"Electronic properties of double-wall carbon nanotubes and the effect of functionalization"

Laflamme Janssen, Jonathan ; Beaudin, Jason ; Côté, Michel

Abstract

Although promising for many electronic applications, further understanding of carbon nanotubes systems are required for practical designs. A difficulty currently hindering further development in this field is the considerable degradation of transport properties in a single-wall carbon nanotube (SWCNT) when it is subjected to ambient conditions or functionalized. Double-wall carbon nanotubes (DWCNT) could solve this problem, by allowing the outer tube to be functionalized while the inner tube would retain a pristine structure and it's promising electronic properties. However, our understanding of interactions between the tubes and their consequences on the system's electronic properties is still incomplete. In this presentation, we investigate those interactions using density-functional theory (DFT) calculations. In particular, we investigate separately the effects of structural deformations, Fermi energy realignment and electronic orbital overlap on the band structure of DWCNT. The e...

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Electronic properties of double-walled carbon nanotubes (DWNT) and the effect of functionalization

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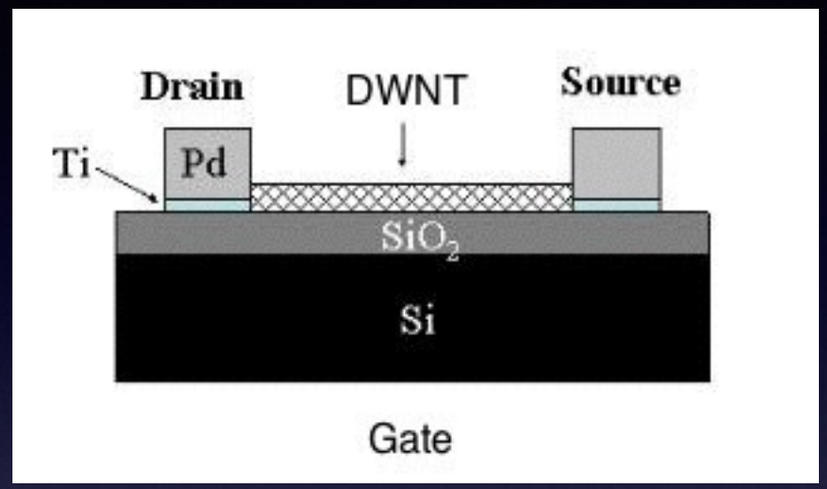
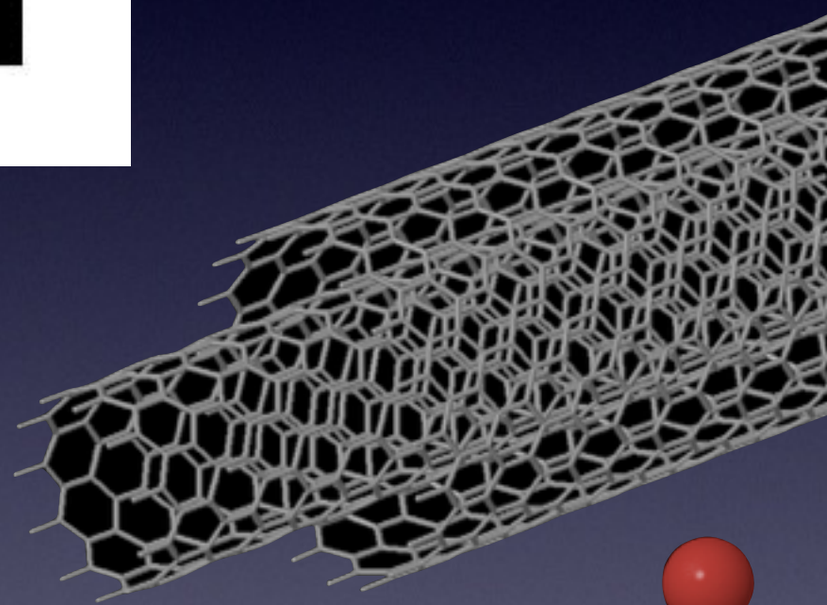
Peter Haynes
Imperial College, London, United Kingdom

Motivation

- DWNT : easier FETs

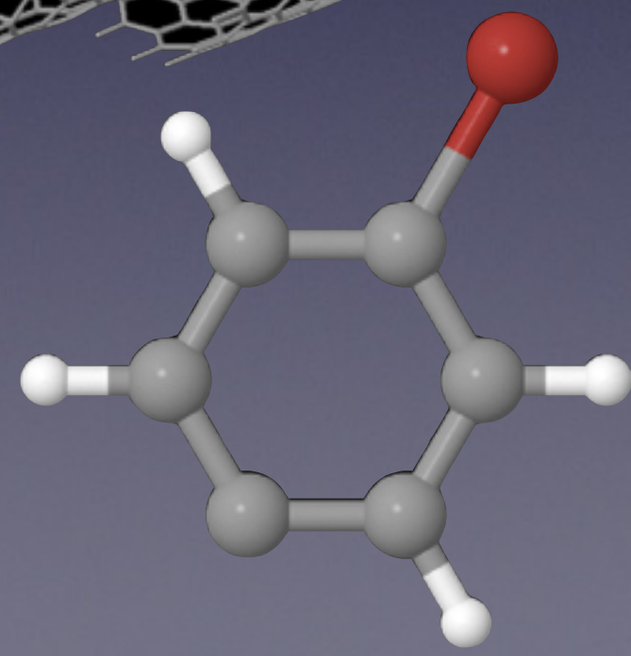


- S@S DWCNT



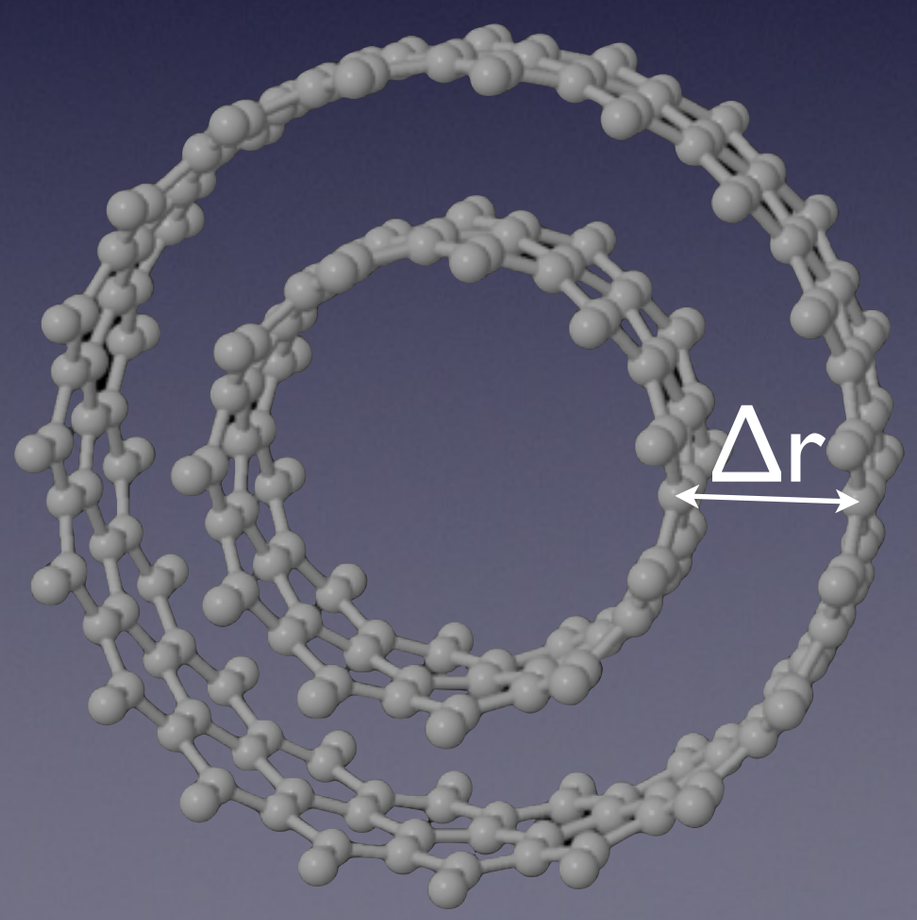
- Part 1 : wall interaction in DWNT?

- Part 2 : effect of functionalization? (bromo-phenyls)



Part I : interaction in DWNT

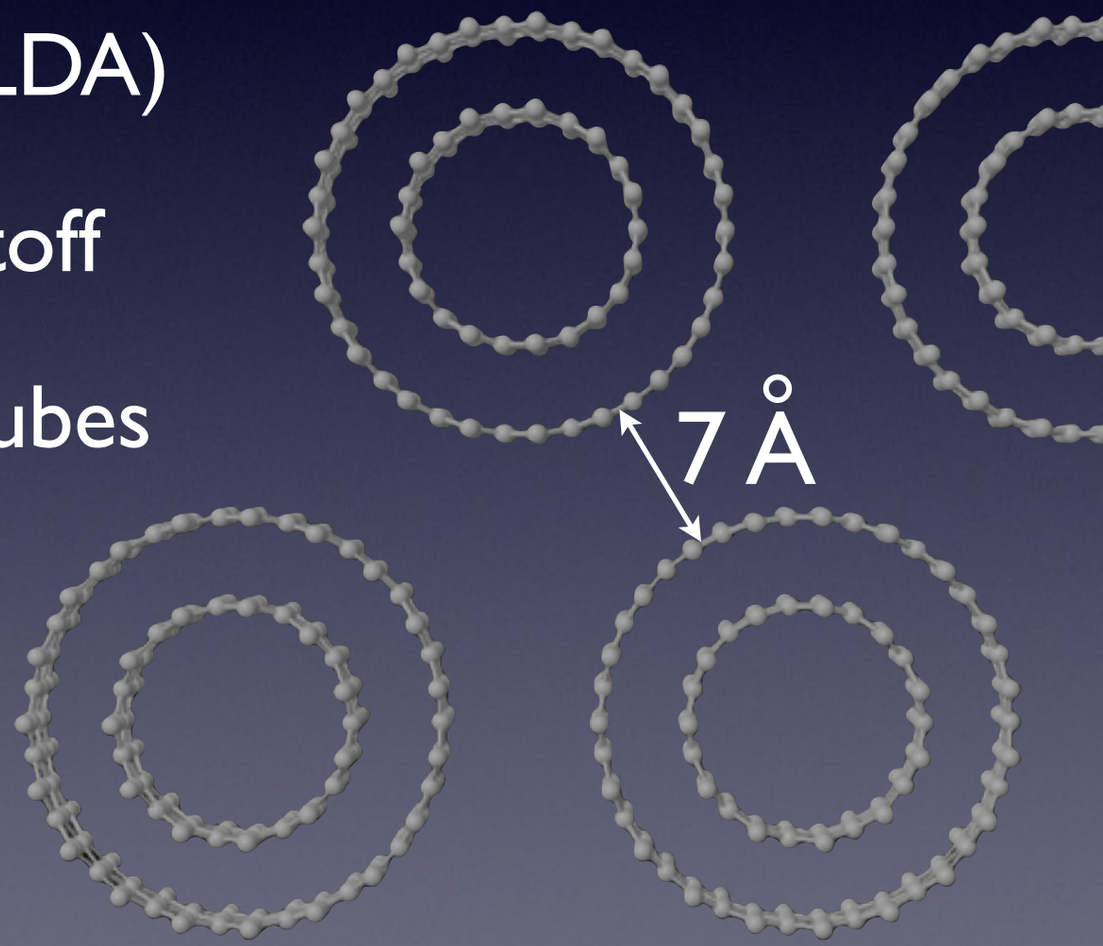
- Litterature :
  - S@S DWNT : semiconducting or metallic [1-3]
  - metallicity : comes from differences in work functions of NTs [4]
- Effect of interaction beyond mismatched work functions?
  - Structural deformation
  - Electronic interaction
- Importance of those effects with respect to interwall distance (Δr)



[1] : Okada and Oshiyama, PRL **91**, 216801 (2003)
[2] : Song et al., Chem. Phys. Lett. **414**, 429-433 (2005)
[3] : Pudlak and Pincak, Eur. Phys. J. B **67**, 565-576 (2009)
[4] : Shan and Cho, Phys. Rev. B **73**, 081401(R) (2006)

Method

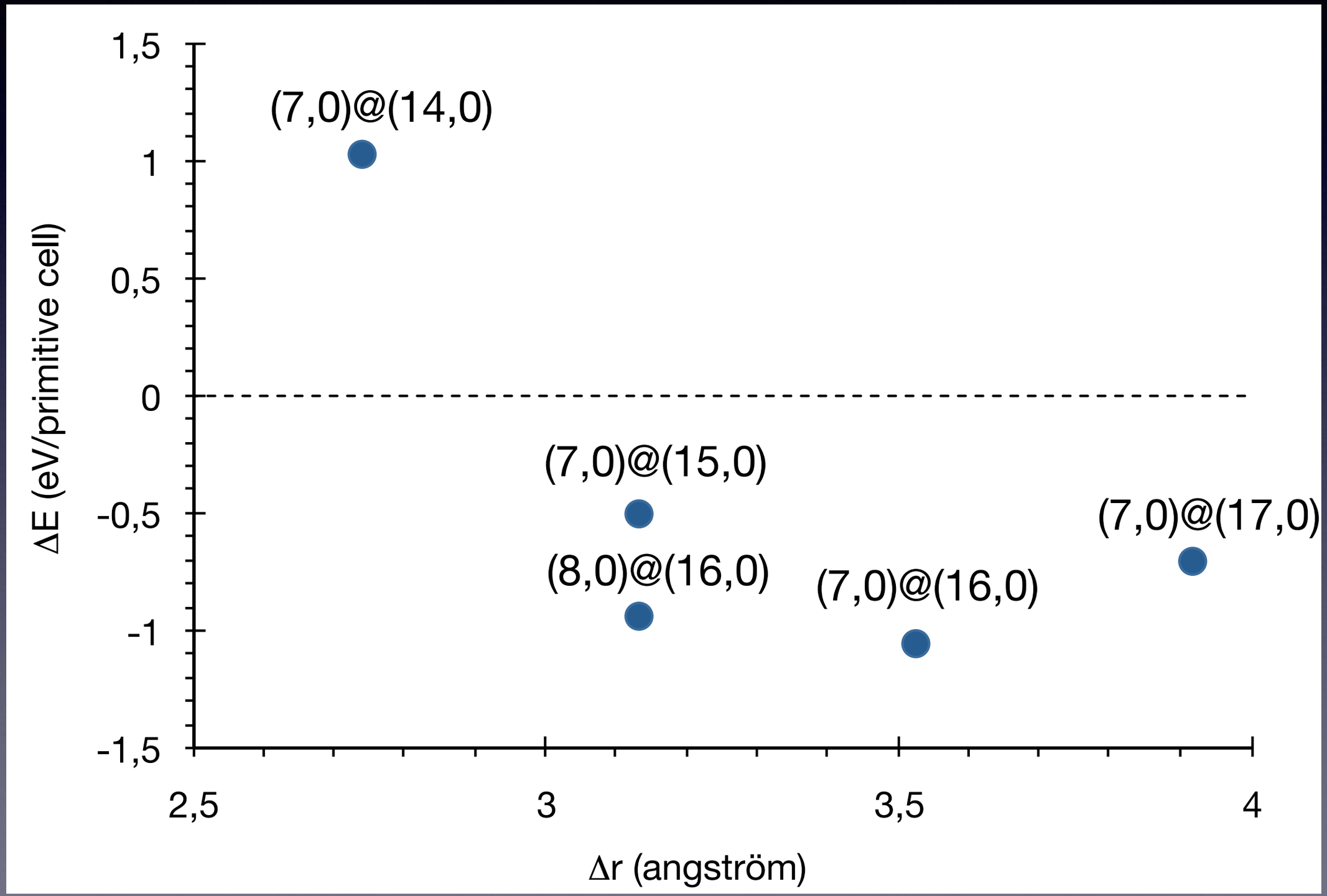
- Method : Density Functional Theory (DFT) as implemented in Abinit [5]
  - Local Density Approximation (LDA)
  - Plane wave basis set : 35 Ha cutoff
  - 7 angström distance between tubes
  - 1 1 6 k-points grid
  - Forces fully relaxed
  - (n,0)@(n,0) DWNT



[5] : Gonze et al. , Computer Phys. Commun. **180**, 2582-2615 (2009).

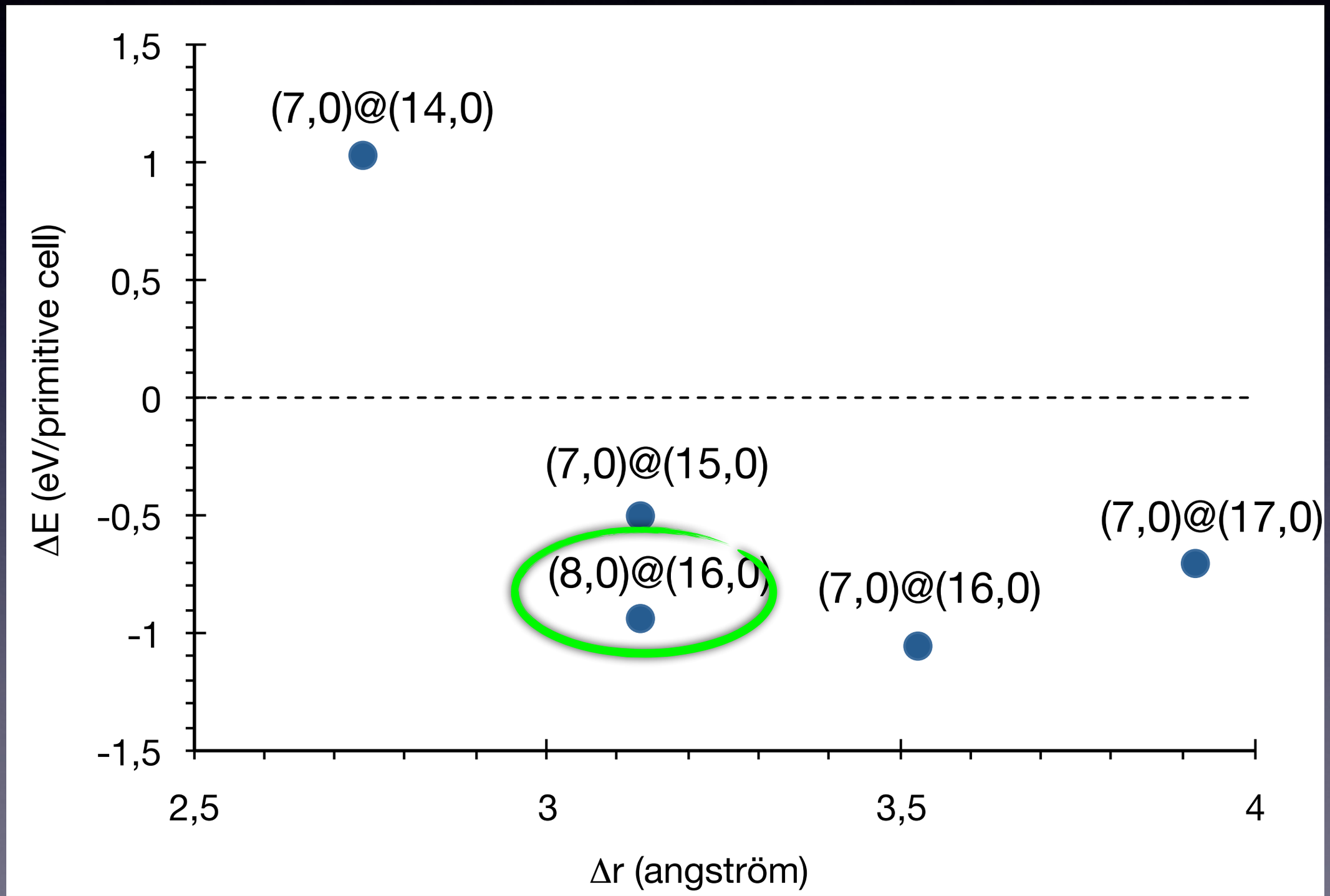
Bonding energy

dependance on Δr



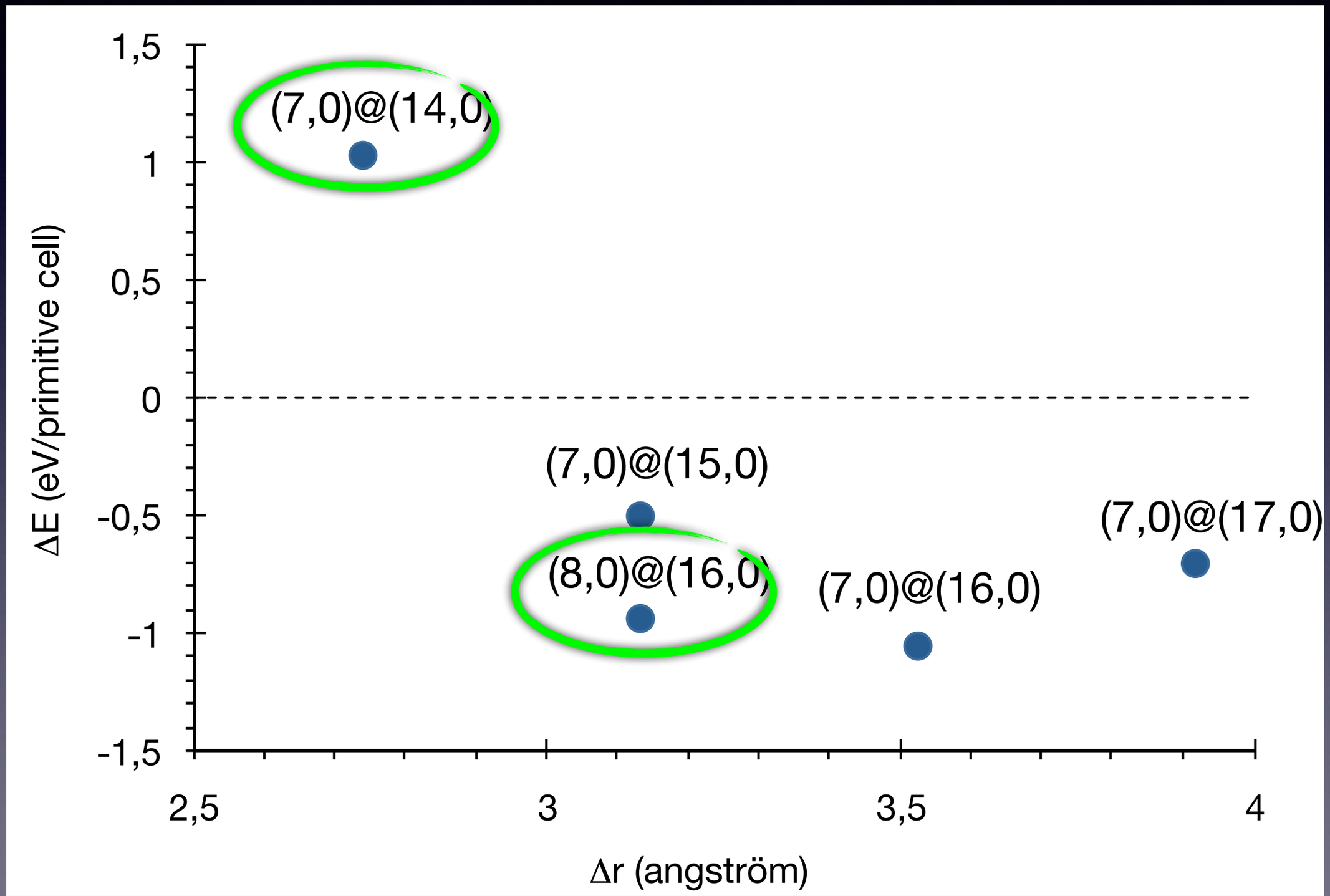
Bonding energy

dependance on Δr



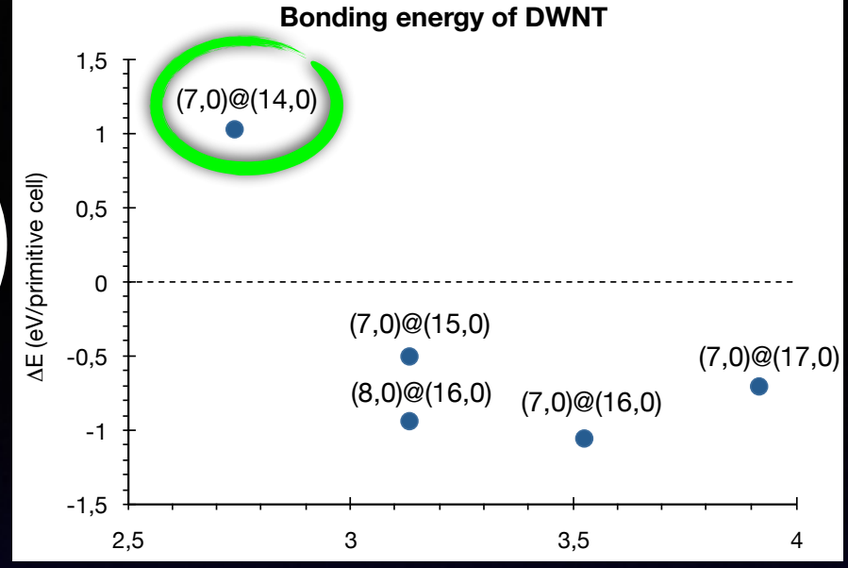
Bonding energy

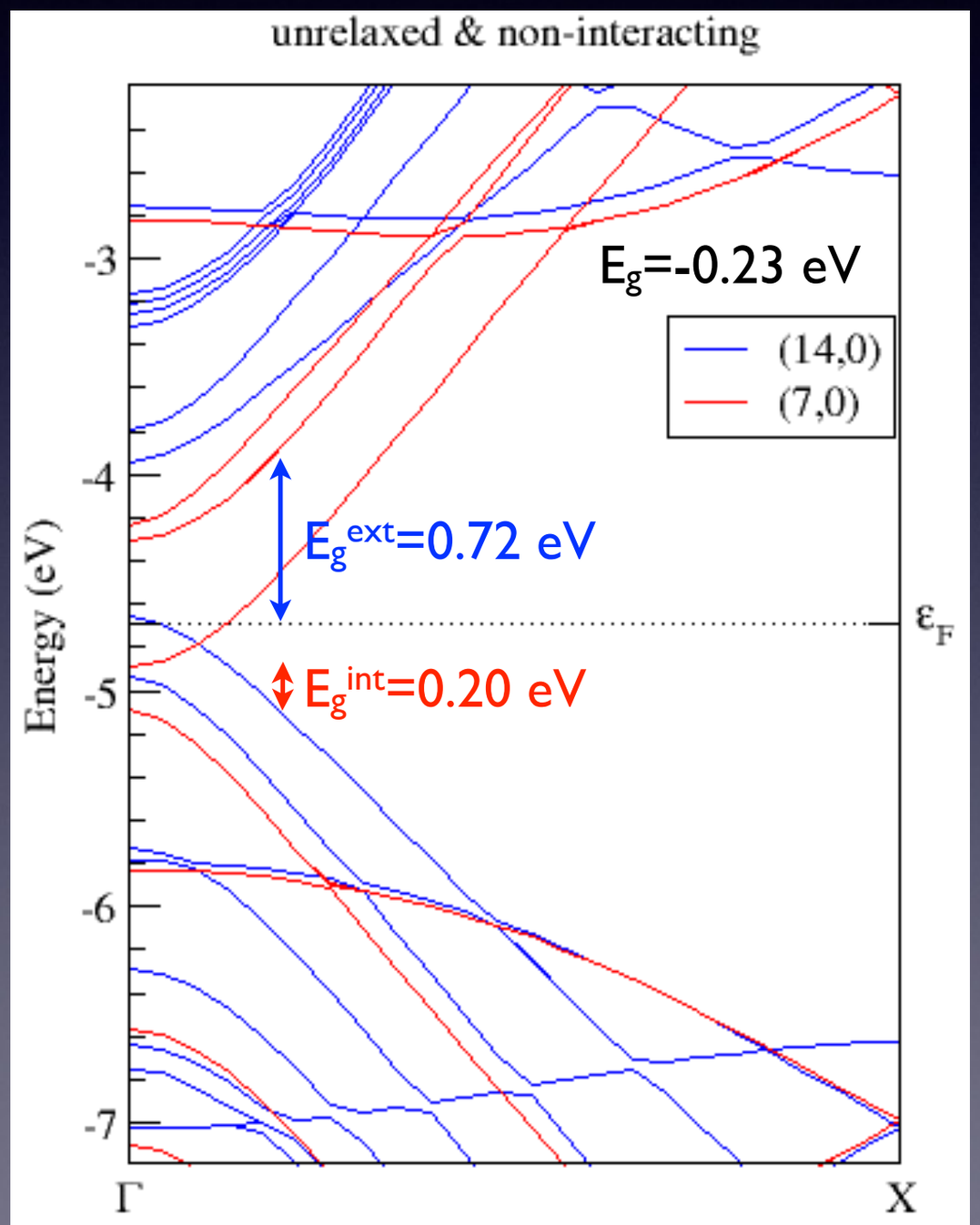
dependance on Δr

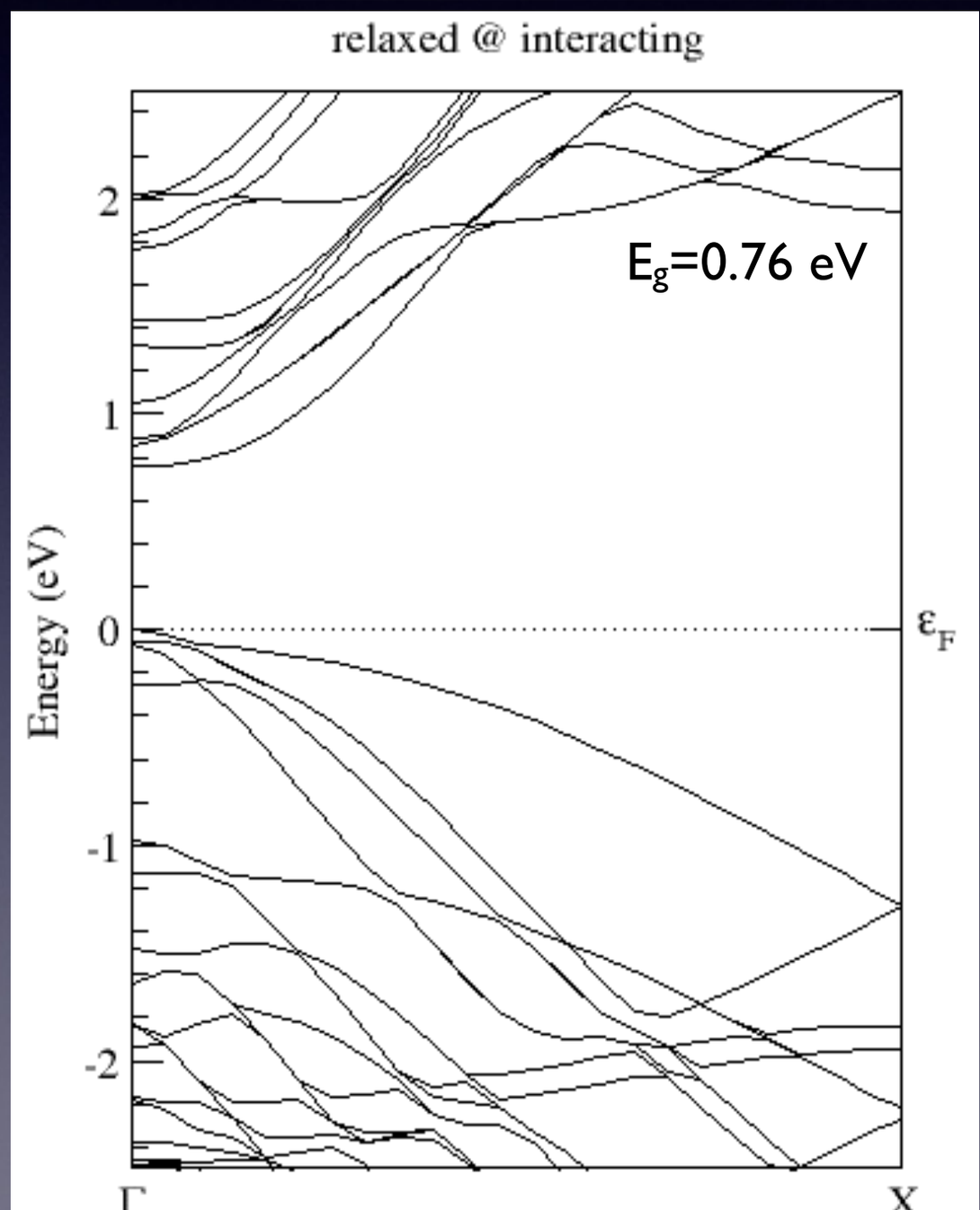


(7,0)@(14,0)

Δr = 2,7 Å

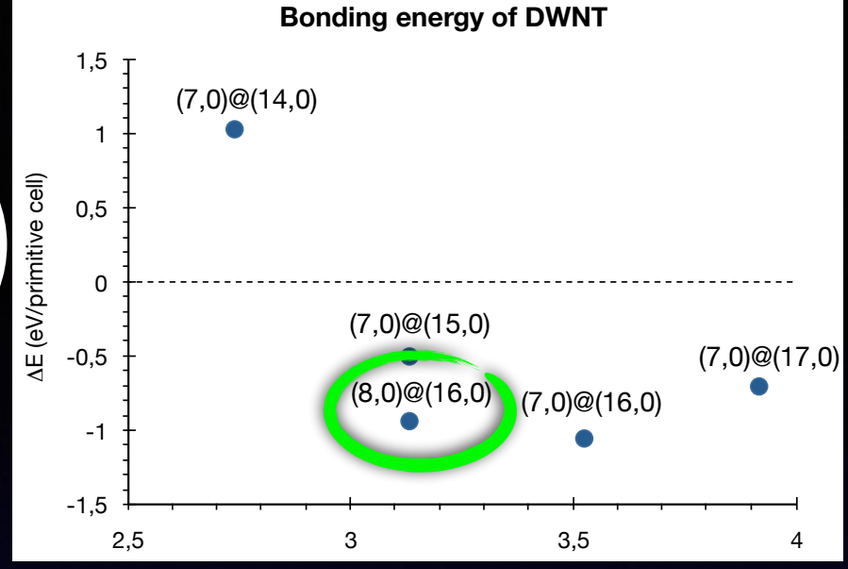

Bonding energy of DWNT
ΔE (eV/primitive cell)
1,5
1
0,5
0
-0,5
-1
-1,5
2,5
3
3,5
4
(7,0)@(14,0)
(7,0)@(15,0)
(8,0)@(16,0)
(7,0)@(16,0)
(7,0)@(17,0)

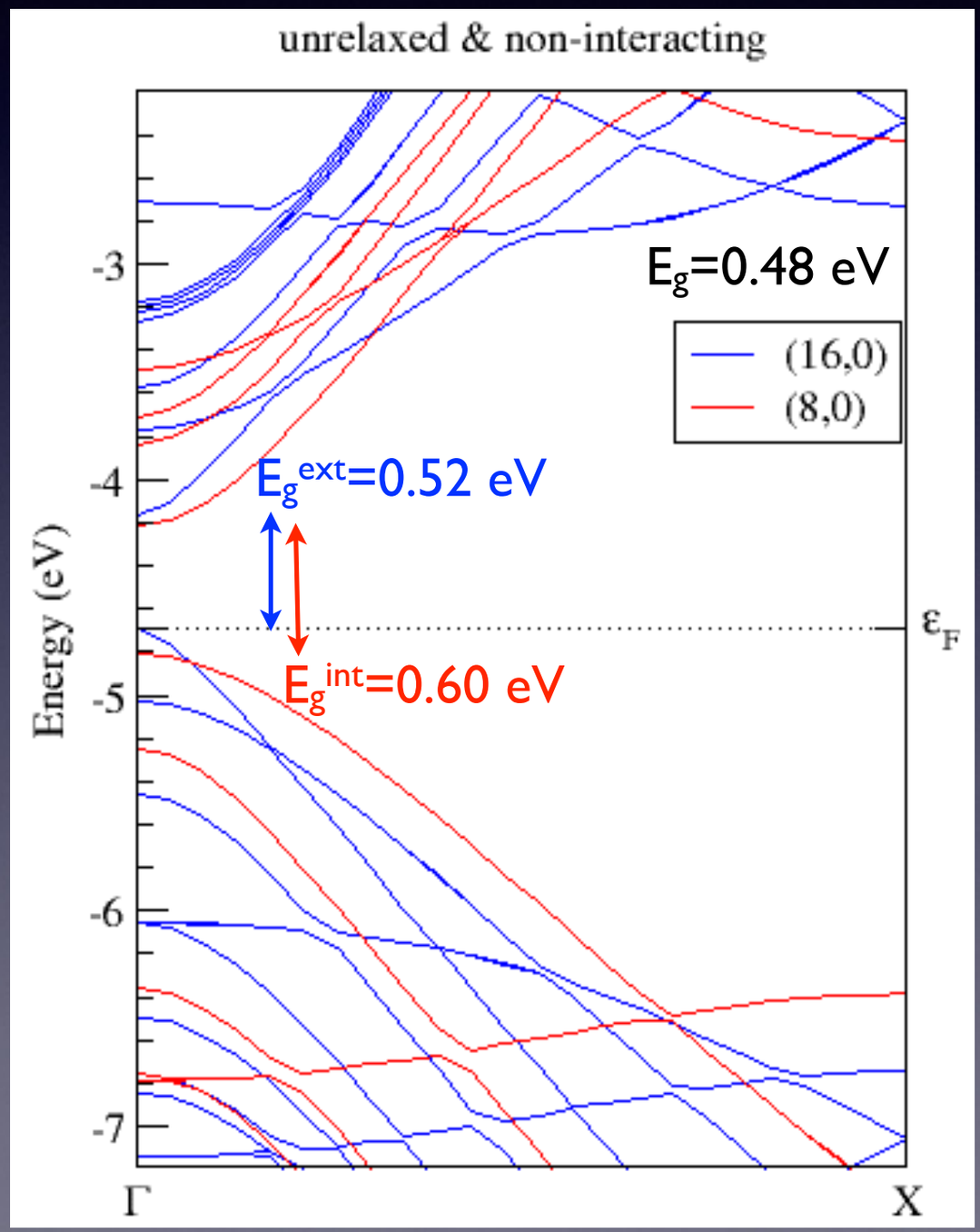

unrelaxed & non-interacting
E_g=-0.23 eV
(14,0)
(7,0)
E_g^{ext}=0.72 eV
E_g^{int}=0.20 eV
Energy (eV)
-3
-4
-5
-6
-7
ε_F
Γ
X

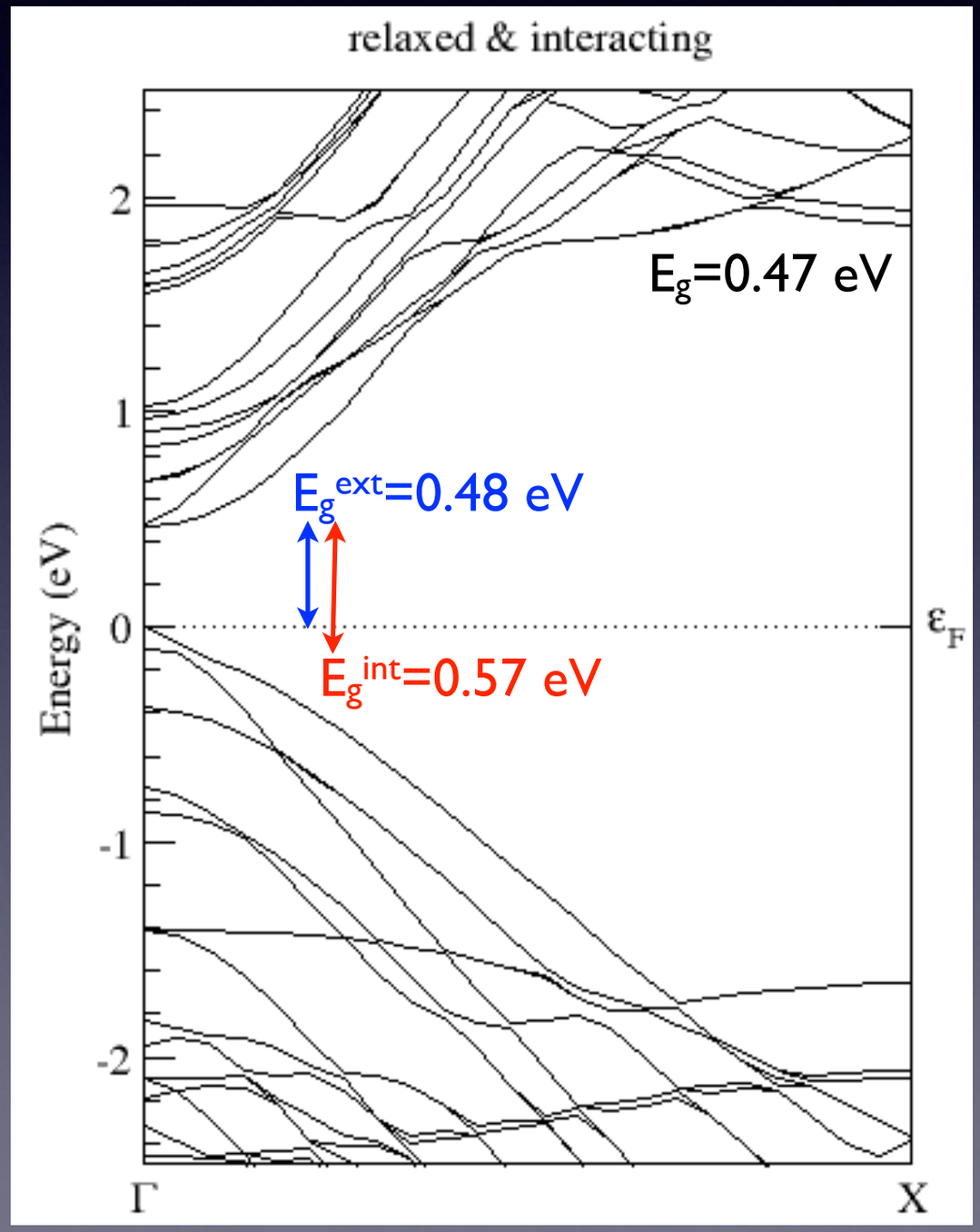

relaxed @ interacting
E_g=0.76 eV
Energy (eV)
2
1
0
-1
-2
ε_F
Γ
X

(8,0)@(16,0)

Δr = 3,1 Å


Bonding energy of DWNT
ΔE (eV/primitive cell)
1,5
1
0,5
0
-0,5
-1
-1,5
2,5
3
3,5
4
(7,0)@(14,0)
(7,0)@(15,0)
(8,0)@(16,0)
(7,0)@(16,0)
(7,0)@(17,0)

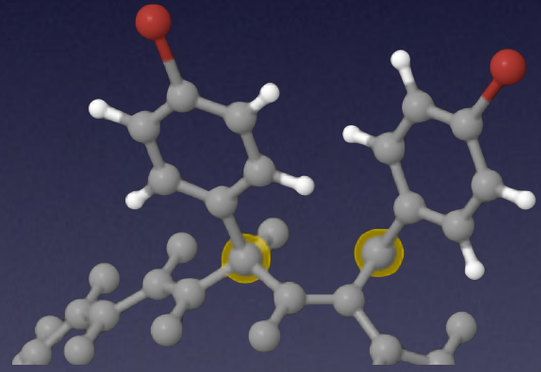

unrelaxed & non-interacting
Energy (eV)
-3
-4
-5
-6
-7
Γ
X
ε_F
(16,0)
(8,0)
E_g=0.48 eV
E_g^ext=0.52 eV
E_g^int=0.60 eV

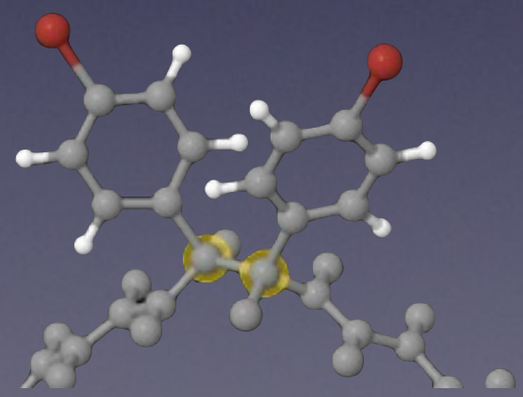

relaxed & interacting
Energy (eV)
2
1
0
-1
-2
Γ
X
ε_F
E_g=0.47 eV
E_g^ext=0.48 eV
E_g^int=0.57 eV

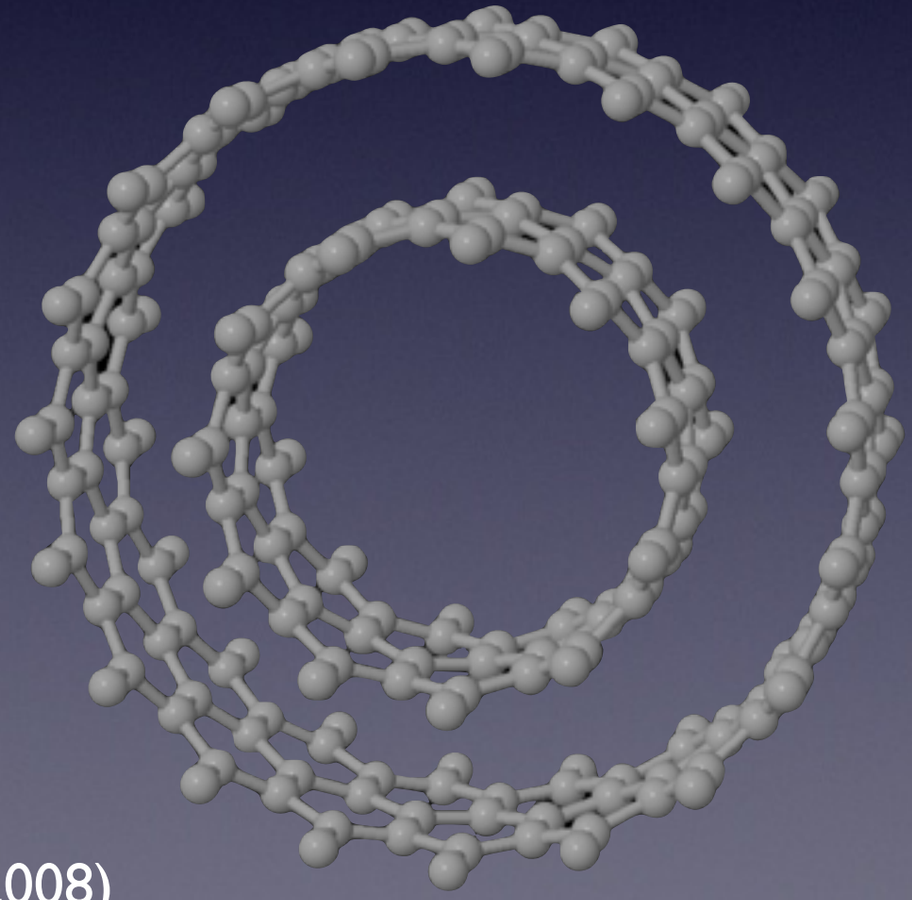
Part 2 : effect of functionalization

- functionalization with bromo-phenyls
- 2 most stables configurations on (5,5) SWNT [6] and graphene [7] (11,0)@(19,0)

- para :
  -1.51eV/pair
  (graphene)
- ortho :
  -1.25eV/pair
  (graphene)





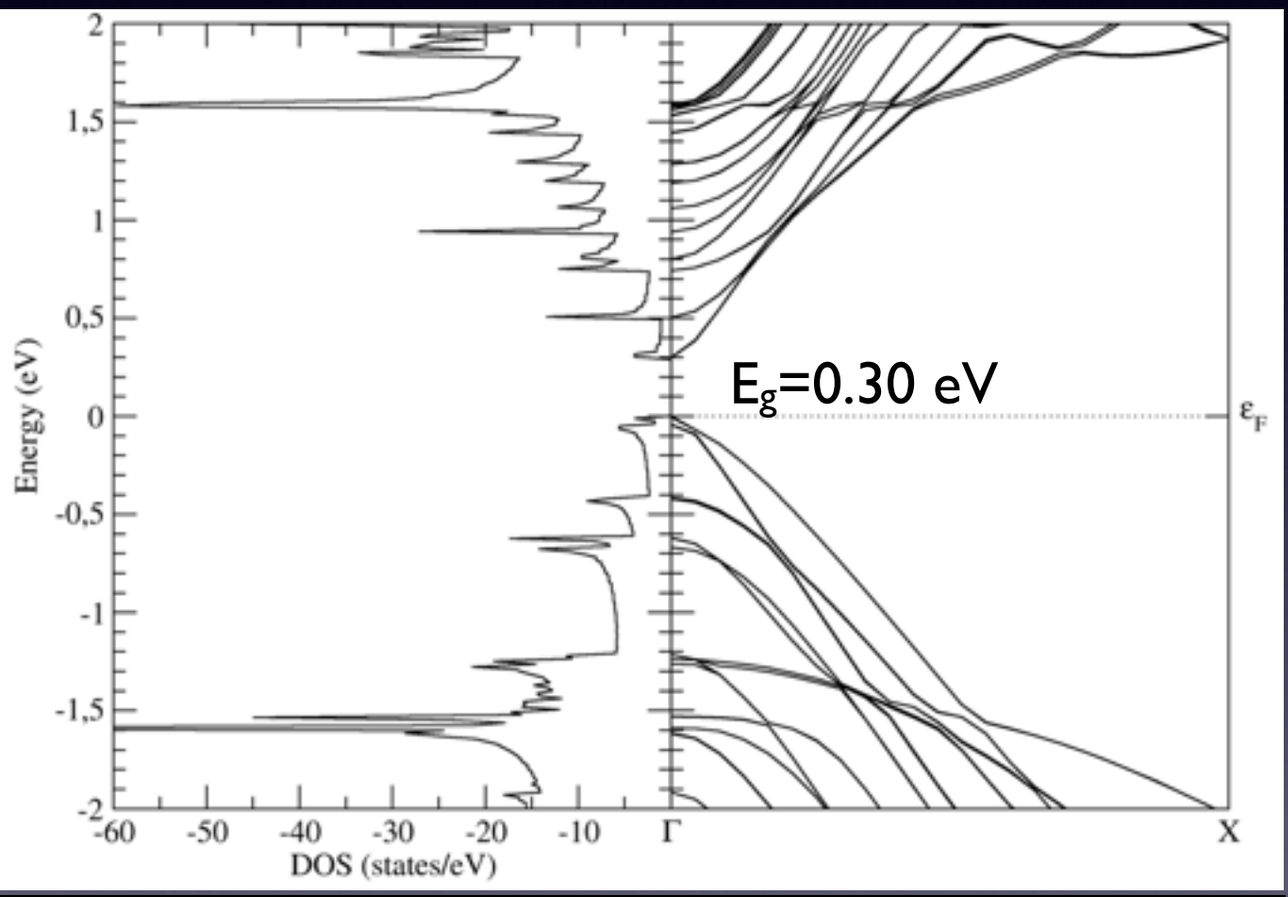


[6] : Lee, Nardelli and Marzari, PRL **95**, 076804 (2005)
[7] : Margine, Bocquet, Blase, Nano Letters **8**, 3315-3319 (2008)

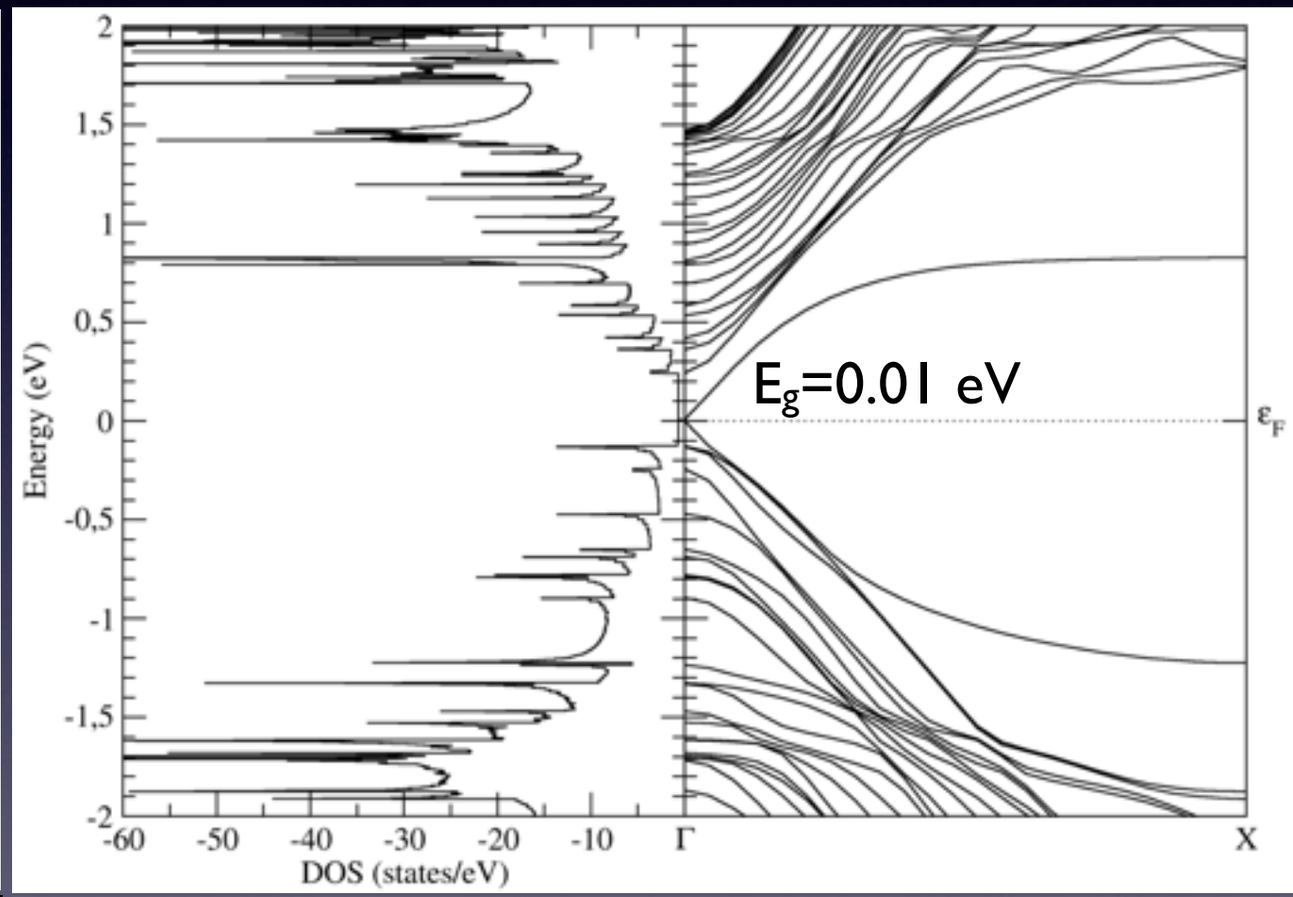
(11,0)@(19,0)

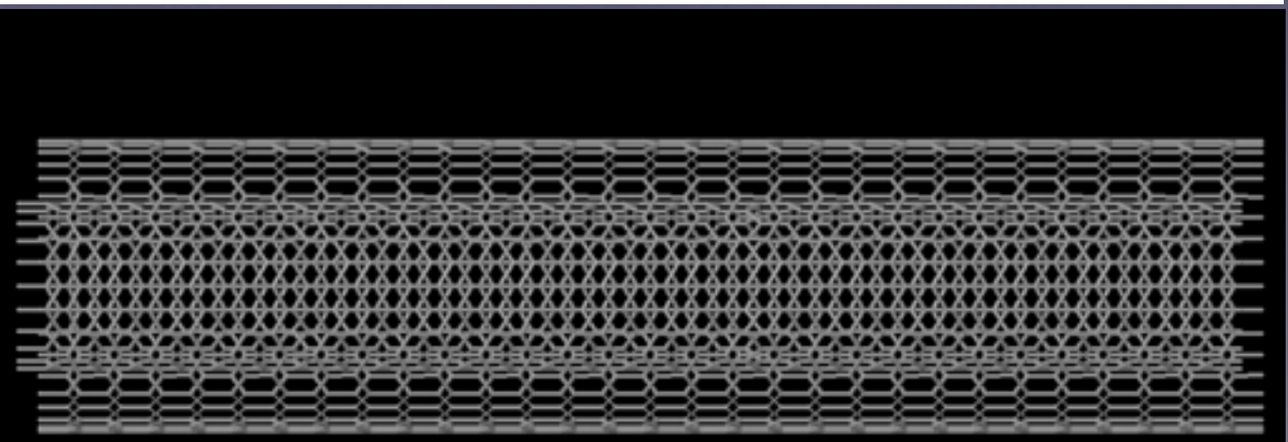
functionalized with bromo-phenyls

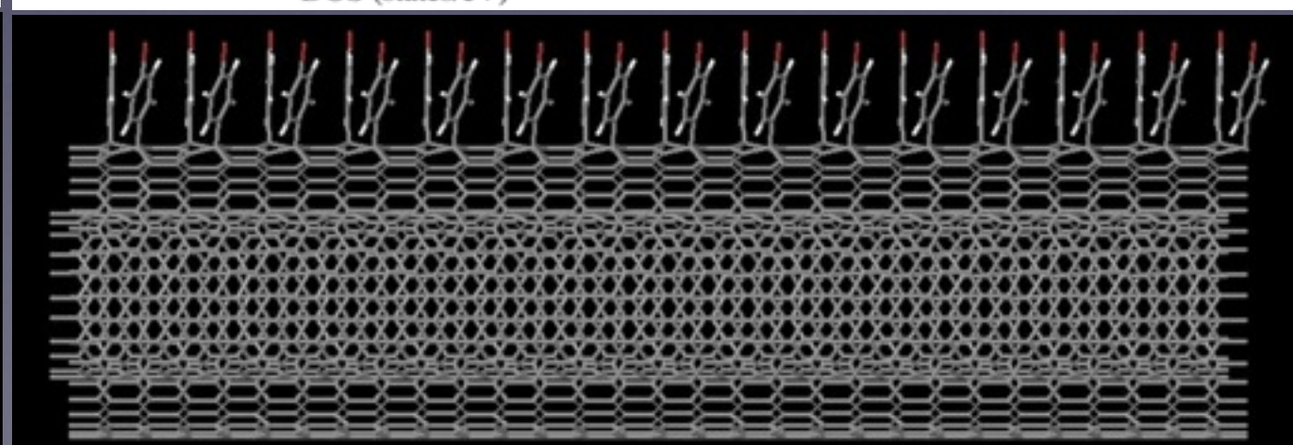
pristine



functinalized (para)



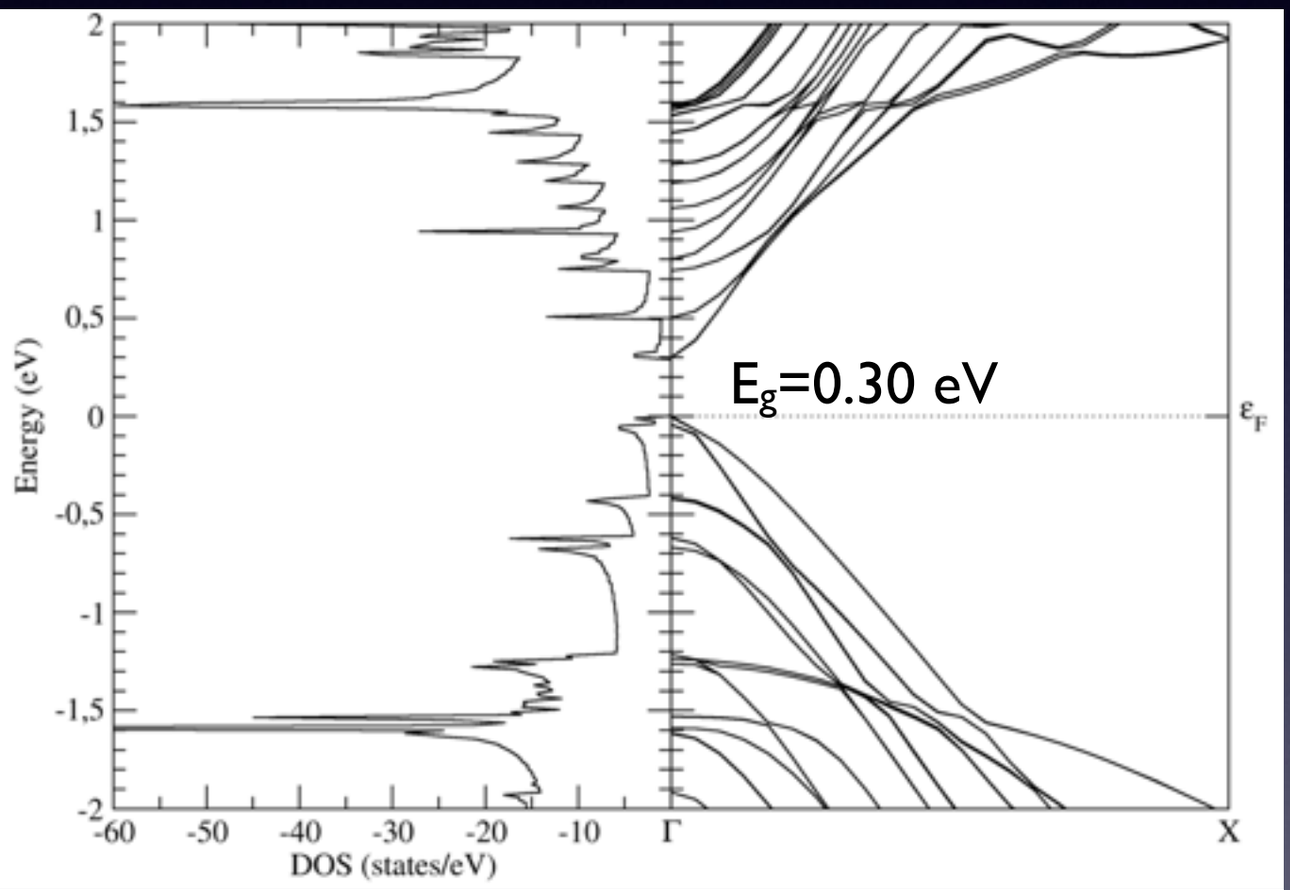




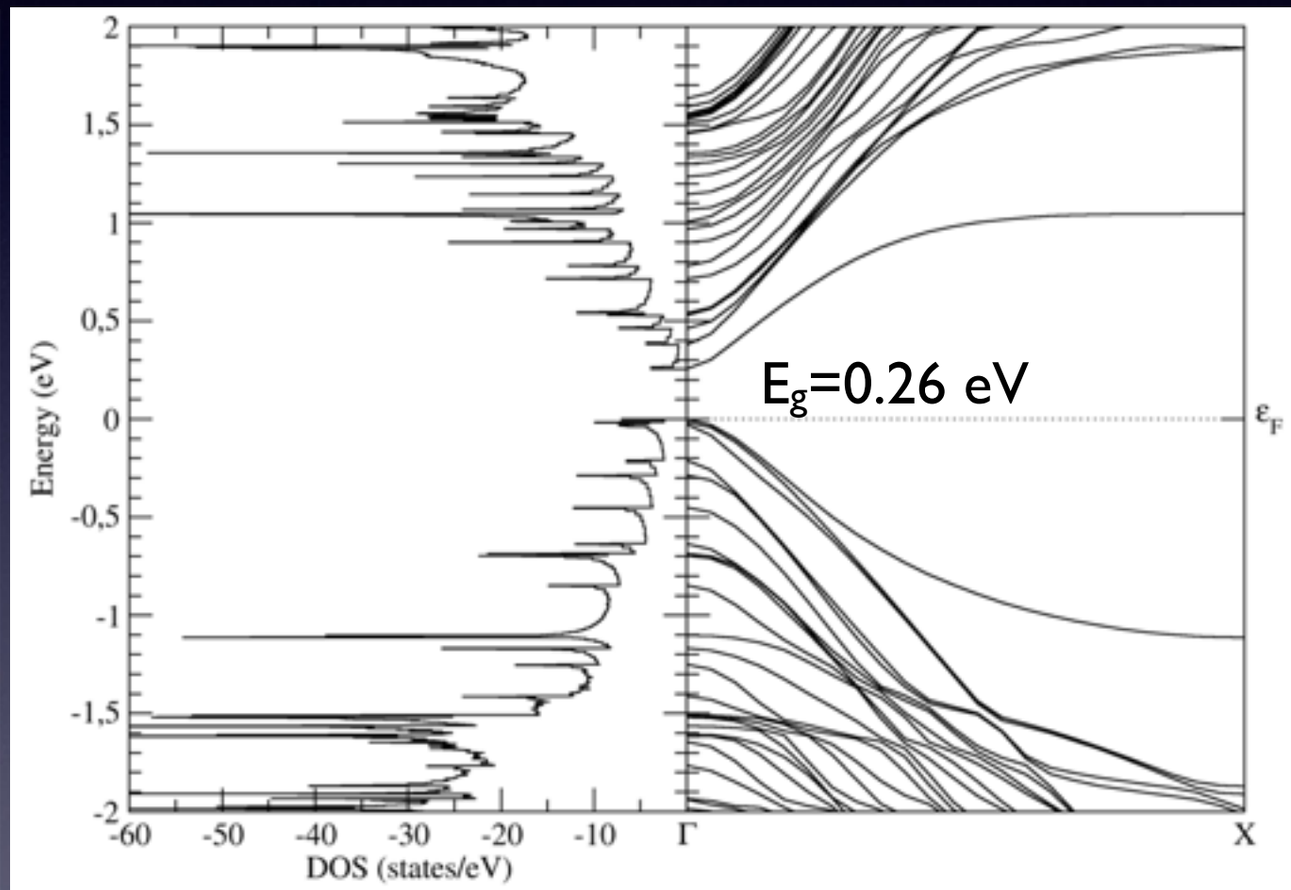
(11,0)@(19,0)

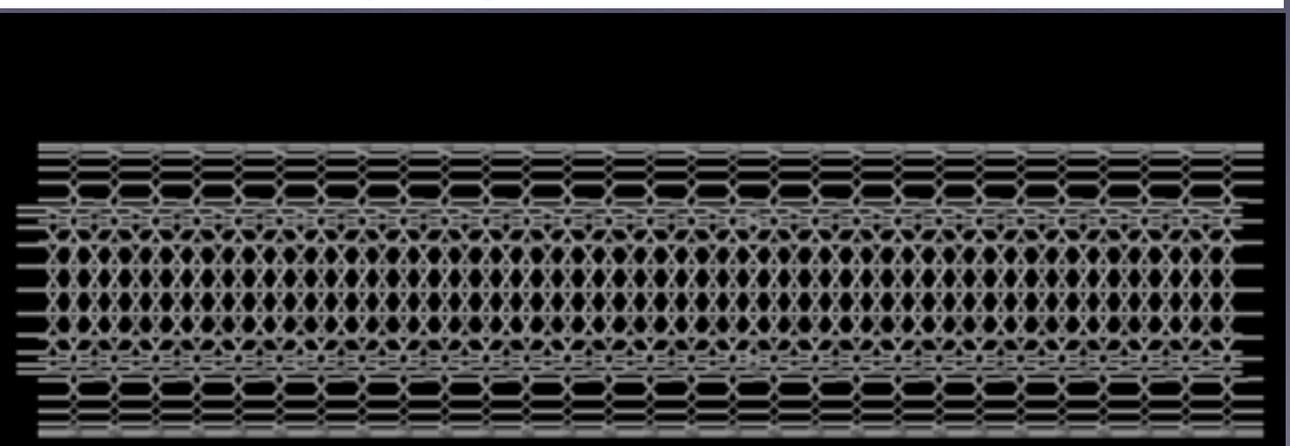
functionalized with bromo-phenyls

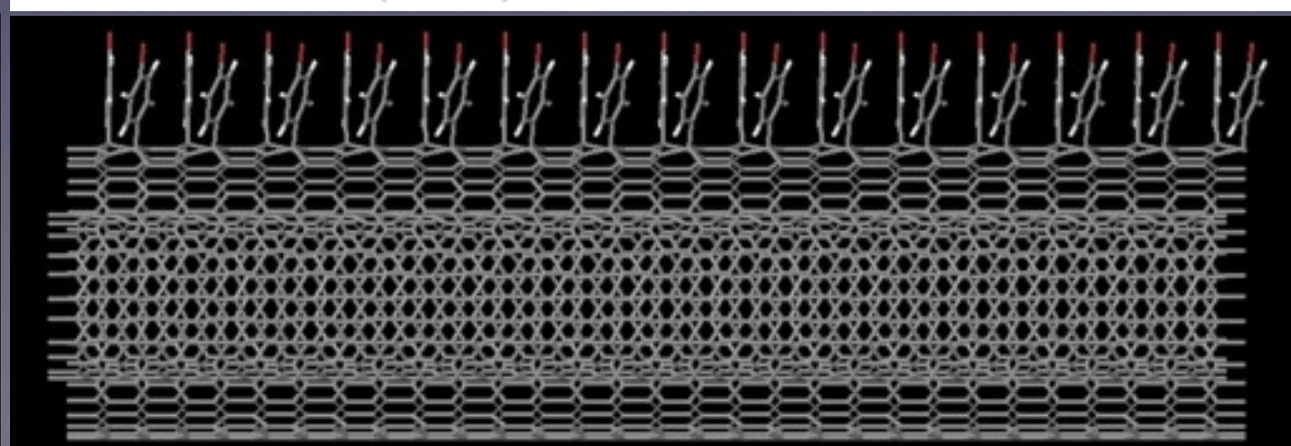
pristine



functionalized (ortho)

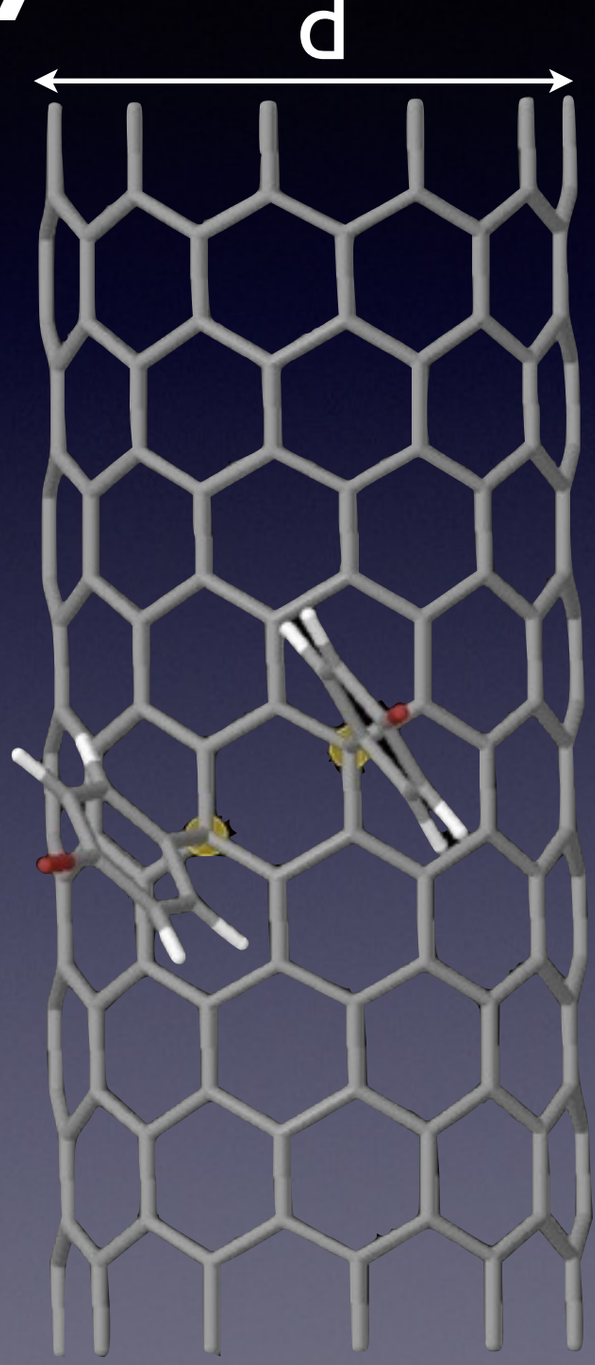






Bonding energy

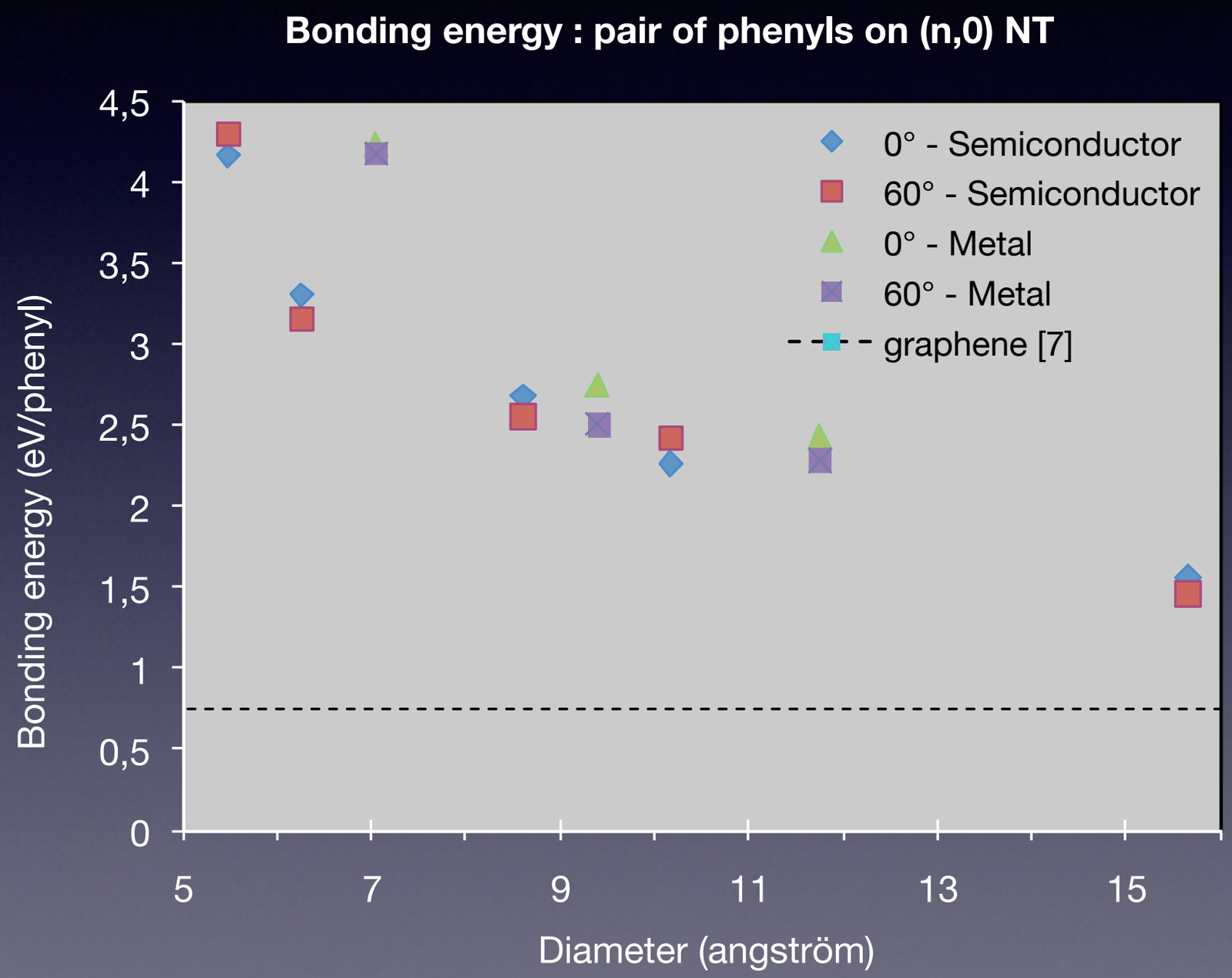
- Which tubes are functionalized?
  - Isolated pairs
  - on zigzag SWNT
  - Para configuration
- Bonding energy (ΔE) with respect to
  - tube diameter (d)
  - metallicity or semiconductivity
  - angle w/r to tube axis (0° or 60°)
- Calculations done using ONETEP [8]



[8] Skylaris, Haynes, Mostofi and Payne, J. Chem. Phys. **122**, 084119 (2005)

Bonding energy

- Trend :
  - E_b ↘ if d ↗ tend to graphene's
  - E_b for M > E_b for S
  - no clear trend for angle



[7] : Margine, Bocquet, Blase, Nano Letters **8**, 3315-3319 (2008)

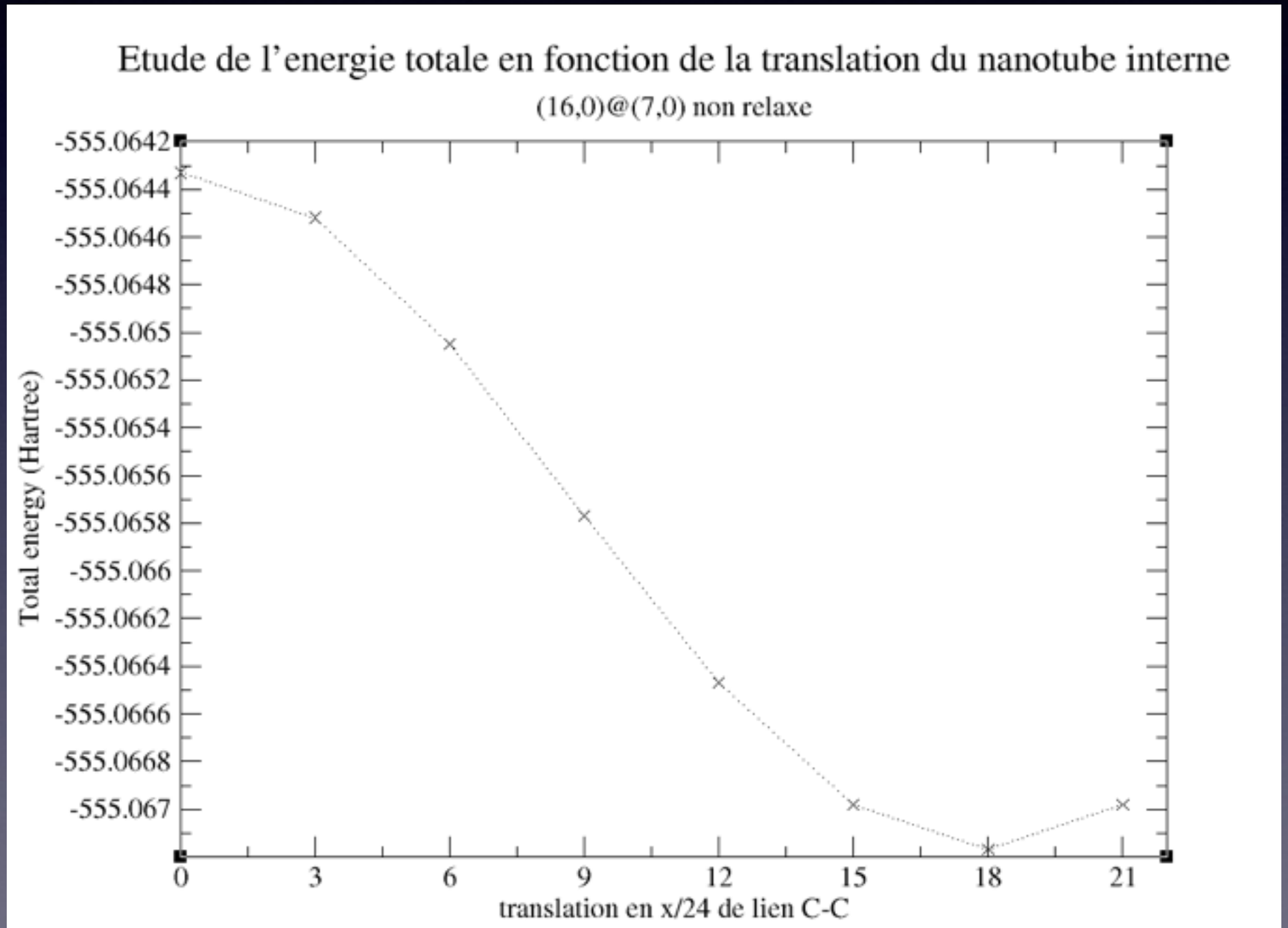
Conclusion

- Band structure of DWNT :
  ~ superposition of SWNT for bonded DWNT
- Effect of functionalisation (bromo-phenyl) :
  electronic states in the gap
- Pairs of phenyls : more sable for
  - small diameters
  - metallic tubes

Acknowledgments

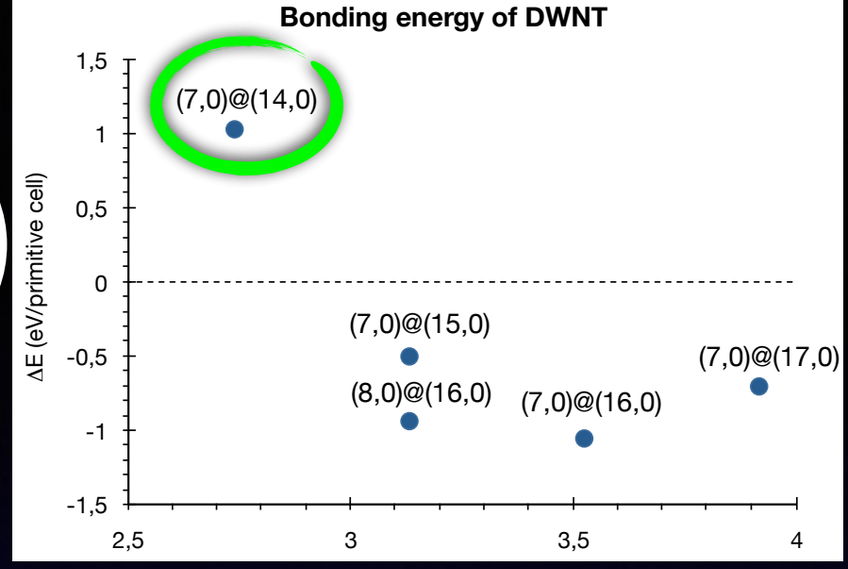
- Delphine Bouilly, Janie Cabana and Richard Martel for the expermiental data on DWNT FETs

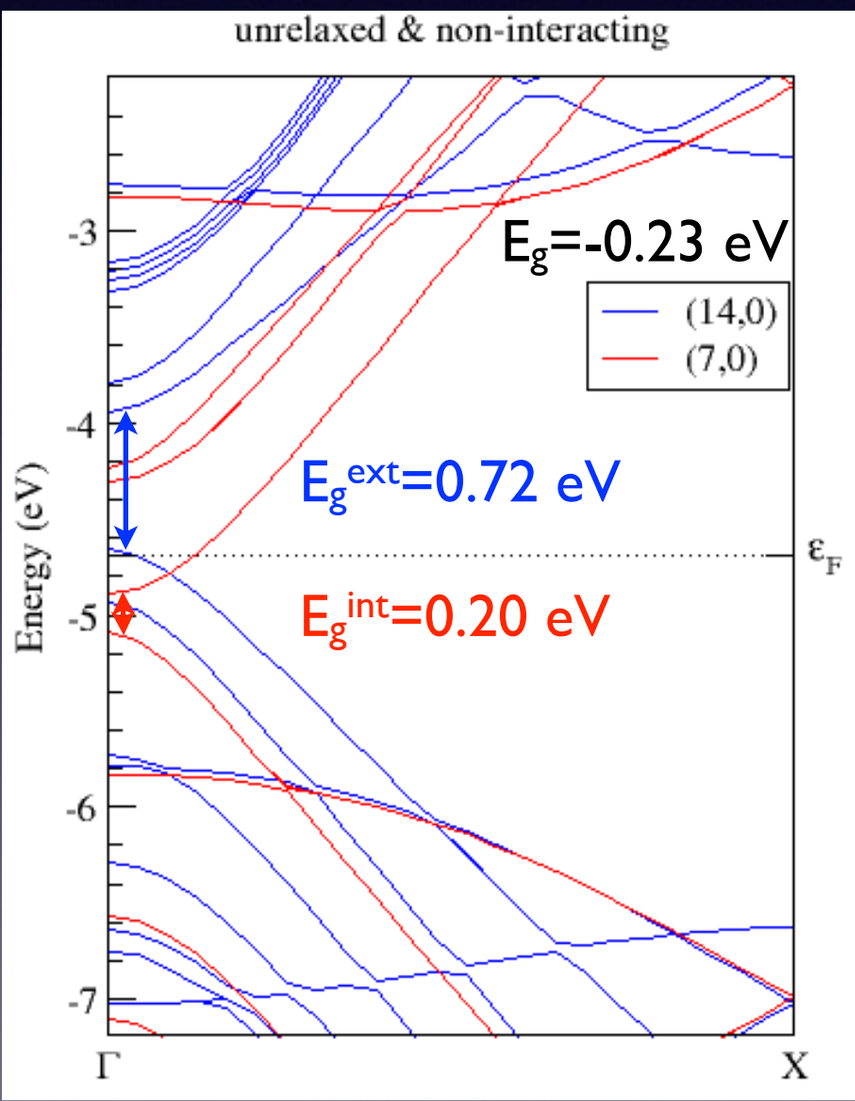
Supplements :
DWNT coaxial translation

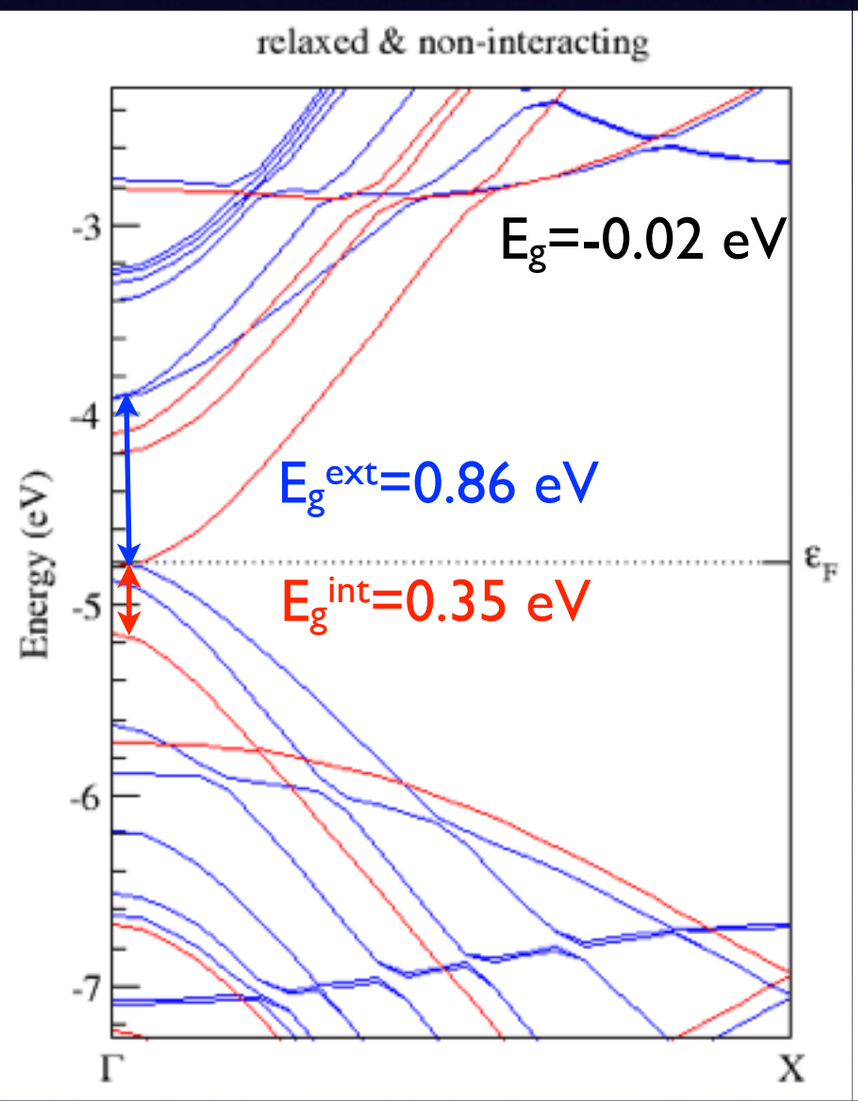


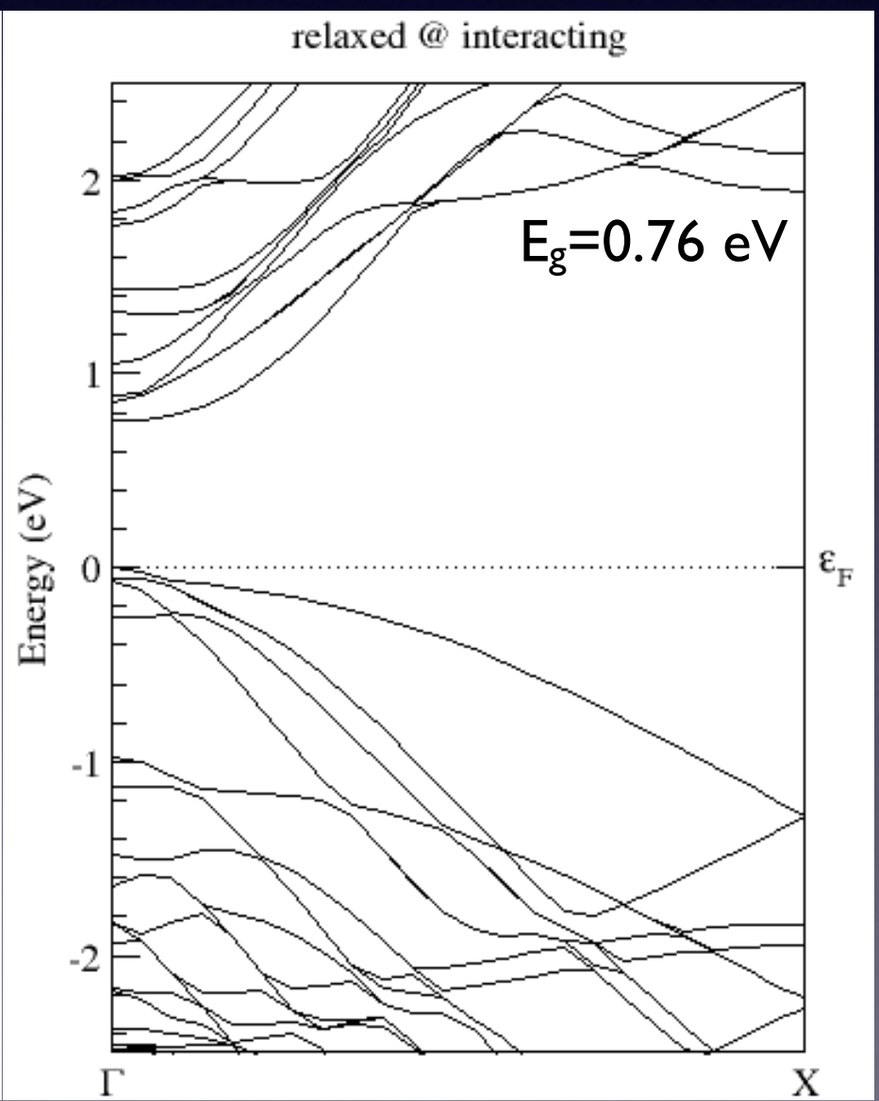
(7,0)@(14,0)

Δr = 2,7 Å


Bonding energy of DWNT
ΔE (eV/primitive cell)
1,5
1
0,5
0
-0,5
-1
-1,5
2,5
3
3,5
4
(7,0)@(14,0)
(7,0)@(15,0)
(8,0)@(16,0)
(7,0)@(16,0)
(7,0)@(17,0)

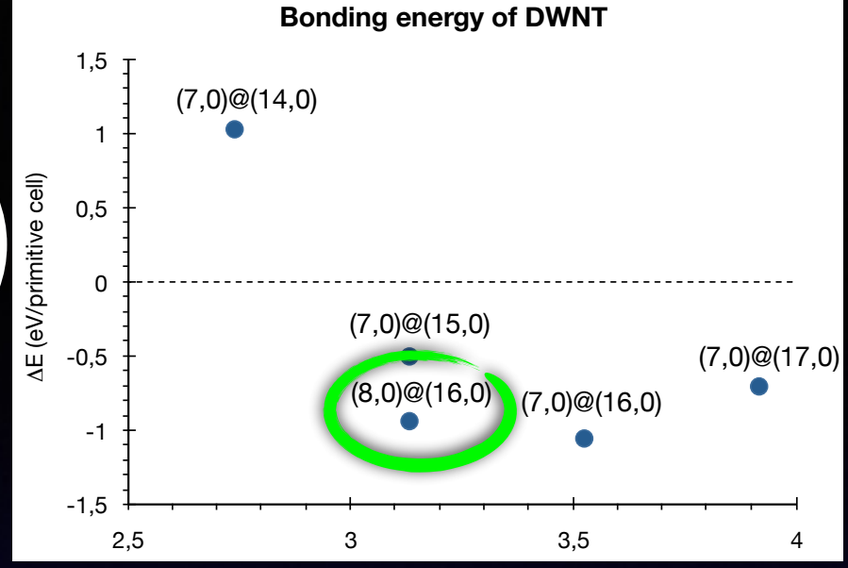

unrelaxed & non-interacting
Energy (eV)
-3
-4
-5
-6
-7
Γ
X
ε_F
E_g=-0.23 eV
(14,0)
(7,0)
E_g^{ext}=0.72 eV
E_g^{int}=0.20 eV

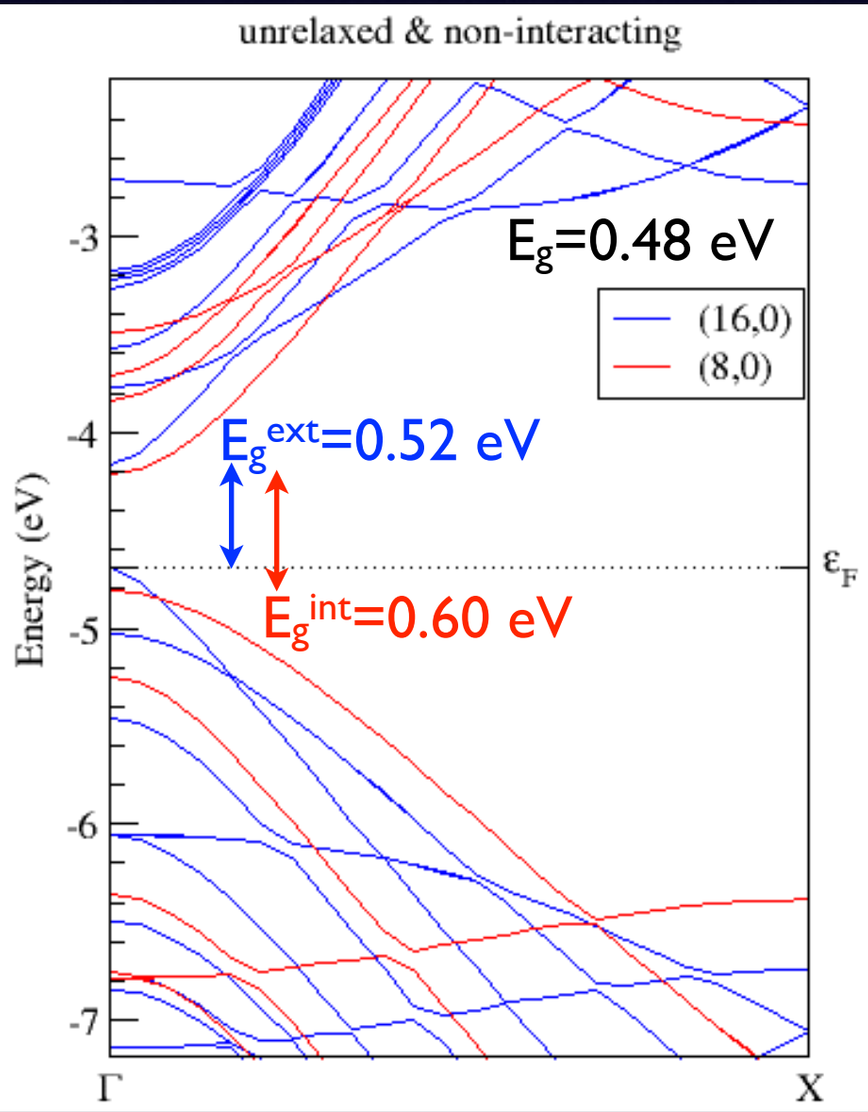

relaxed & non-interacting
Energy (eV)
-3
-4
-5
-6
-7
Γ
X
ε_F
E_g=-0.02 eV
E_g^{ext}=0.86 eV
E_g^{int}=0.35 eV

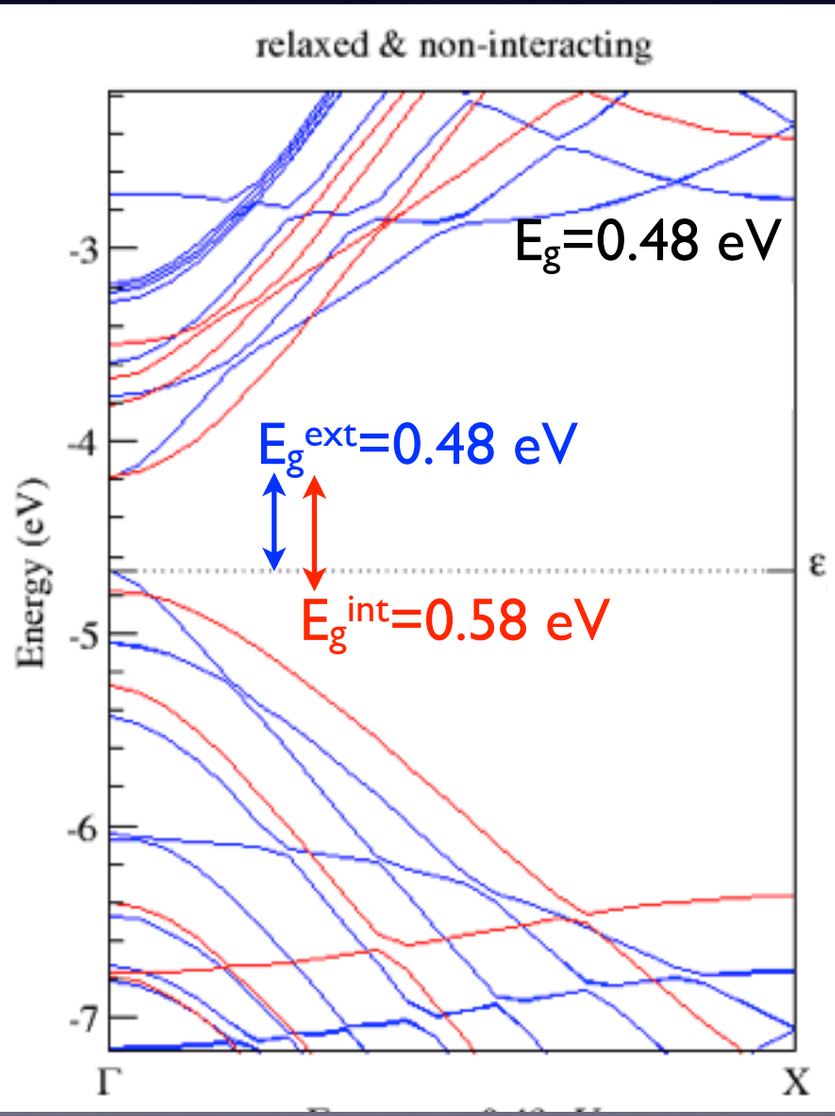

relaxed @ interacting
Energy (eV)
2
1
0
-1
-2
Γ
X
ε_F
E_g=0.76 eV

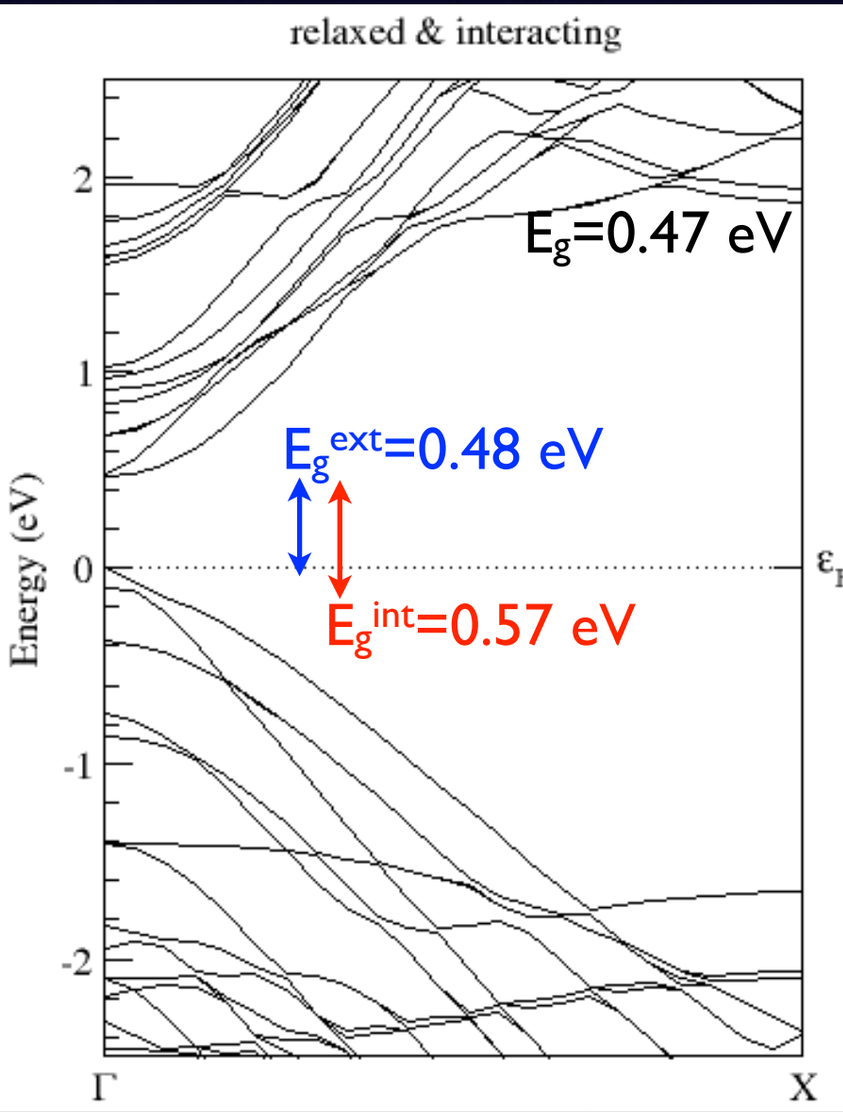
(8,0)@(16,0)

Δr = 3,1 Å


Bonding energy of DWNT
ΔE (eV/primitive cell)
1,5
1
0,5
0
-0,5
-1
-1,5
2,5
3
3,5
4
(7,0)@(14,0)
(7,0)@(15,0)
(8,0)@(16,0)
(7,0)@(16,0)
(7,0)@(17,0)

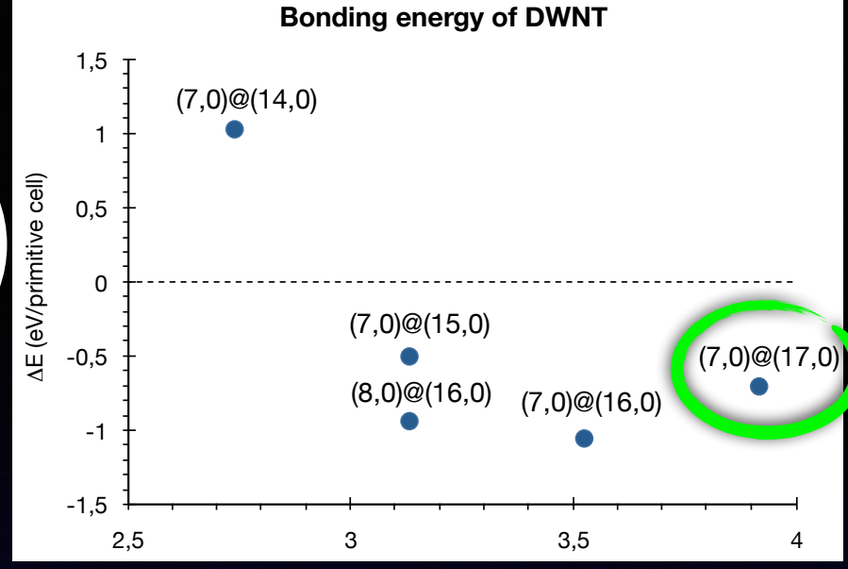

unrelaxed & non-interacting
Eg=0.48 eV
(16,0)
(8,0)
Eg ext=0.52 eV
Eg int=0.60 eV
Energy (eV)
εF
Γ
X

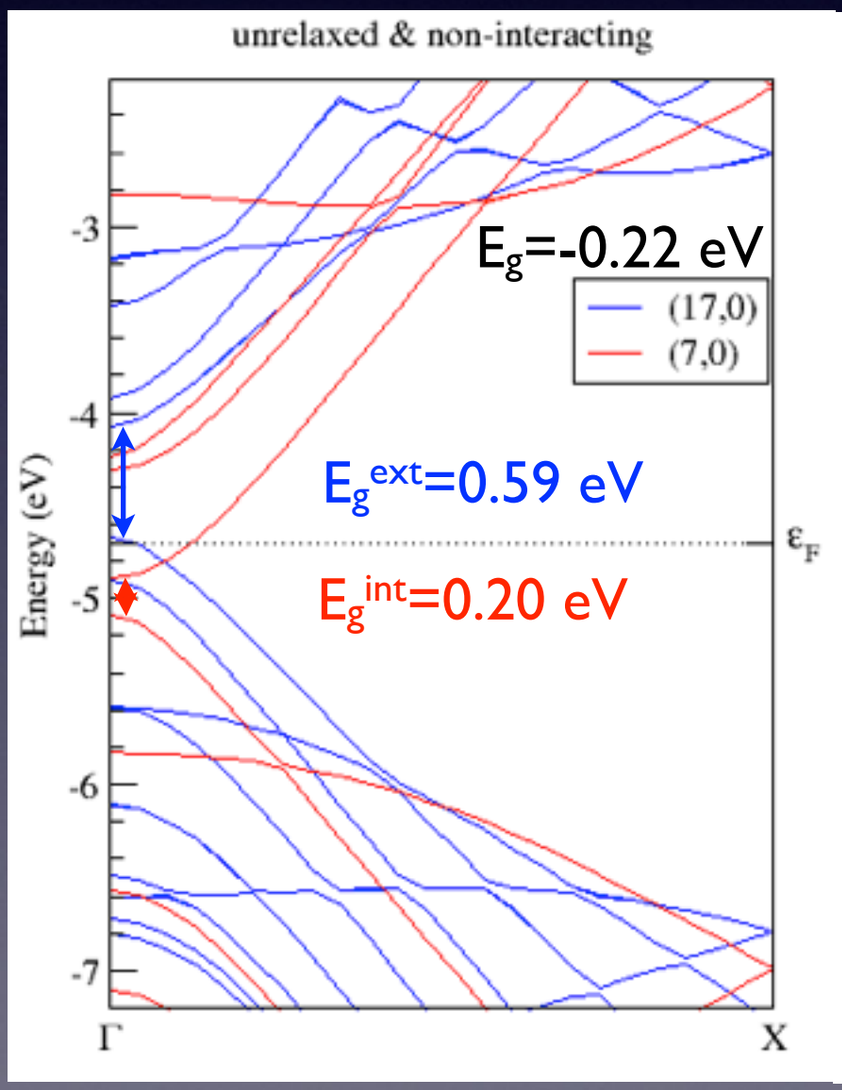

relaxed & non-interacting
Eg=0.48 eV
Eg ext=0.48 eV
Eg int=0.58 eV
Energy (eV)
Γ
X

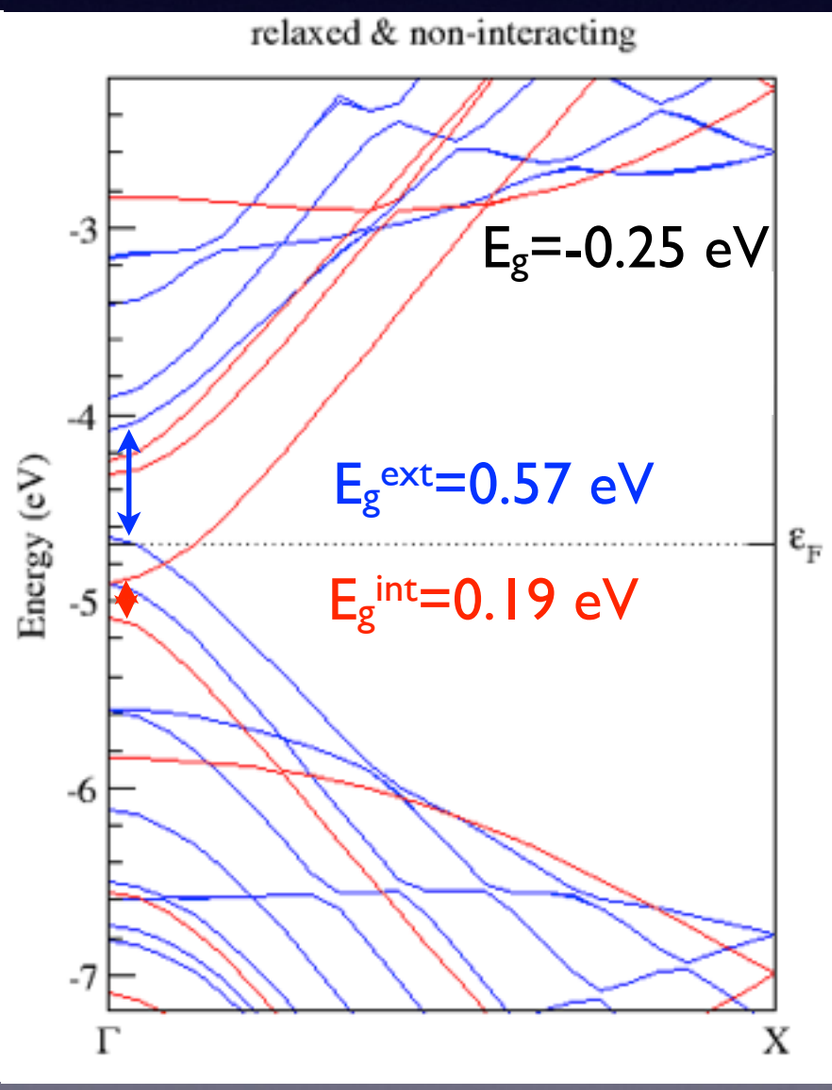

relaxed & interacting
Eg=0.47 eV
Eg ext=0.48 eV
Eg int=0.57 eV
Energy (eV)
εF
Γ
X

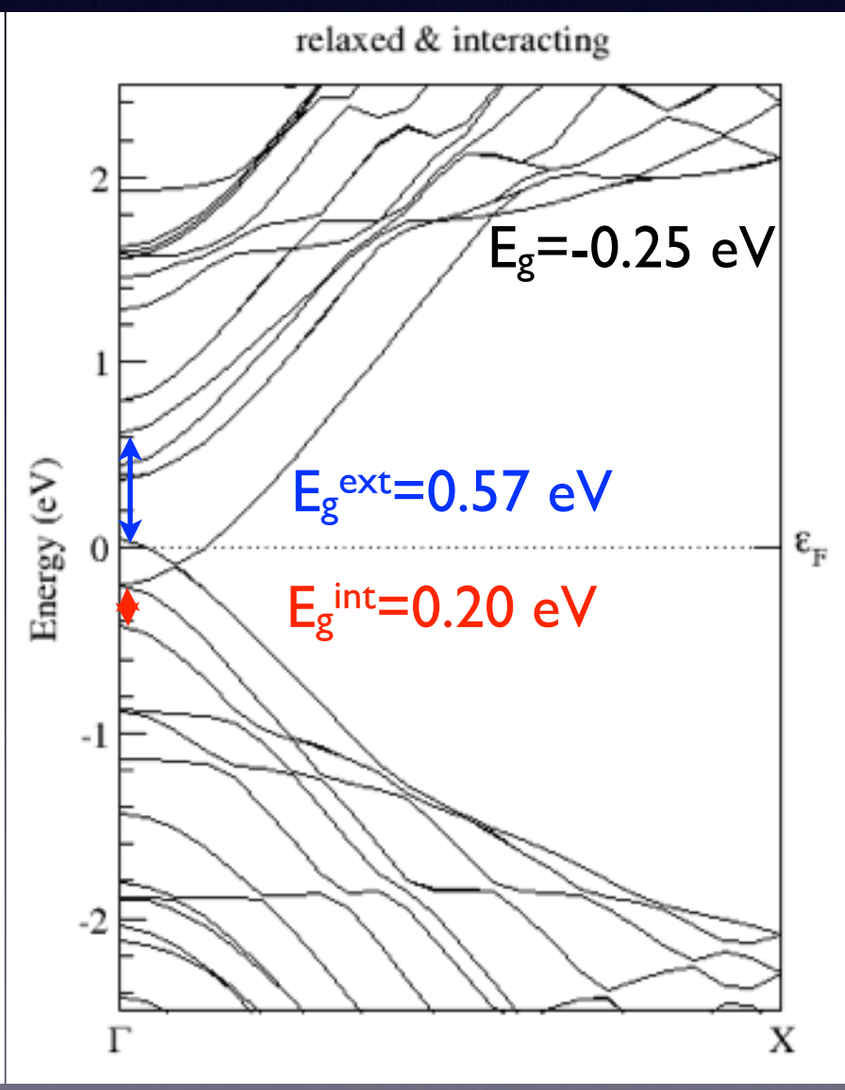
(7,0)@(17,0)

Δr = 3,9 Å


Bonding energy of DWNT
ΔE (eV/primitive cell)
1,5
1
0,5
0
-0,5
-1
-1,5
2,5
3
3,5
4
(7,0)@(14,0)
(7,0)@(15,0)
(8,0)@(16,0)
(7,0)@(16,0)
(7,0)@(17,0)


unrelaxed & non-interacting
E_g=-0.22 eV
(17,0)
(7,0)
E_g^{ext}=0.59 eV
E_g^{int}=0.20 eV
Energy (eV)
ε_F
Γ
X


relaxed & non-interacting
E_g=-0.25 eV
E_g^{ext}=0.57 eV
E_g^{int}=0.19 eV
Energy (eV)
ε_F
Γ
X


relaxed & interacting
E_g=-0.25 eV
E_g^{ext}=0.57 eV
E_g^{int}=0.20 eV
Energy (eV)
ε_F
Γ
X