Junctions of left- and right-handed chiral carbon nanotubes – nanobamboo

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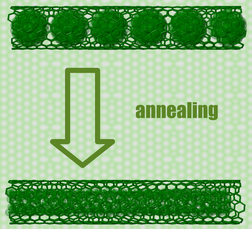
Motivation



Measurements on **peapod** grown double-wall carbon nanotubes show anomalies:

NMR - metallic spin relaxation for all inner tubes [1],

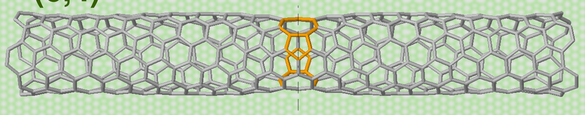
ESR - features reminiscent of localized states appear during annealing,

mechanically breakable - e.g. Raman signal of inner tubes disappears after grinding the samples.

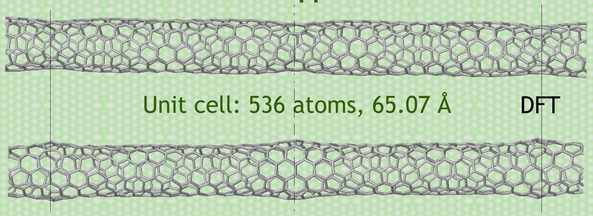
Introduction

- For a given outer tube more inner tubes are possible (selected by van der Waals distance)
- Inner tube growth can start at different places
- Connection of different chiralities form a defect (pentagon-heptagon pairs were considered so far)
- Simplest possibility: a junction of a left-handed and a right-handed chiral nanotube
- Junctions should be more-less straight

(6,4)



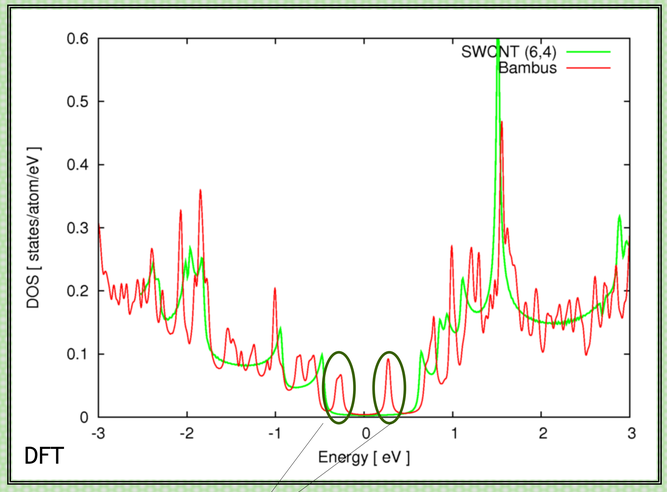
For a realistic system size: periodic boundary condition should be applied.

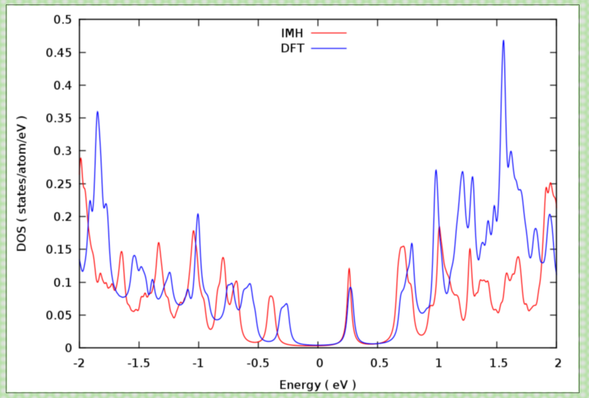


Methods

- density functional theory (DFT) based Vienna ab-initio Simulation Package [2], local density approximation (LDA) and projector augmented-wave method (PAW),
- DFT-optimized geometries (plane-wave cutoff energy of 500 *eV*),
- screw-axis symmetry was used to create longer geometries, if needed,
- density of states (DOS) calculated by DFT with a Gamma-centered (1×1×20) Monkhorst-Pack set of kpoints,
- Hückel-type calculation (IMH, [3]) for DOS, with a single Gamma-point, but a sufficiently large supercell of at least 5000 atoms were used,
- LCAO coefficients of the Hückel-type calculation gives us an approximation of the wavefunctions of the molecular orbitals.

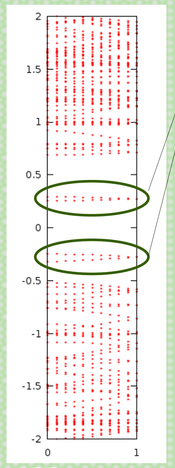
Density of states for our nanobamboo





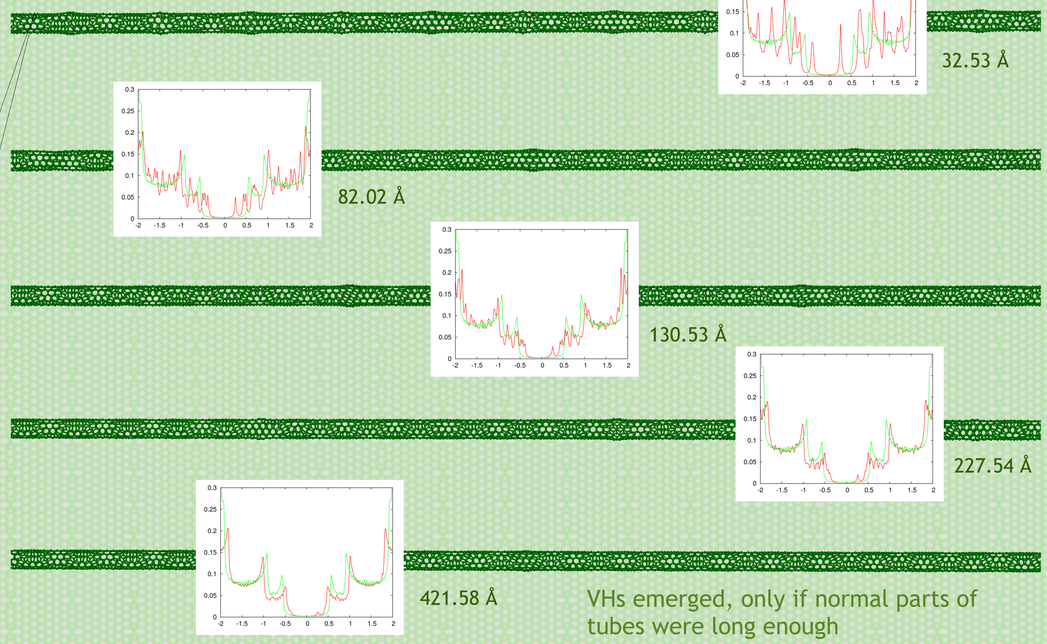
- Excellent agreement of the two methods
- IMH can treat up to 20000 atoms/u.c.

Band structure



Localized states?

Van Hove singularities



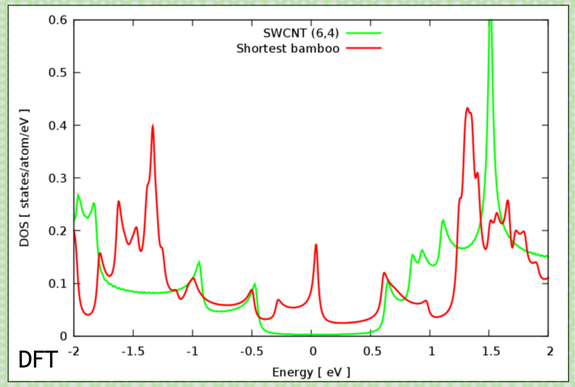
VHs emerged, only if normal parts of tubes were long enough

Energetics

	Number of atoms	*Total energy**	*Energy/ atom*	*Distance* of bumps*	*Energy/ bump*
Pristine (6,4)	152	-1510.309	-9.936	-	-
Bamboo	536	-5311.407	-9.909	32.53	7.21
Shorter	216	-2131.743	-9.869	13.01	7.24
Shorter+neck	520	-5152.376	-9.908	13.01; 49.88	7.24
Shortest	104	-1022.318	-9.83	6.39	5.53

* All energies are in units of eV, all lengths are in ångstroms.

Decreasing the distance between the bumps can bring the localized states to the Fermi level

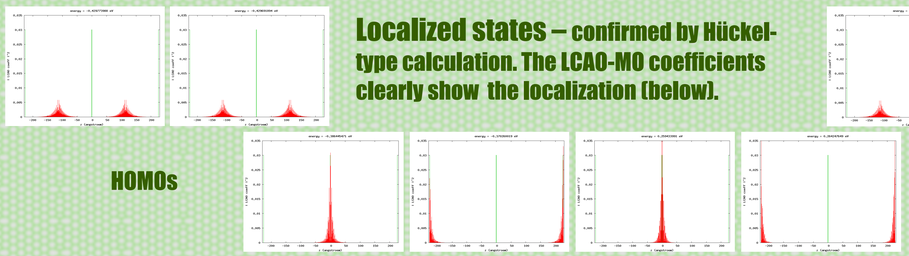


To have both sharp Van Hove singularities and localized states at the Fermi level, a random distribution of bump distances should be considered.

Conclusions

- **localized states were found around the Fermi level by DFT calculations on a bamboo-like geometry,**
- **and confirmed by Hückel-type calculations,**
- **these localized states might account for the ESR signal seen in experiments,**
- **the rigid structure of the bumps makes the inner tubes mechanically unstable,**
- **more chiralities should be investigated.**

Localized states – confirmed by Hückel-type calculation. The LCAO-MO coefficients clearly show the localization (below).



References

[1] PM Singer, P Wzietek, H Alloul, F Simon and H Kuzmany, PRL **95**, 236403 (2005)

[2] G Kresse and J Furthmüller, PRB **54**, 11169 (1996)

[3] Lázár A, Surján P, Paulsson M and Stafström S, Int. J. Quantum Chem. **84**, 216 (2002)

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