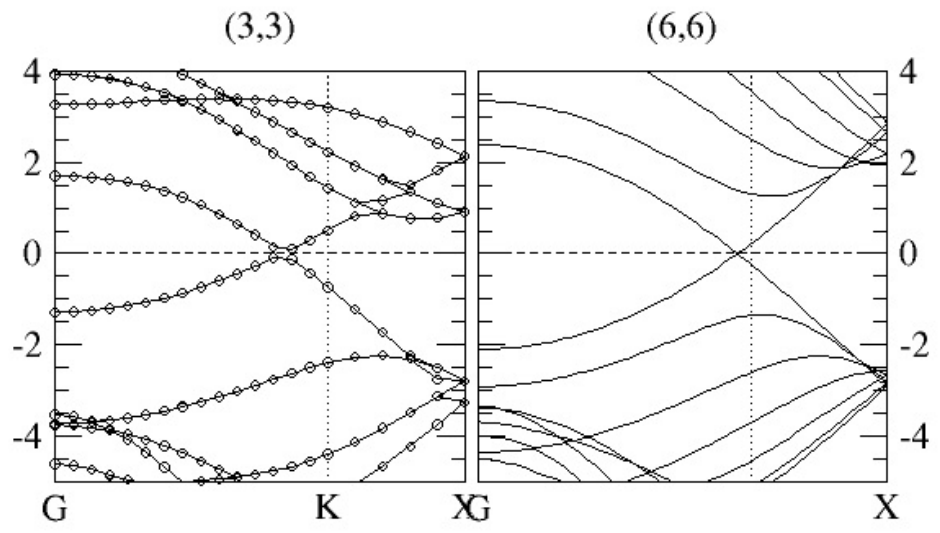
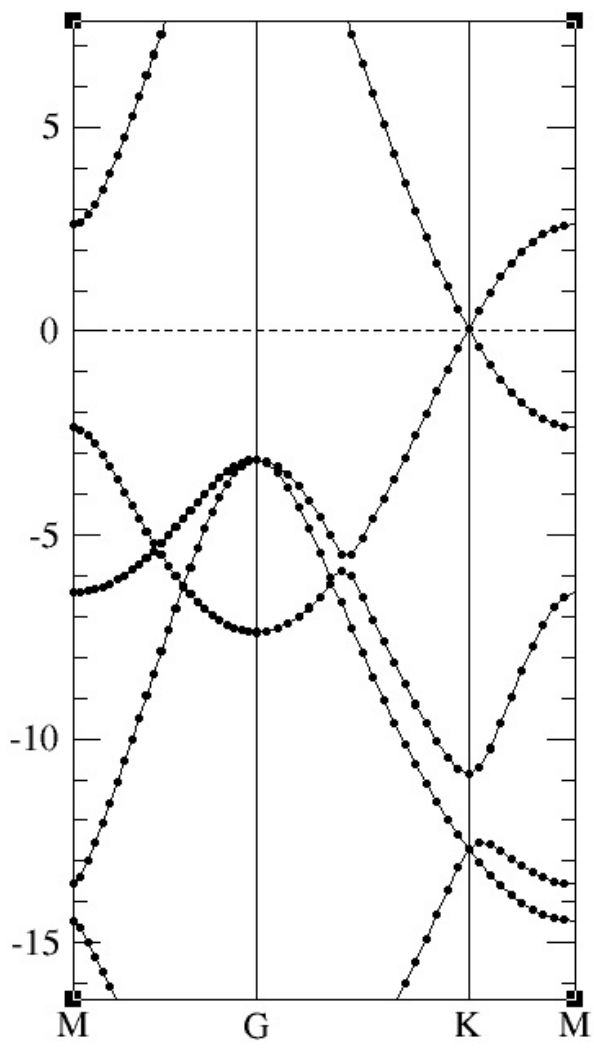
- Feel free to try other nanotubes.
 - Change (n,n) , $(n,0)$.
 - Could you do (n,m) ?
- Try substitutional defects in the tube
- Try BN nanotubes
- ...



Navigation and control panel:

- Search: A_3
- Zoom: Z
- Navigation: \leftarrow , \rightarrow , \downarrow , \uparrow
- AutoT
- AutoO
- View: ZX, ZY, AX, AY, PZ, Pu, Po, Cy
- SD:1
- CW:0
- Exit

Graphene





Local Density of States

