Theoretical Study of Hydrogen @ Carbon Nanotubes and Nanoscrolls

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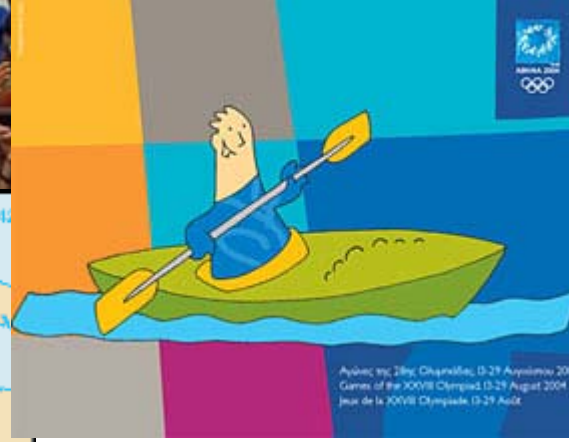
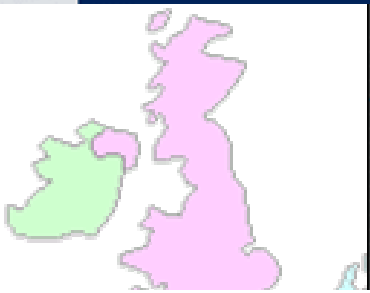
Collaborators : G. Lithoxoos, J. Samios @ UoAthens


ΑΘΗΝΑ 2004



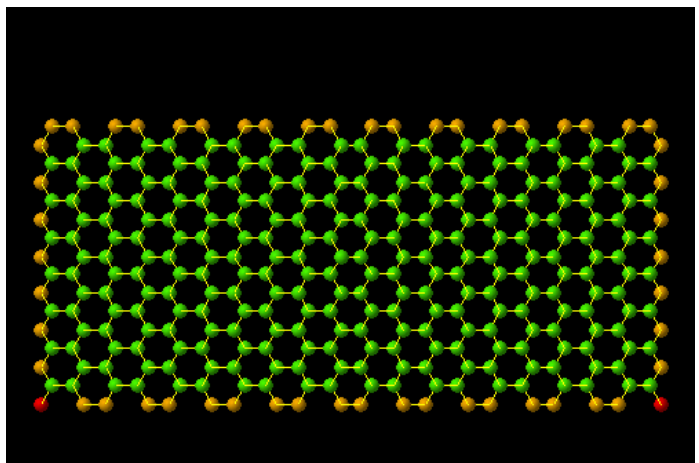



BULGARIA
F.Y.R.O.M.
ALB.
TUR.
Kavála
Alexandroúpolis
Thessaloníki
Mount Olympus
Kérkyra
Ioánnina
Lárisa
Igoumenítsa
Vólos
Límnos
Lésvos
Aegean Sea
TURKEY
Chalkís
Chíos
Elefsís
ATHENS
Pátrai
Sámos
Ionian Sea
Corinth Canal
Peiraiéfs
Lávrion


CRETE island
Agia Pelagia
Amnissos
Gouves
Hersonissos
Agios Nikolaos
Vai Beach
Palekastron
Sitia
Kato Zakros
Makrygialos
Ierapetra
Kritsa
Heraklion
Knossos
Rethimnon
Georgioupolis
Almirida
Chania
Kalamaki
Gerani
Nopigia
Kastelli
Spila
Platanyas
Stalos
Kalives
Megala Horafia
Sfinari
Kefali
Elefonisi
Paleohora
Loutro
Chora Sfakion
Rodakino
Plakias
Agia Galini
Matala
Lentas

Outline

- Quantum chemistry calculations in XXL systems
- Hydrogen @ SWNTs
- Hydrogen @ *doped* SWNTs
- Hydrogen @ *Nanoscrolls*



1997 Dillon et. al Hydrogen storage @ SWNTs

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Monday, November 8, 1999 Published at 09:16 GMT

Sci/Tech

Carbon tubes could store hydrogen fuel

Hydrogen-powered cars are already in development

1999 Chen et. al. Higher capacity of Alkali Doped CNT

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method of storing high quantities of hydrogen inside tiny tubes of carbon just two nanometres (billionths of a

Sci/Tech Contents

Relevant Stories

20 May 99 | Sci/Tech
'Artificial muscles' made from nanotubes

05 Mar 99 | Sci/Tech
World's smallest scales weigh in

Internet Links

Science

Massachusetts Institute of Technology

US National Hydrogen Association

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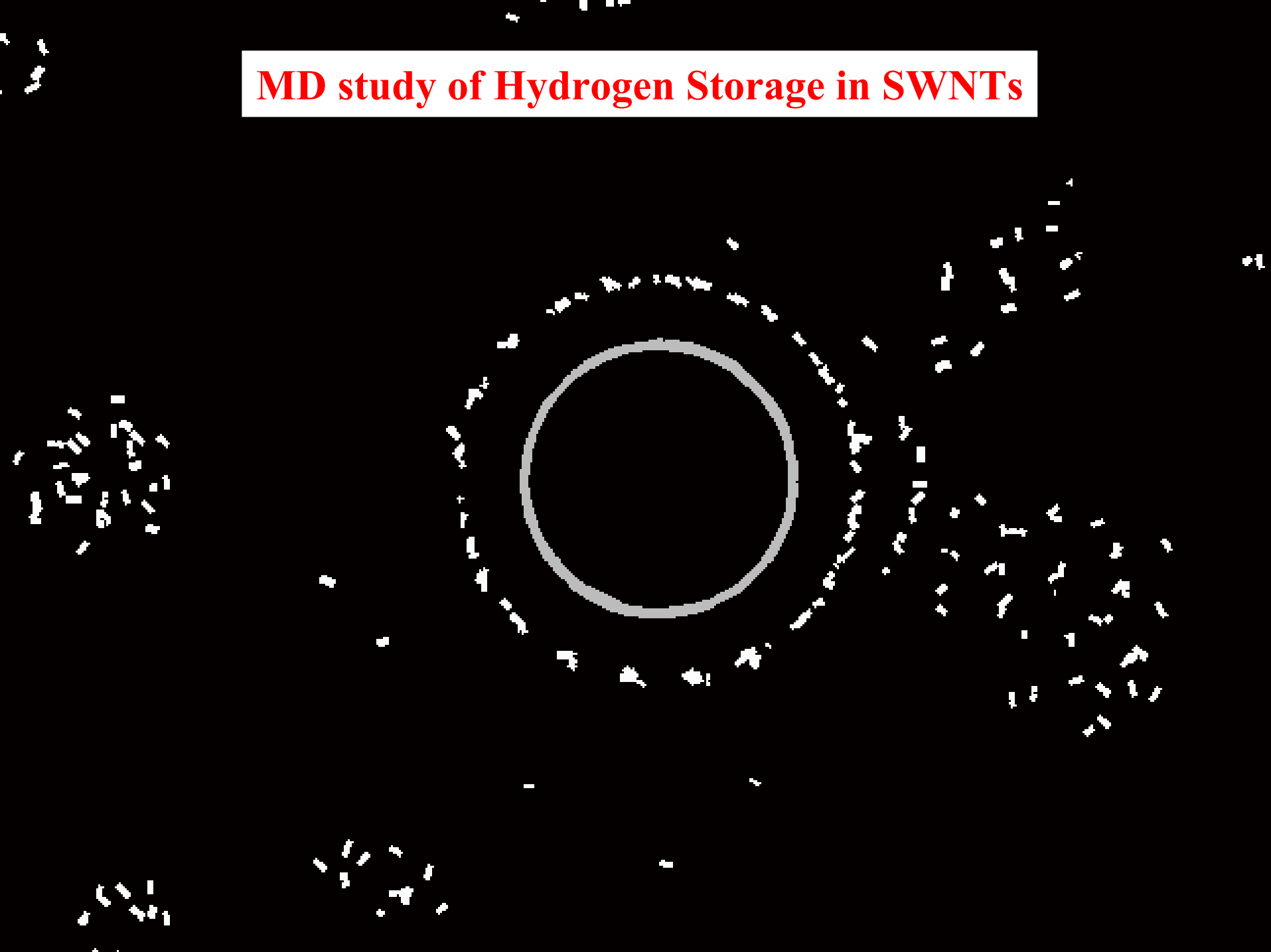
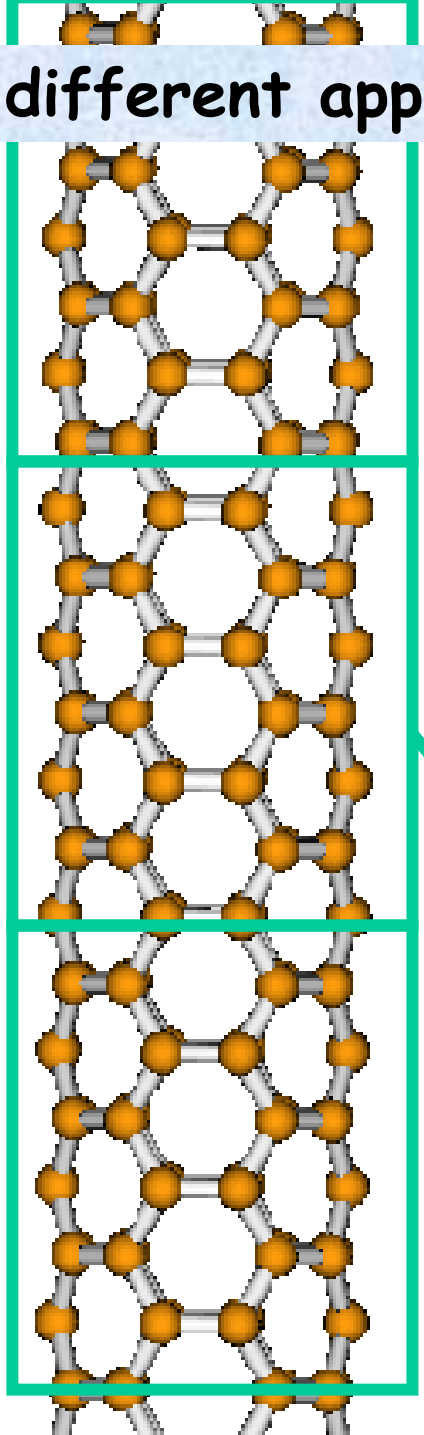
MD study of Hydrogen Storage in SWNTs

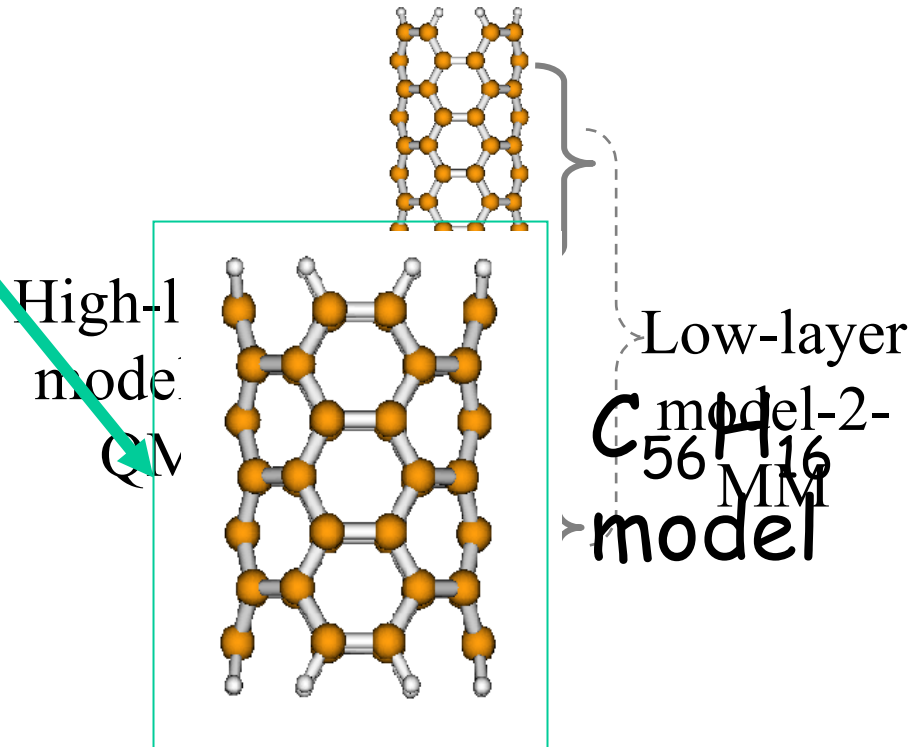


3 different approaches for *ab-initio* treatment

(4,4) SWNT

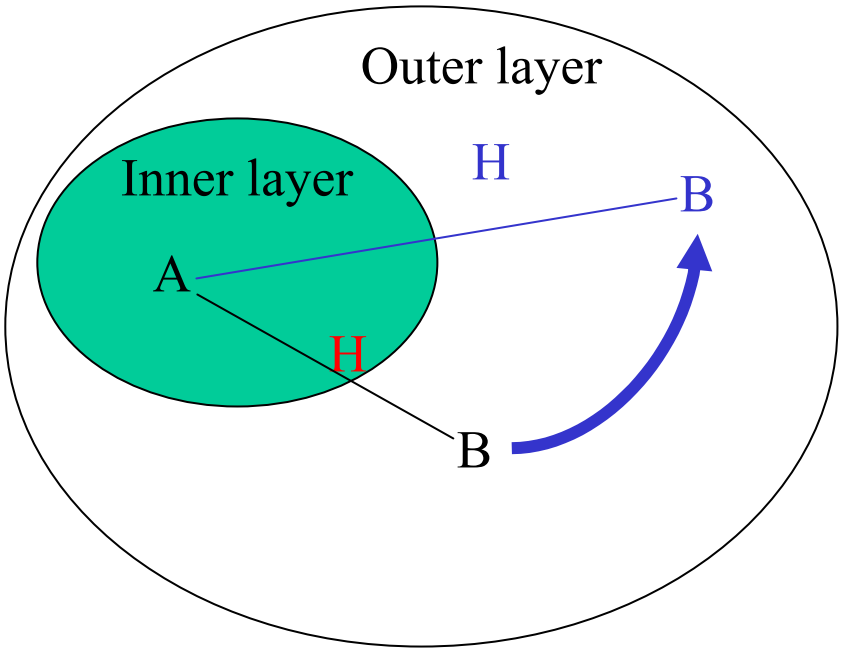


1. The *Cluster* model
2. Periodic DFT models
3. QM/MM mixed models

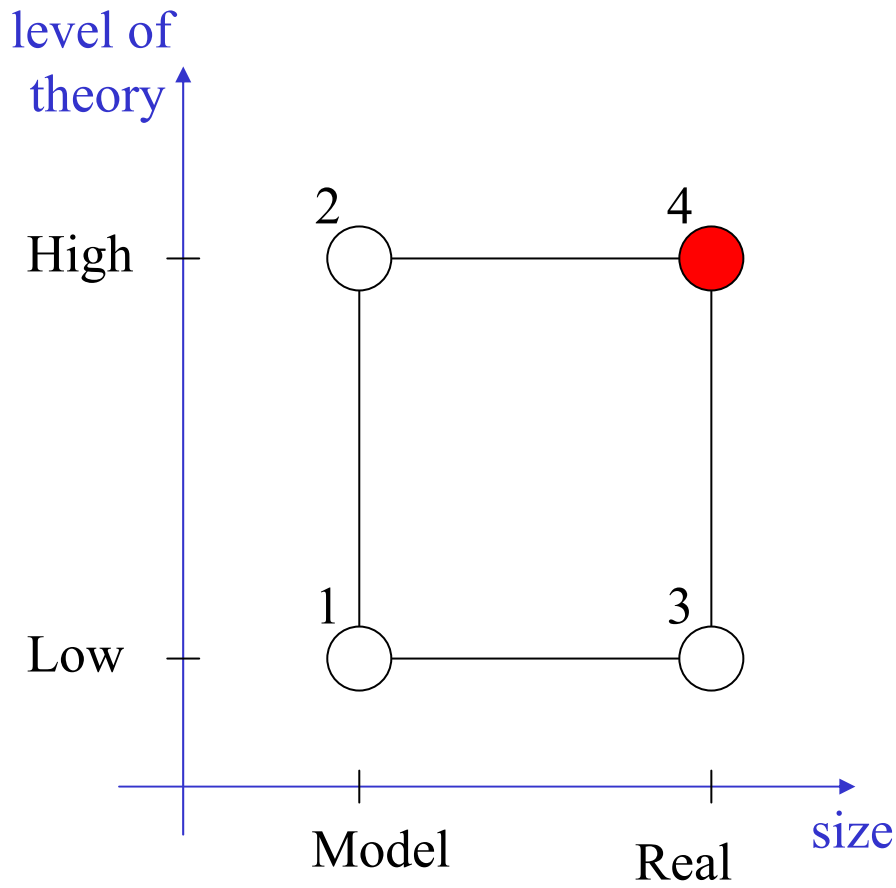


ONIOM

our **O**wn **N**-layer **I**ntegrated molecular **O**rbital and molecular **M**echanics model



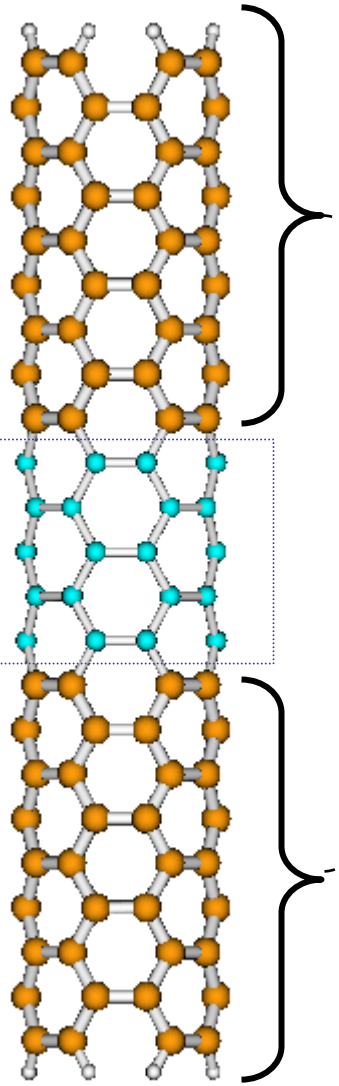
Model System = inner layer + link atoms
Real System = inner layer + outer layer



J. Molecular Structure 461 (1999) 1
Prof. K. Morokuma 65th birthday

$$E_{ONIOM} = E_3 - E_1 + E_2$$

(4,4) SWCN → $C_{200}= C_{40}+C_{144}+H_{16}$

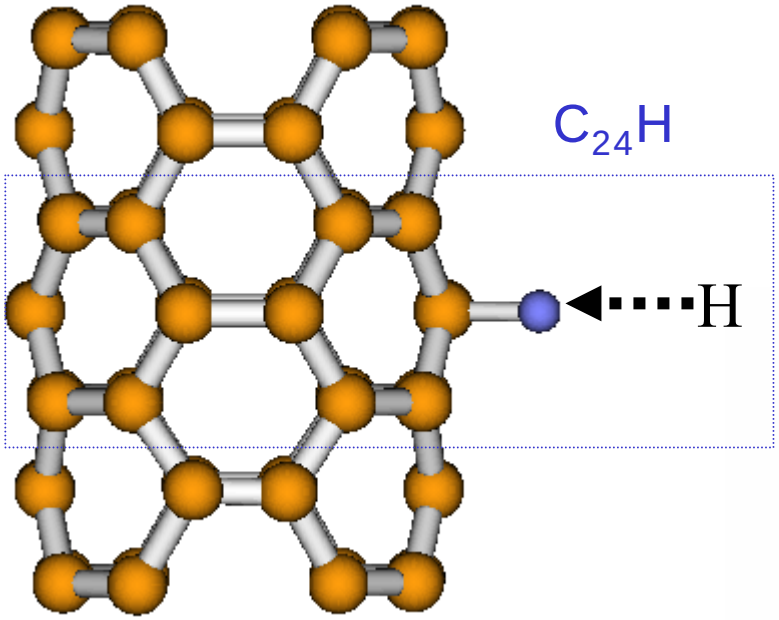


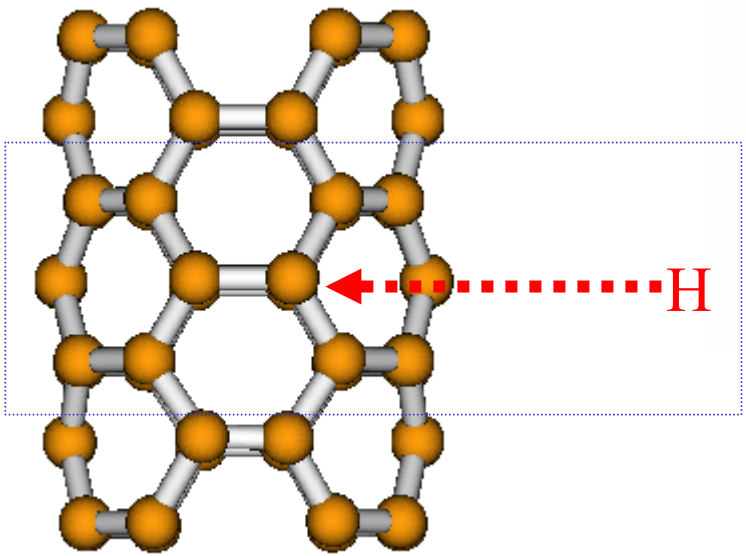
High-layer
model-1-
DFT
(B3LYP/6-31G*)

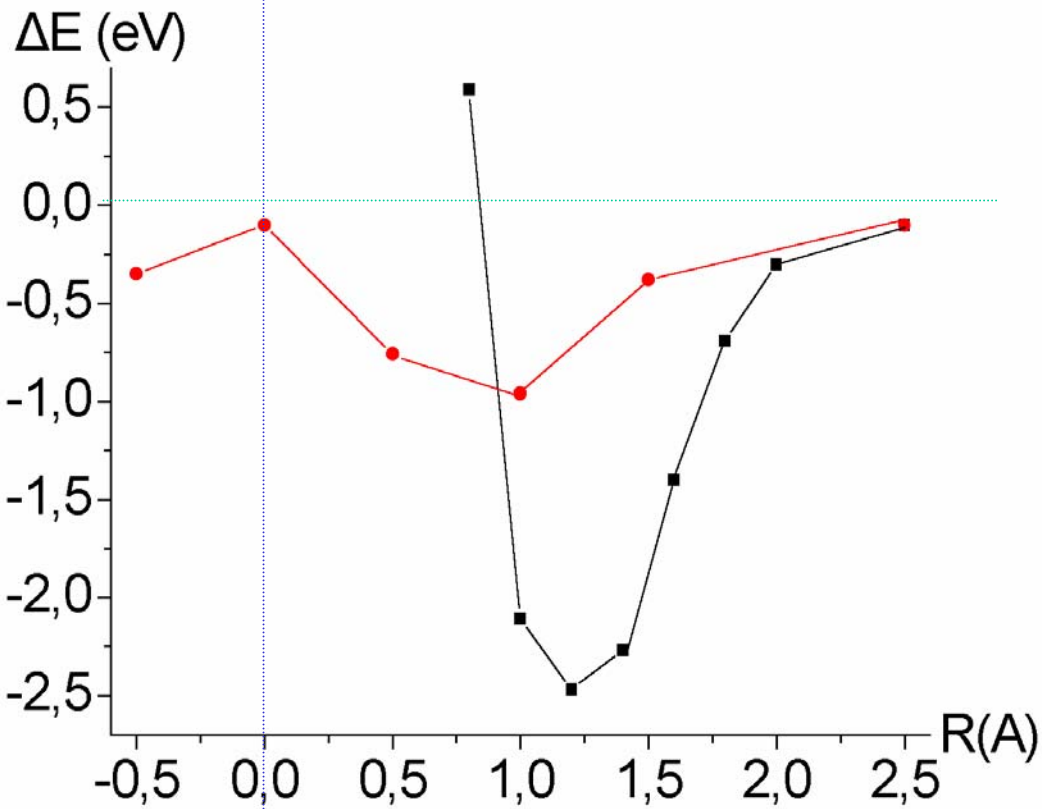
Low-layer
model-2-
UFF

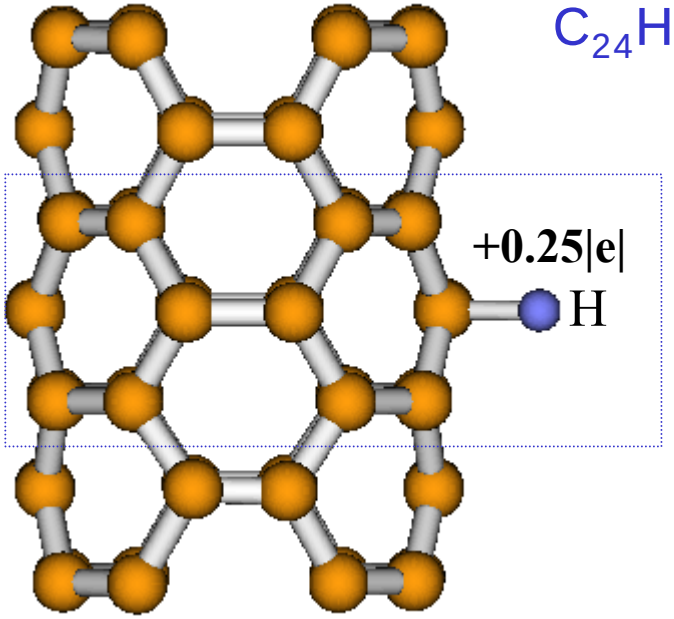
Gaussian '98

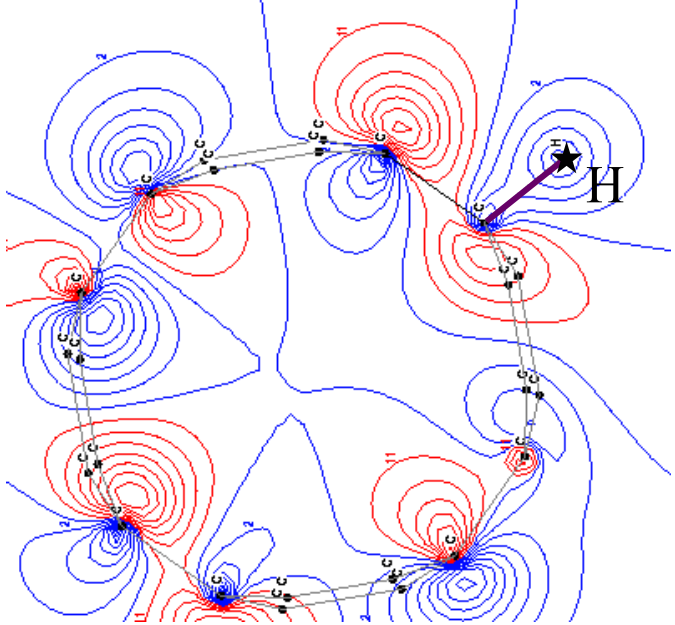
Hydrogen Interaction with SWNTs

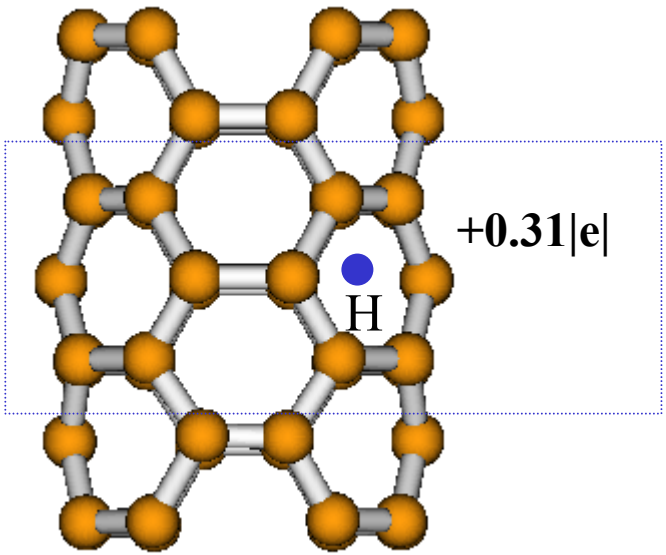


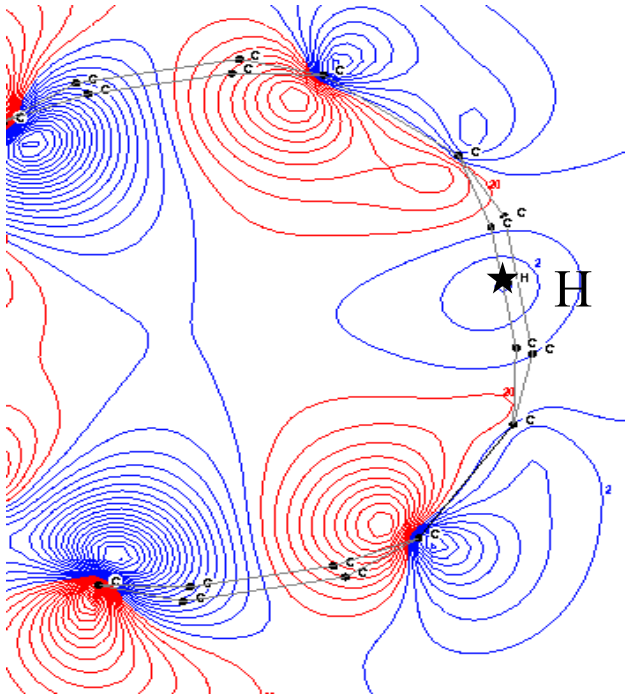


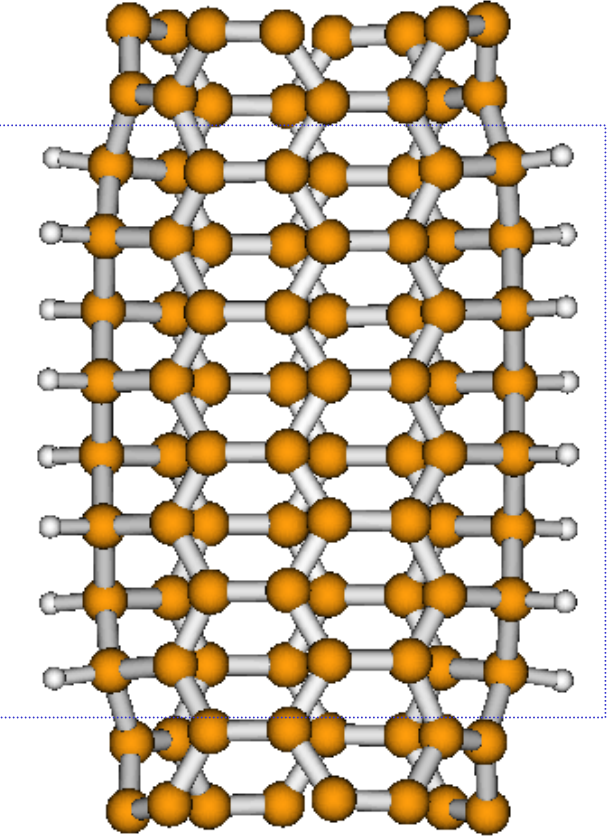



$C_{24}H$
+0.25|e|
H

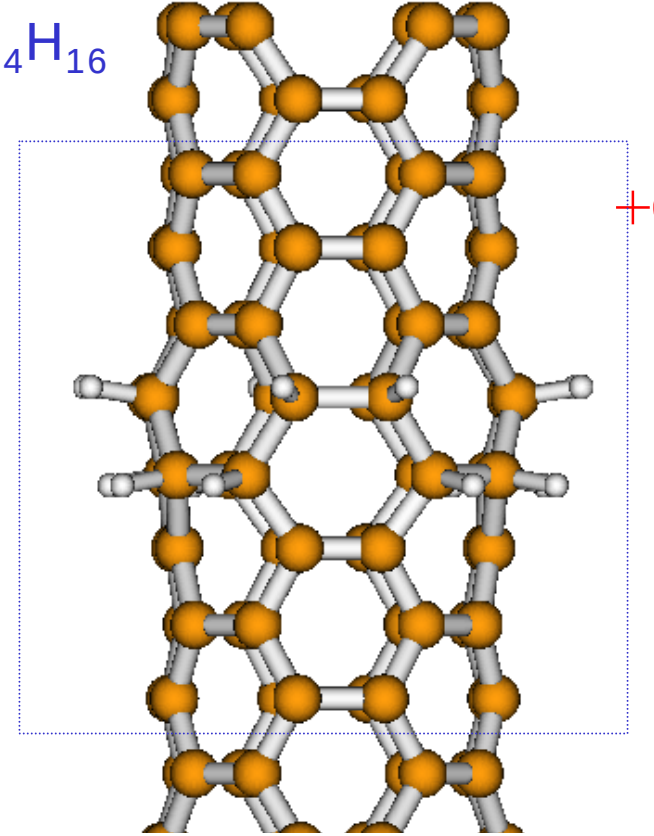

H


+0.31|e|
H

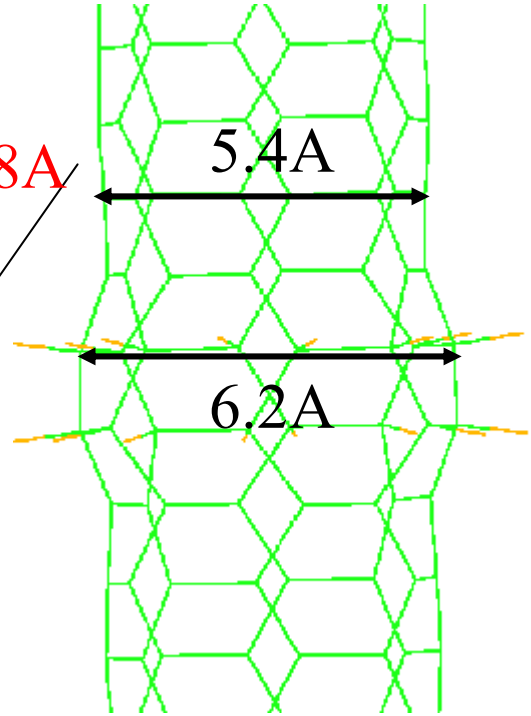

H

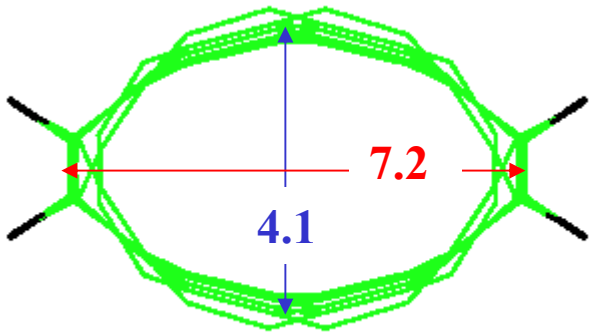


$C_{64}H_{16}$

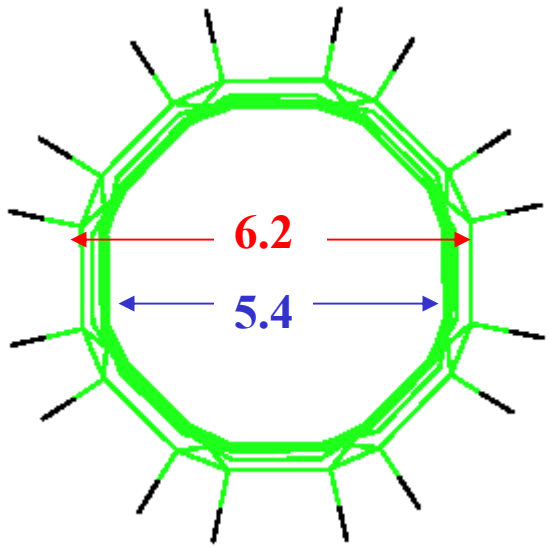


+0.8A





$T=92A^2$



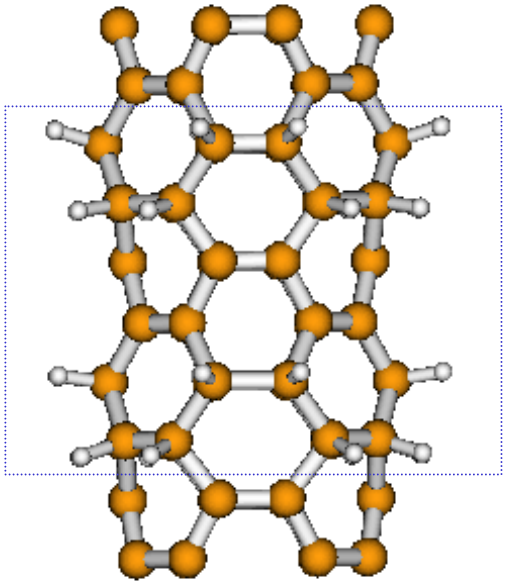
$\Delta E=2.6eV$

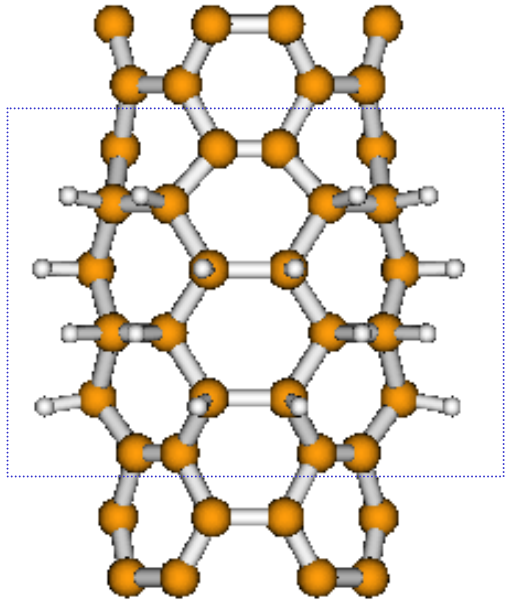
$T=92A^2$

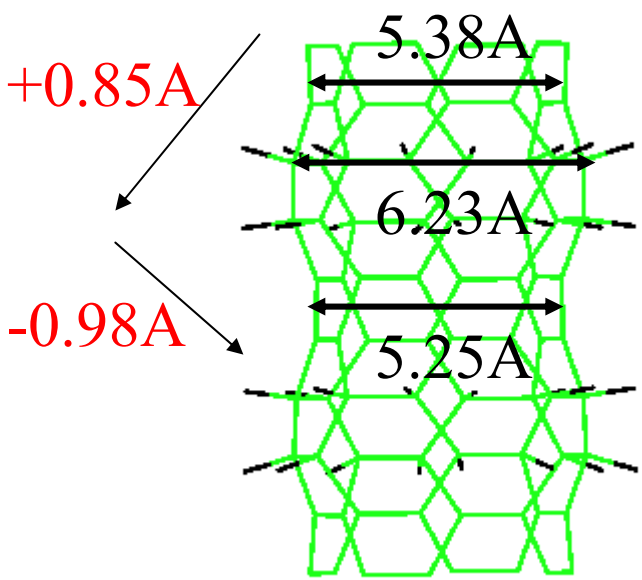
$T=121A^2$

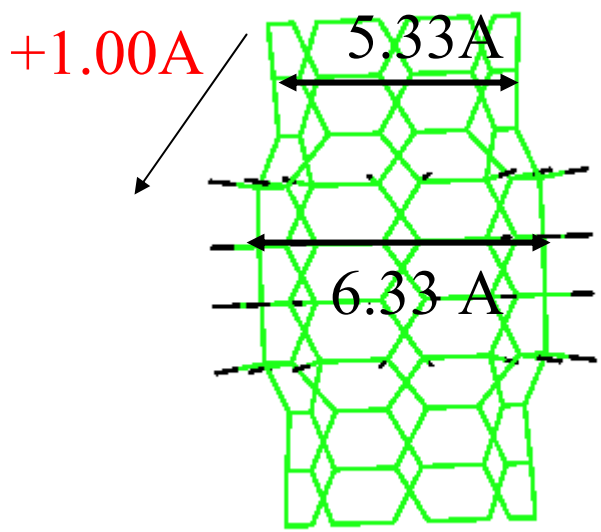
ΔE = 0.0 + 17eV

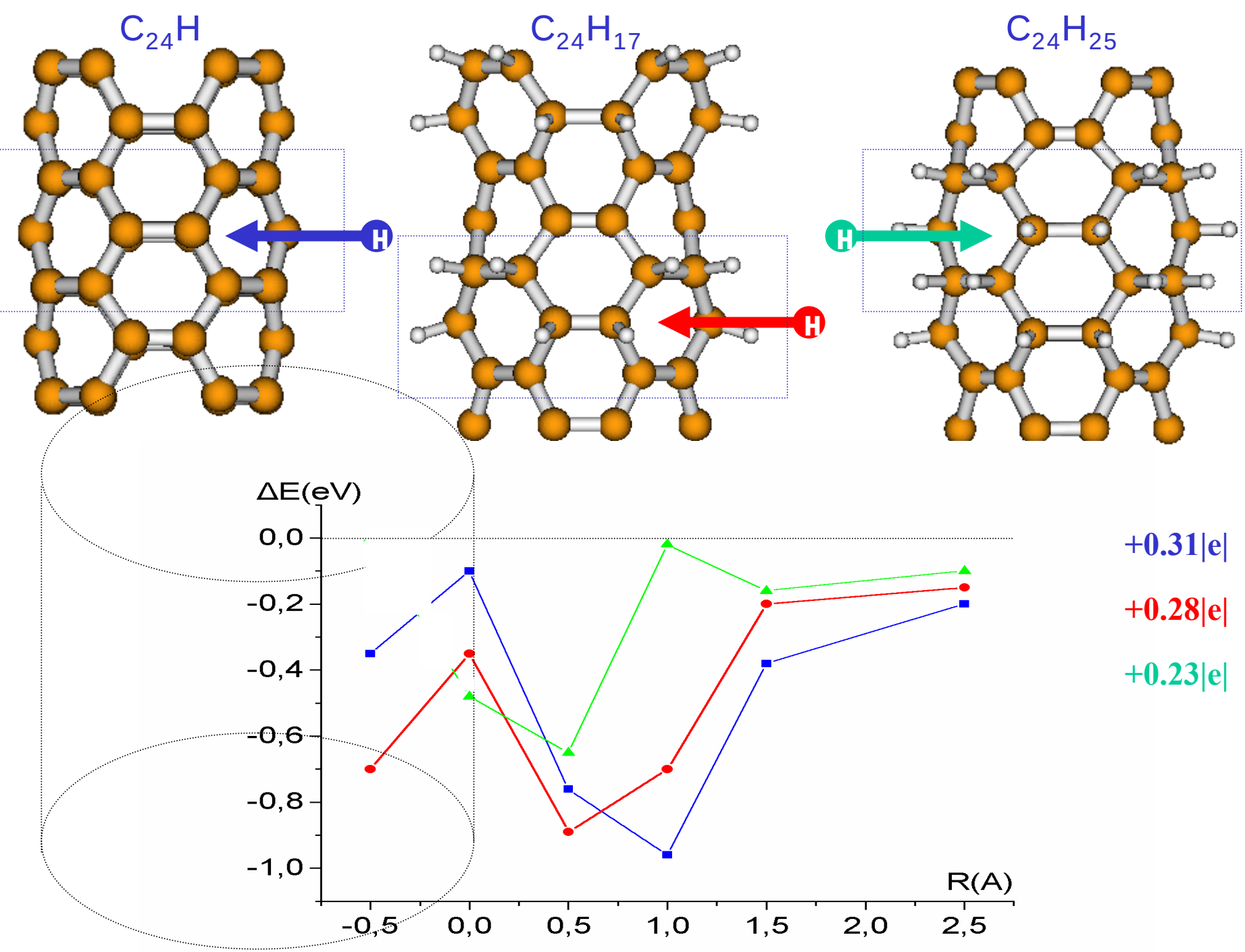
$C_{48}H_{32}$







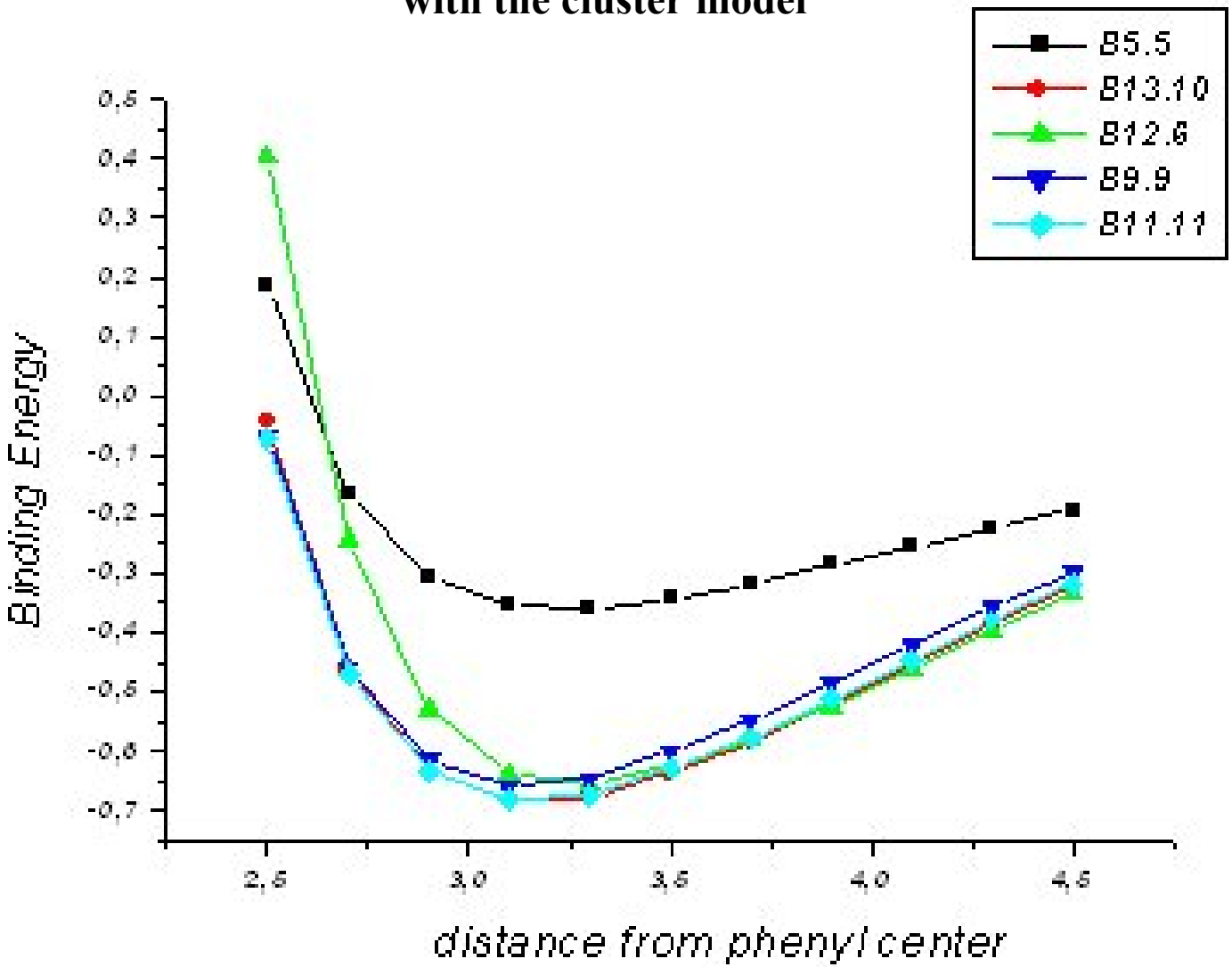



C24H
C24H17
C24H25
H
H
H
ΔE(eV)
0,0
-0,2
-0,4
-0,6
-0,8
-1,0
-0,5
0,0
0,5
1,0
1,5
2,0
2,5
R(A)
+0.31|e|
+0.28|e|
+0.23|e|

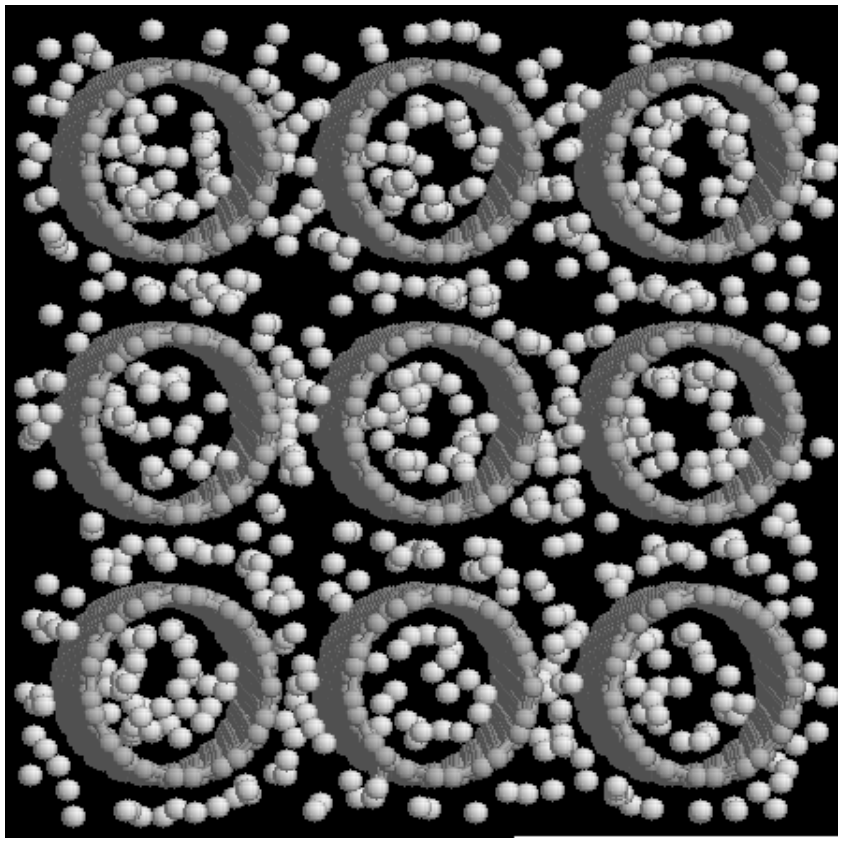
Curvature vs. Chirality in Hydrogen Interaction with SWNTs

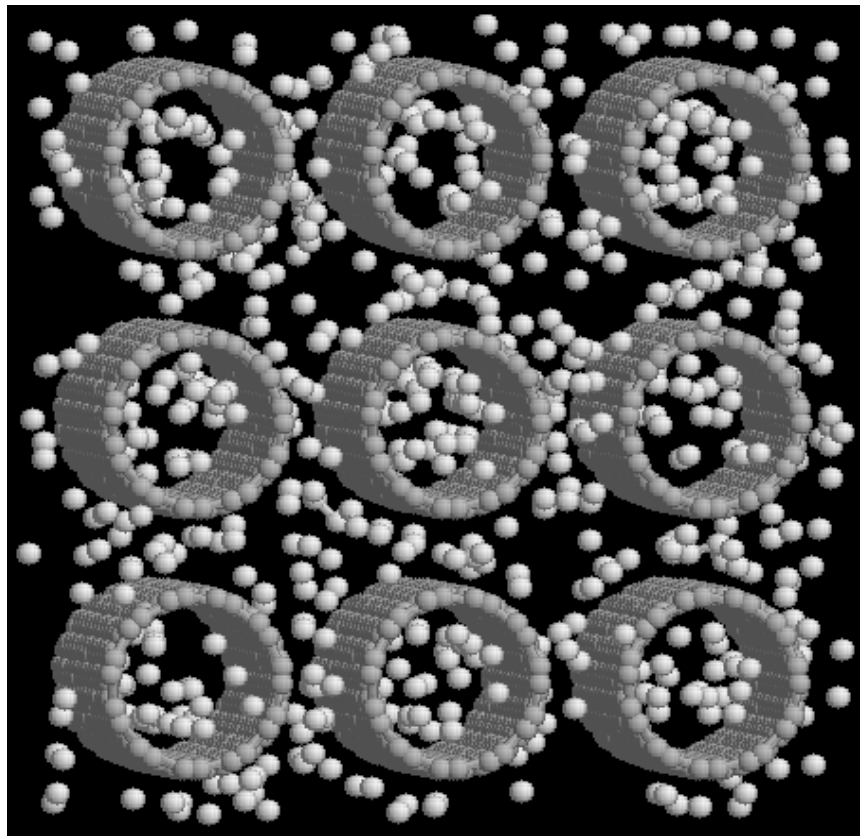
***Ab-initio* DFT calculations**

with the cluster model



GC-MC Snapshots of the simulation boxes
for the thermodynamic state of 175K and 5Mpa



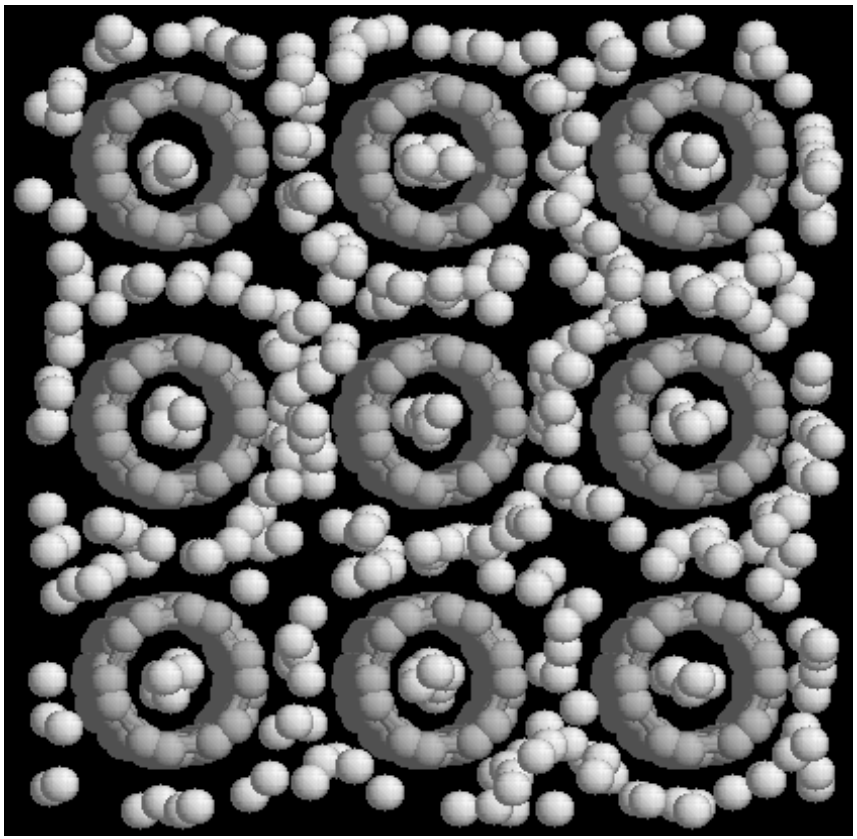


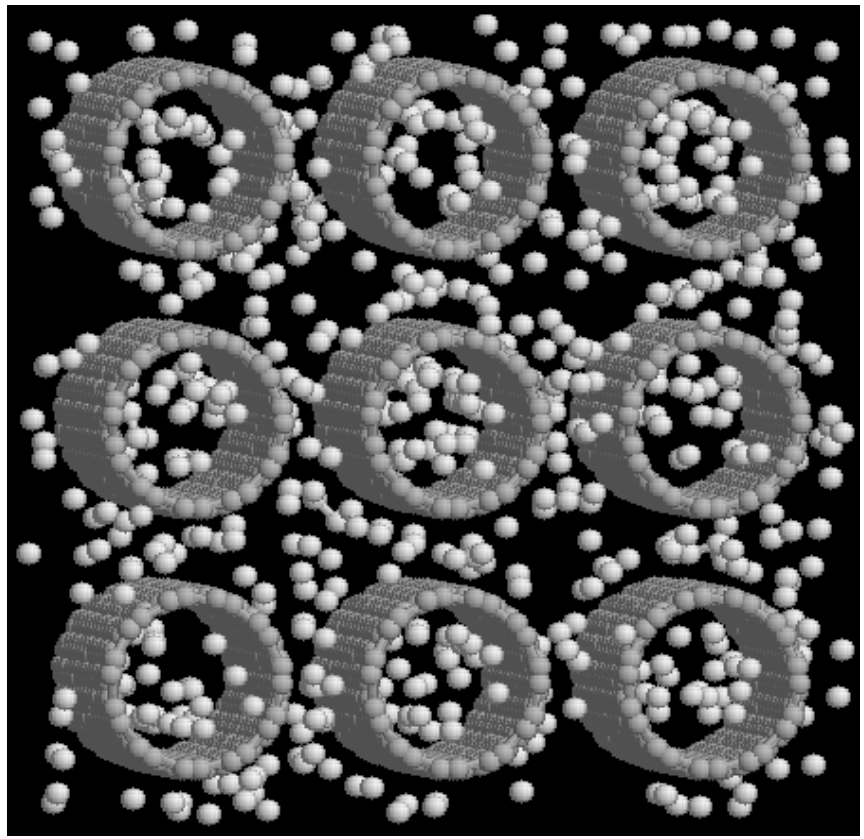
(13,10) SWCN
d=1.56nm
%wt = 1.90

chirality

(11,11) SWCN
d=1.55nm
%wt = 1.92

GC-MC Snapshots of the simulation boxes
for the thermodynamic state of 175K and 10Mpa



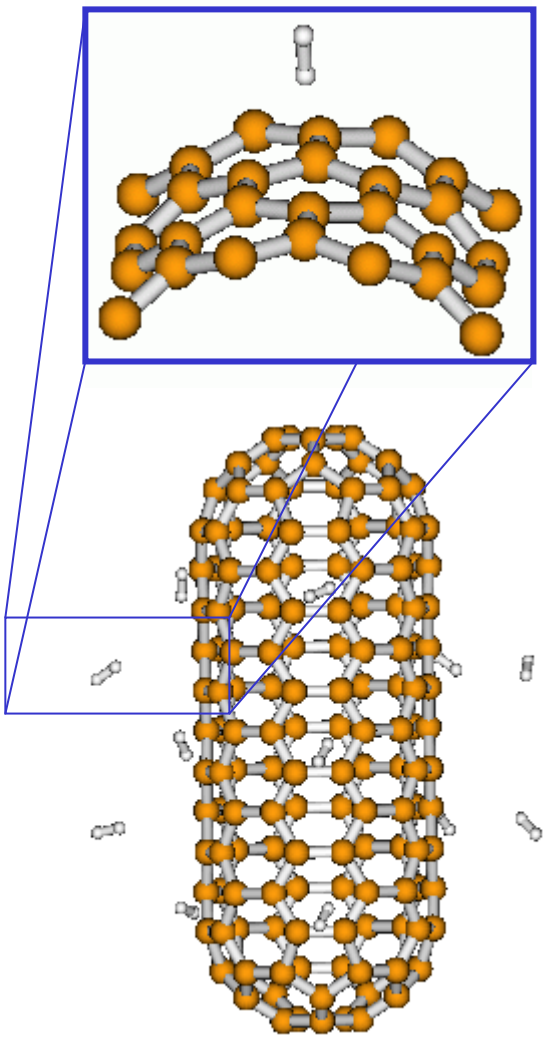


(6,6) SWCN
d=0.81nm
%wt = 2.20

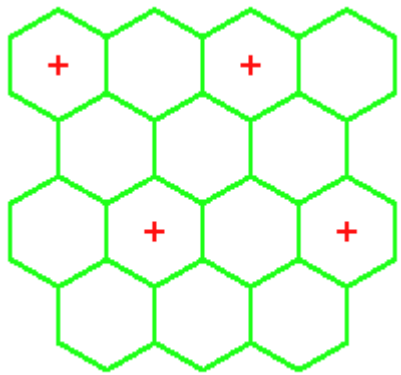
curvature

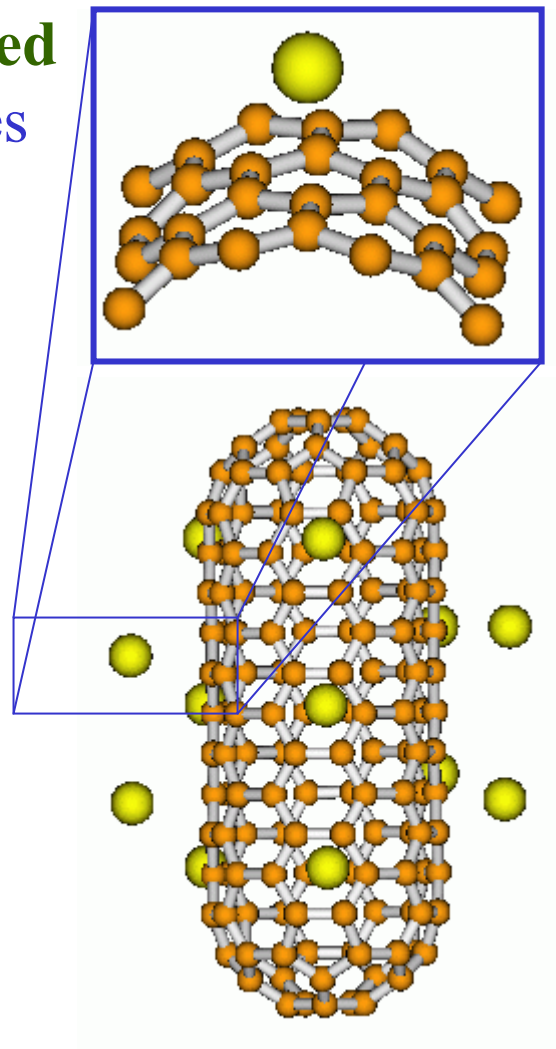
(11,11) SWCN
d=1.55nm
%wt = 3.03

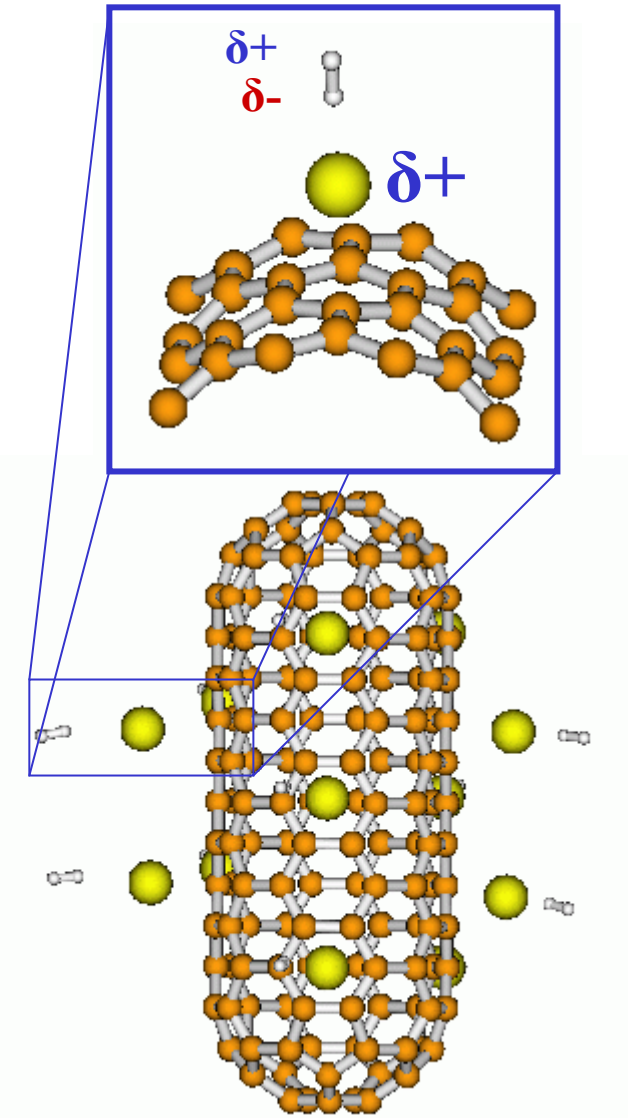
Hydrogen Interaction with doped SWNTs

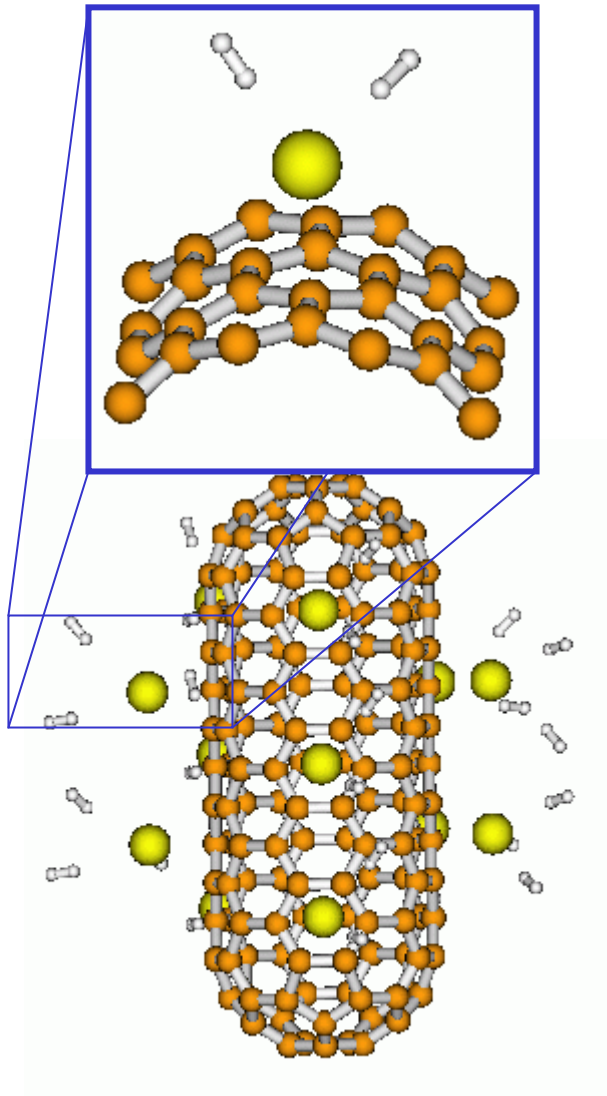


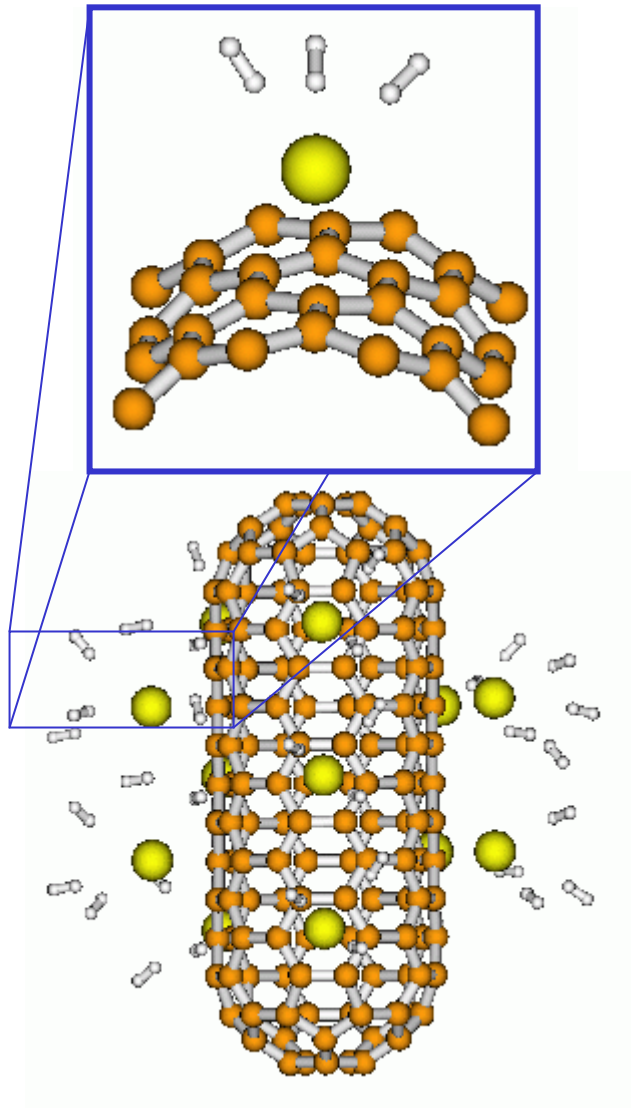
Alkali Metal Doped
Carbon Nanotubes



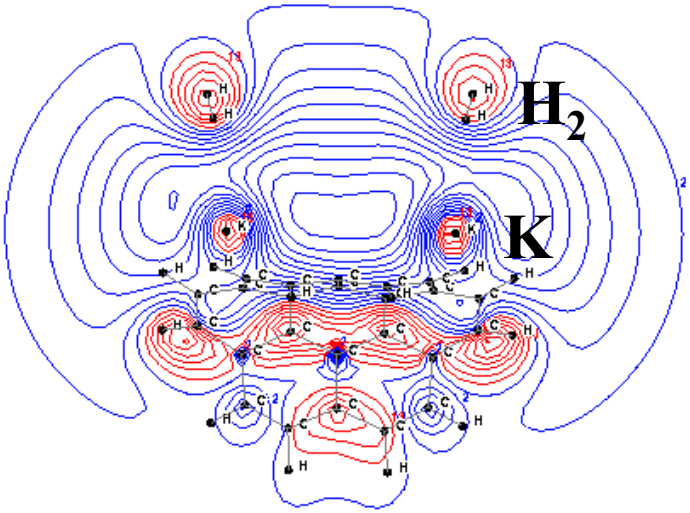


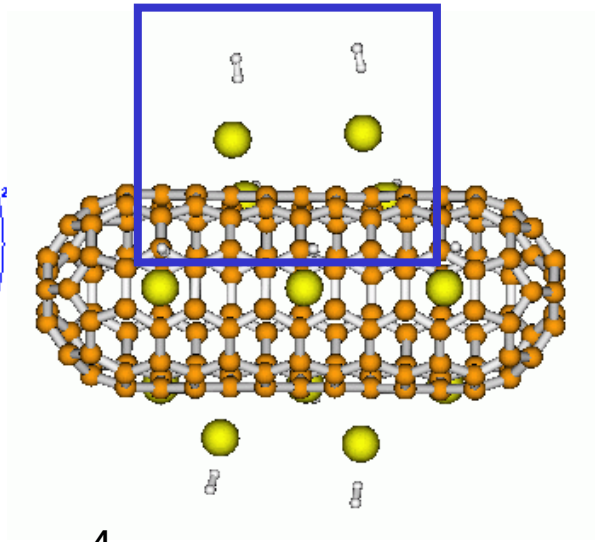






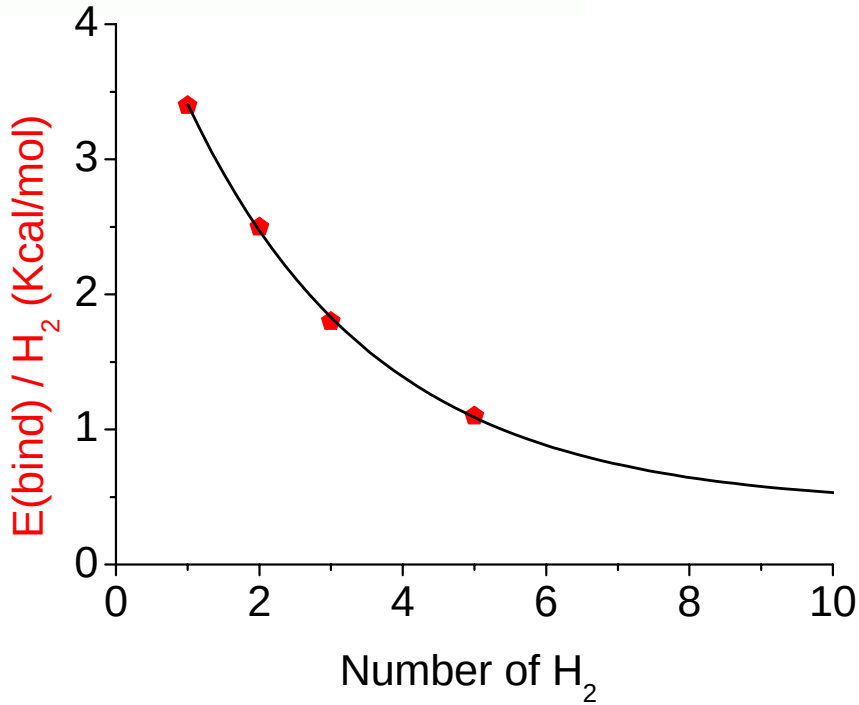
DFT= 3.4 kcal/mol/H_2 2.5 kcal/mol/H_2 1.8 kcal/mol/H_2

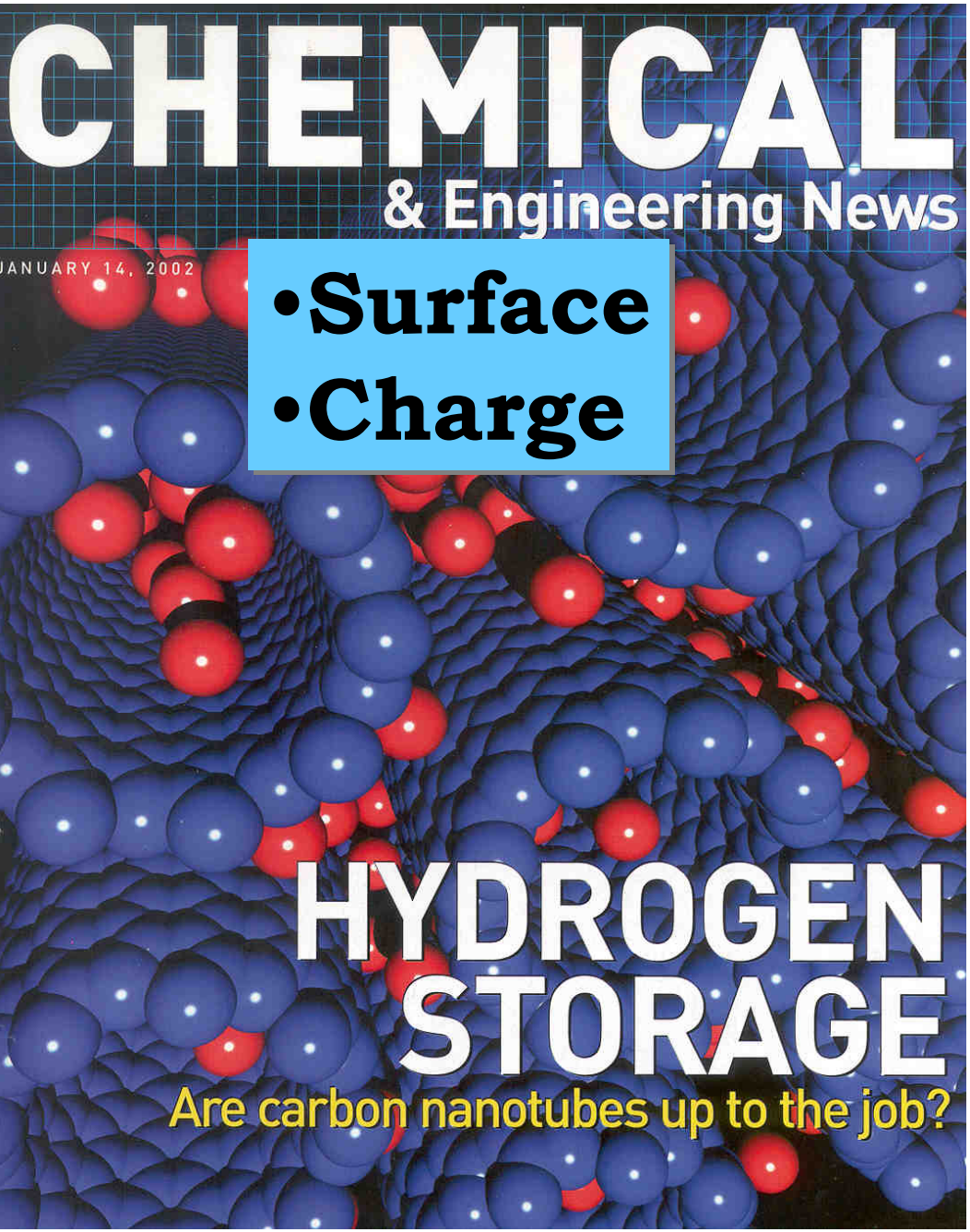




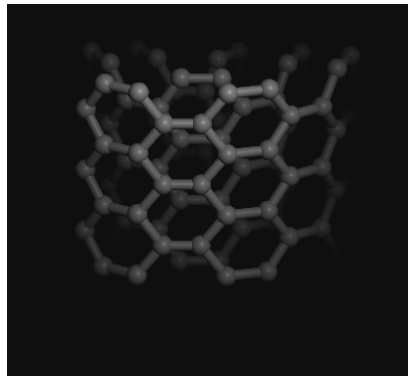
Energetic and structural characteristics for all the different cases of molecular hydrogen adsorption in K-doped (5,5)-carbon nanotube (DFT).

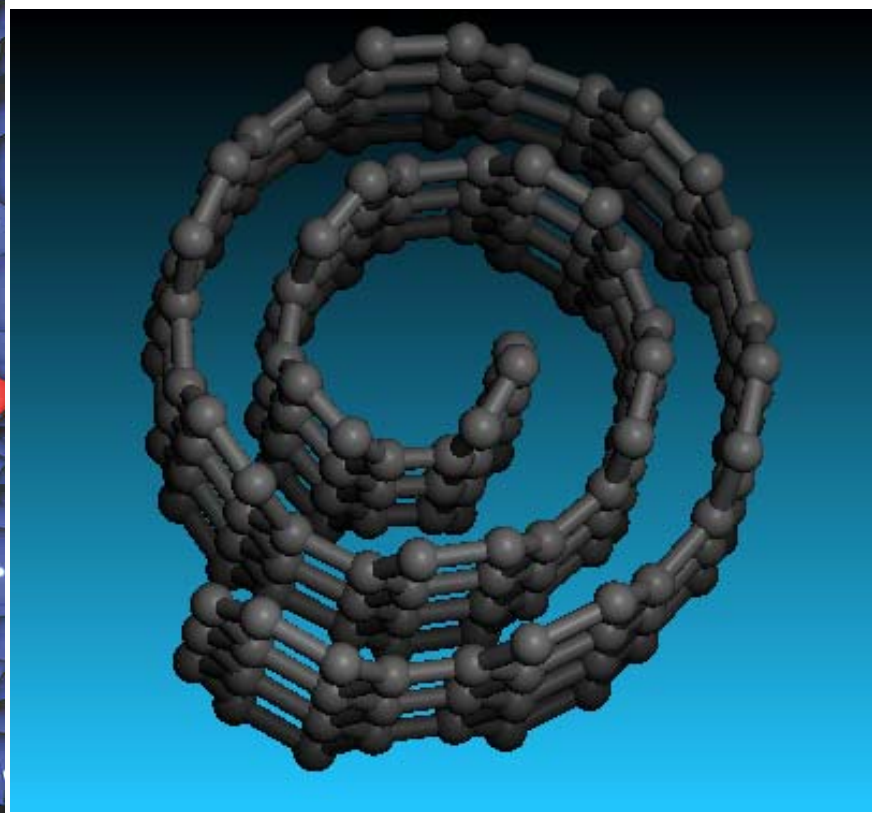
Number of H_2	E_{bind}/H_2 (kcal/mol)	d [K-C_{hex}] (Å)	d [K-H_2] (Å)
1	3.4	3.0	3.0
2	2.5	3.0	3.3
3	1.8	3.0	3.5
5	1.1	3.0	3.8

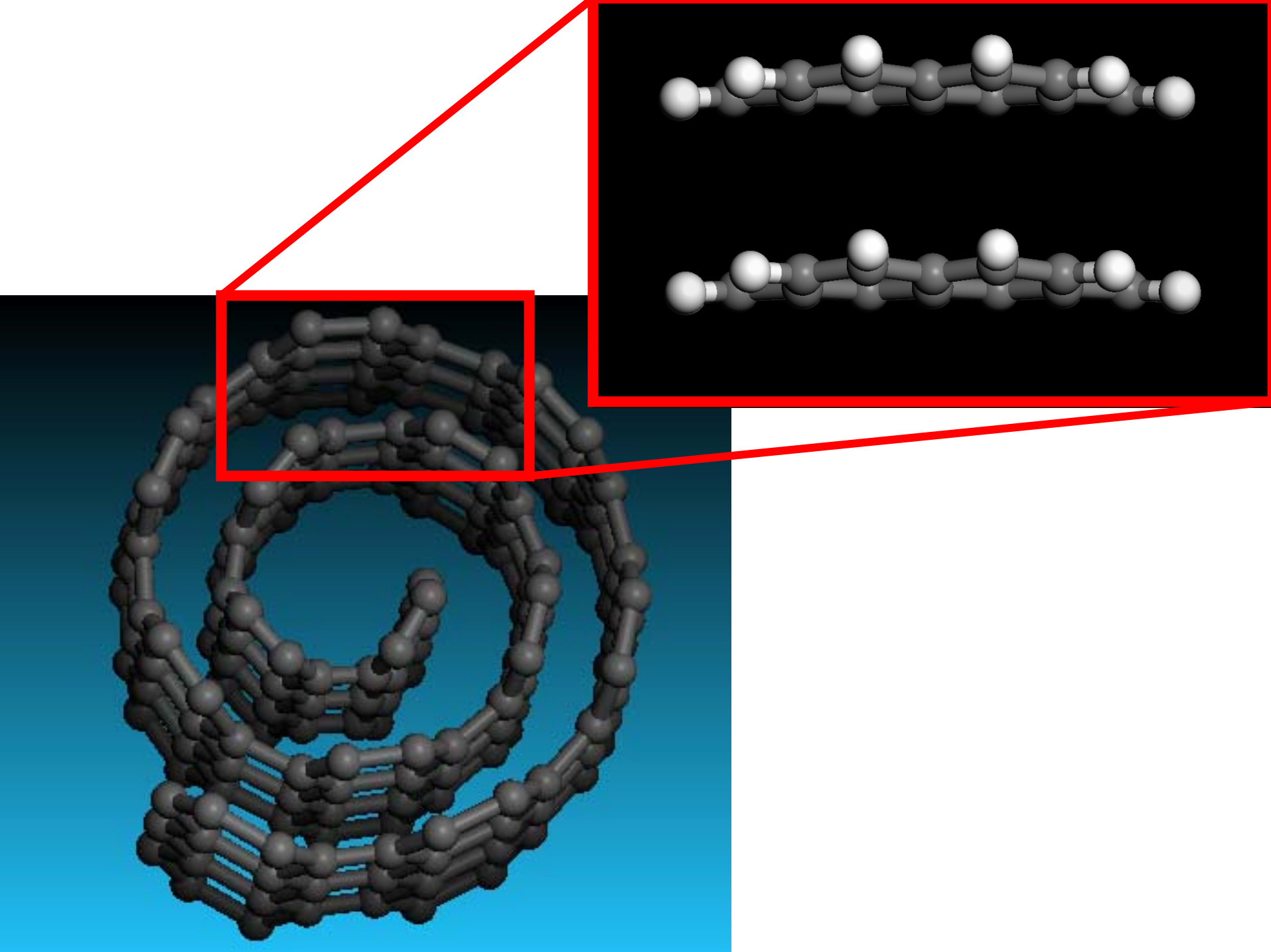


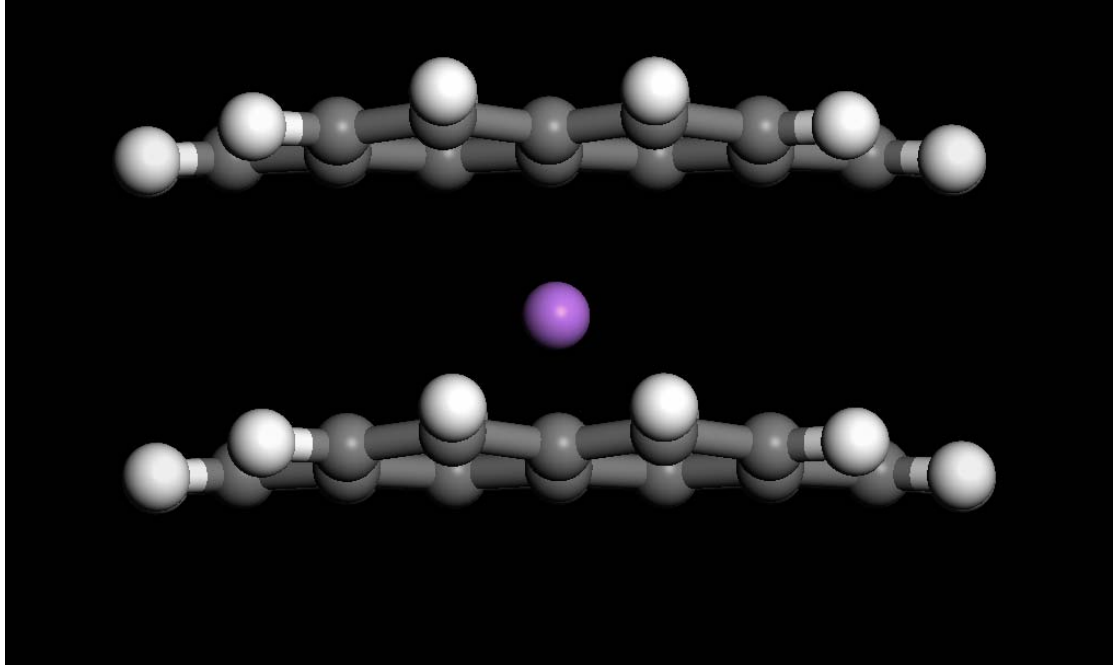


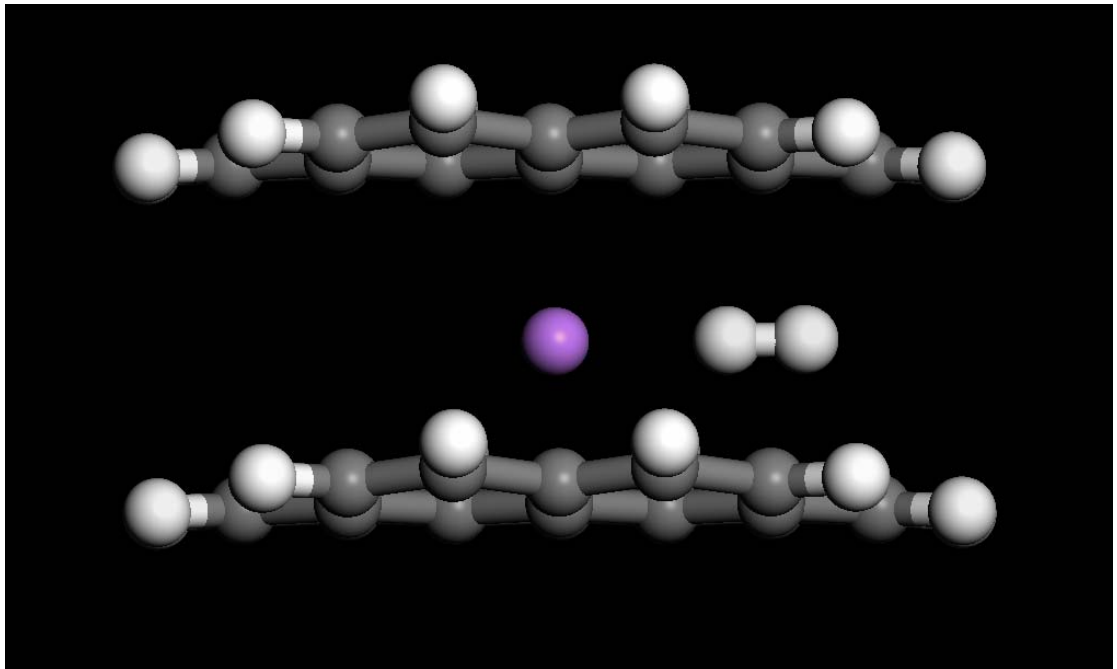
Nano-scrolls











Further reading:

- *Extreme hydrogen sensitivity of the transport properties of Single Wall Carbon Nanotubes,*
  A.Andriotis, M.Menon, D.Srivastava, G.Froudakis, **Physical Review B 64 (2001) 193401.**

- *Hydrogen Interaction with Single Wall Carbon Nanotubes. A Combined QM/MM study,*
  G. E. Froudakis, **Nano Letters 1 (2001) 179.**

- *Why alkali doped Carbon Nanotubes poses high hydrogen uptake,*
  G. E. Froudakis, **Nano Letters 1 (2001) 531.**

- *Hydrogen Interaction with Carbon Nanotubes. A Review of ab-initio studies,*
  G. E. Froudakis, **Journal of Physics – Condensed Matter 14 (2002) 453.**

- *Hydrogen and Oxygen Interaction with Carbon Nanotubes,*
  G. E. Froudakis, **Encyclopedia of Nanoscience and Nanotechnology (2003).**