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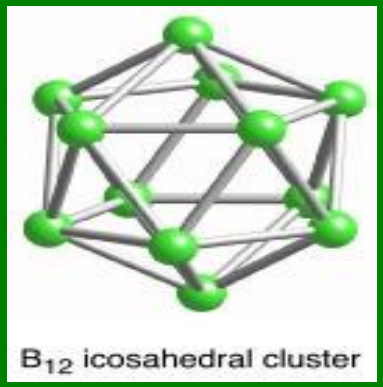
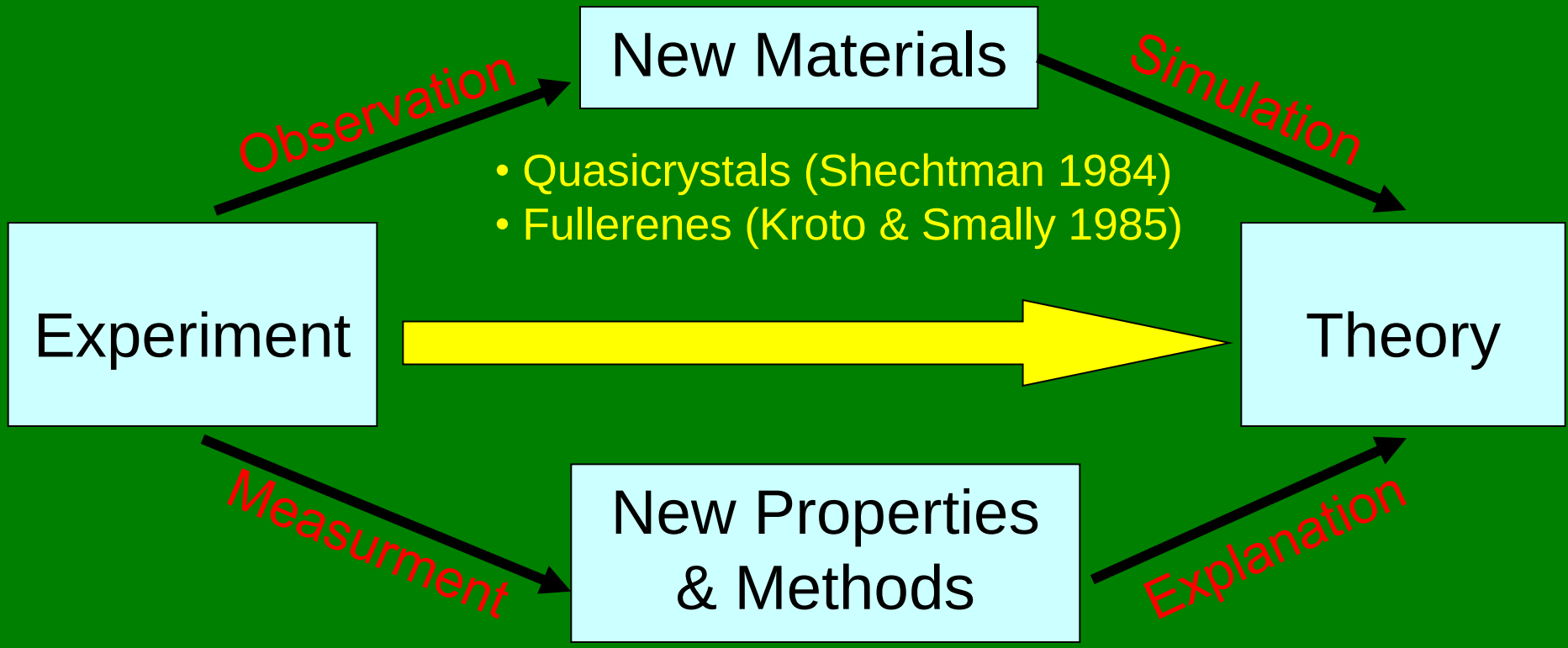
Bergische Universität Wuppertal, Germany

Towards Novel Boron Nanostructured Materials: Theoretical Predictions and Experimental Confirmations.

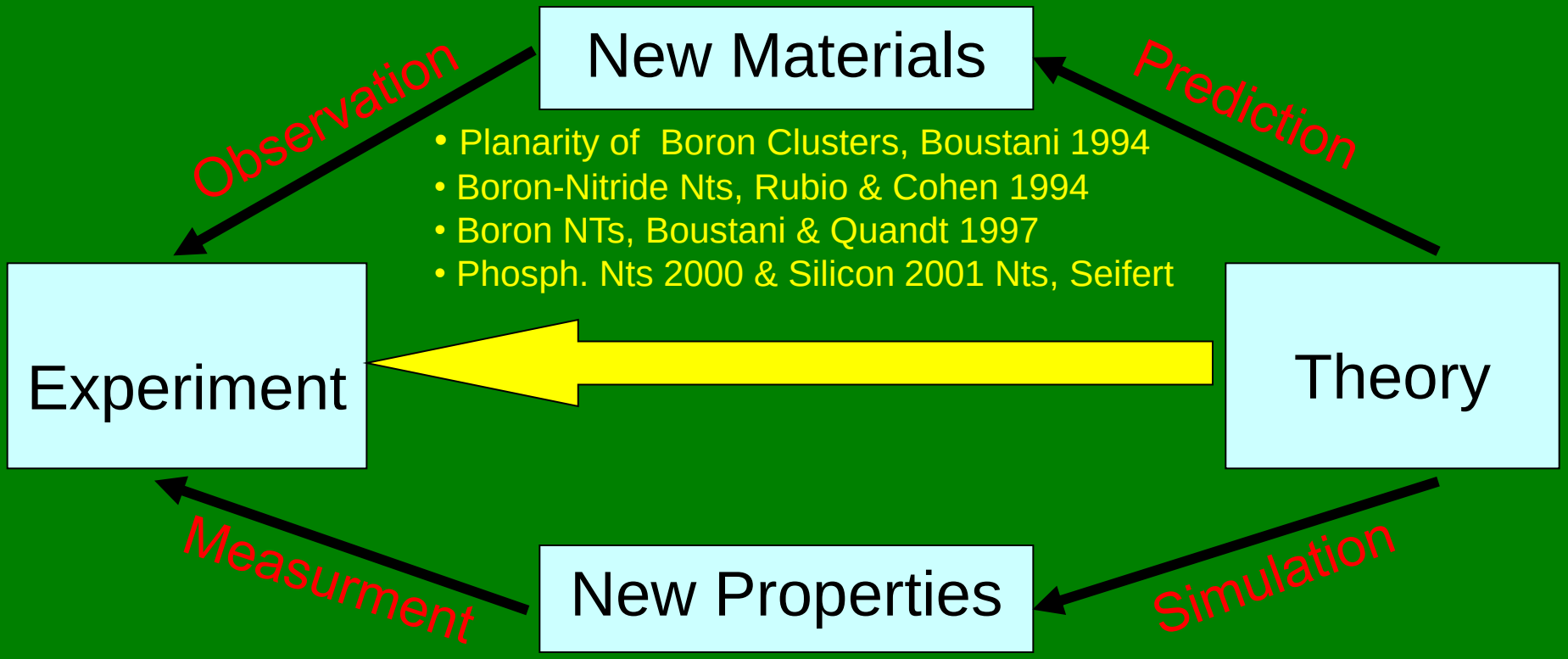


Technische Universität Dresden
Chair Material Science and Nanotechnolgy
April 30, 2009

Conventional Approach



Opposite Approach



Survey of the Talk

- **Outlines**
  - Why Boron
  - Solıd Boron
  - Boron Clusters
- **Novel Boron**
  - Clusters & Cages
  - Sheets & Nanotubes
  - Nanoribbons
- **Theoretical Methods**
  - Basic Concepts
  - Ab Initio Methods
  - Geometry Optimization
- **Applications**
  - Nanotechnology
  - Space Industry
  - Medicine

Motivations

- Mass Spectra of Boron Clusters:

Geometrical Structures | Electronic Properties

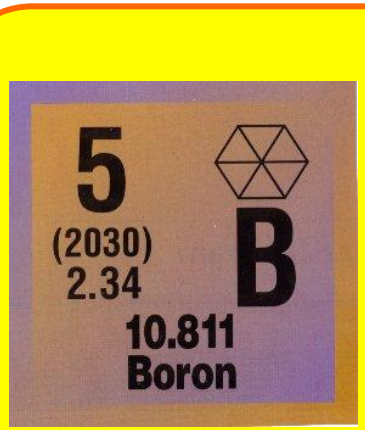
- Search for New Materials with definite properties:

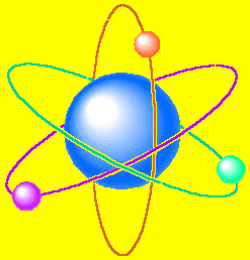
Superlight | Superhardness | High Temperature

Anti-Corrosion | Manufacturable | (Semi) Conductive

- Computationally Applicable

Lightweight Atoms | at Nanoscale Sizes

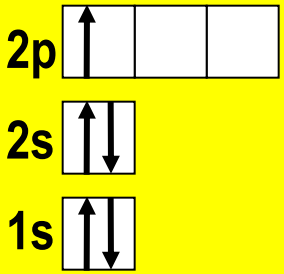




$1s^2 2s^2 2p^1$

Atomic properties

- Electron deficient
- Short covalent radius
- More Orbitals than Valence Electrons



Special properties

- High melting point
- Thermal conductive
- Semi-, Superconductor
- Hardness close to Diamond

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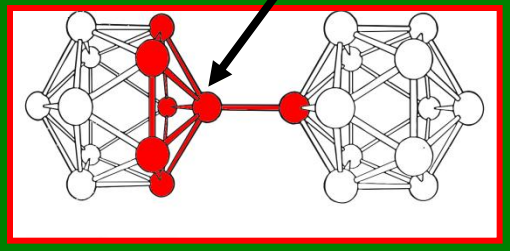
Crystalline Rhombohedral α-Boron

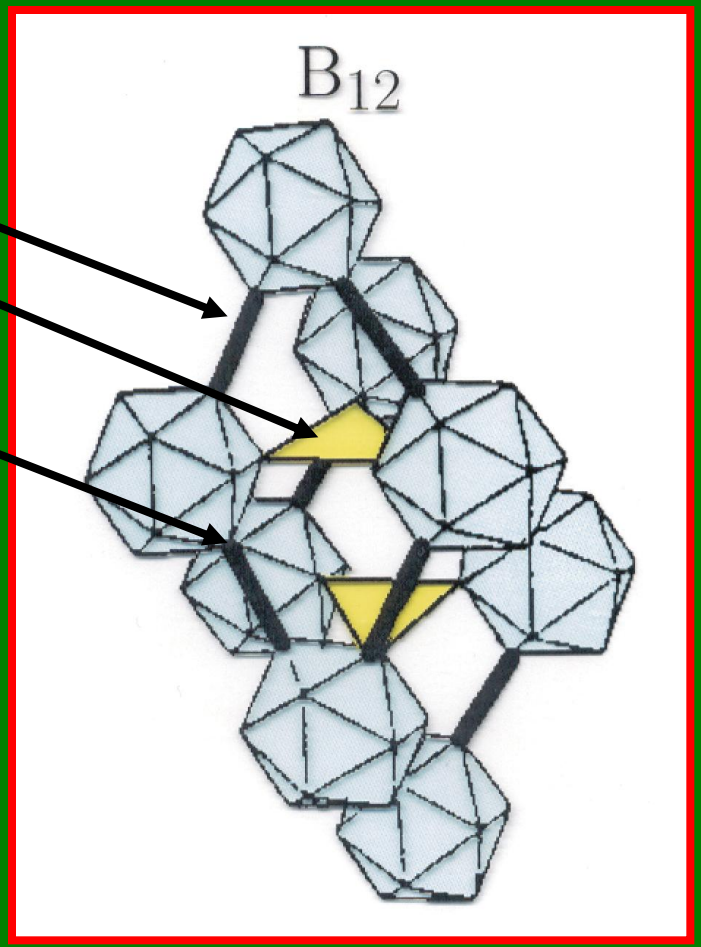
2-center bonds

3-center bonds

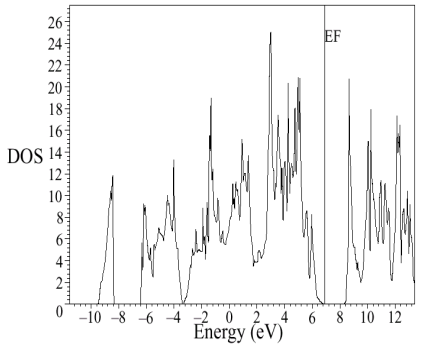
multi-center bonds



Inverse umbrella
bonding (along edges of unit cell)



Density of States:
Semiconductor with
Bandgap of 1.57 **eV**



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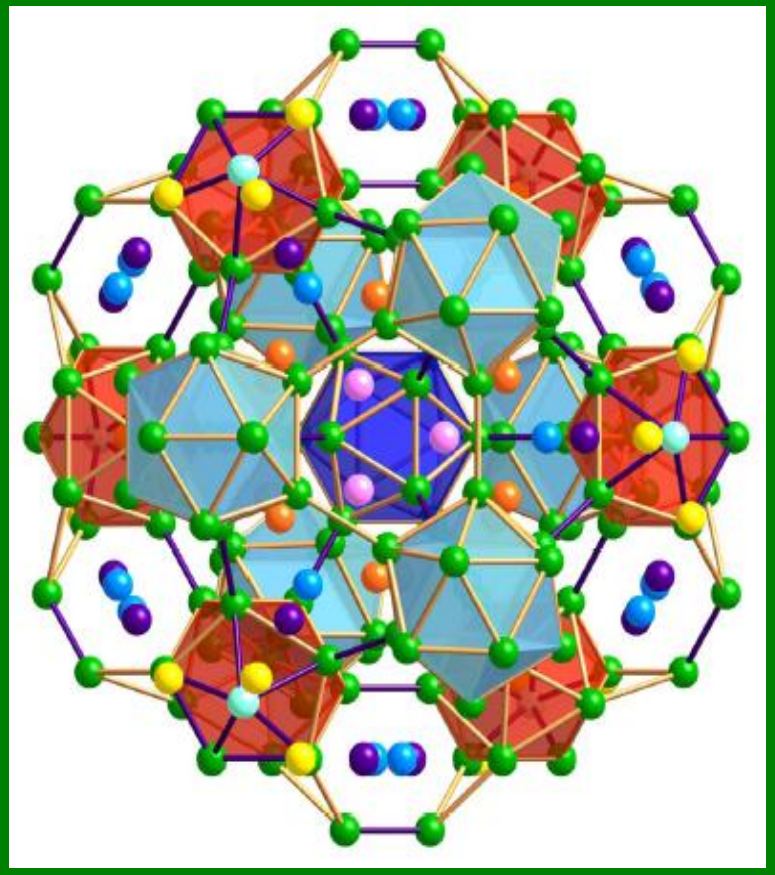
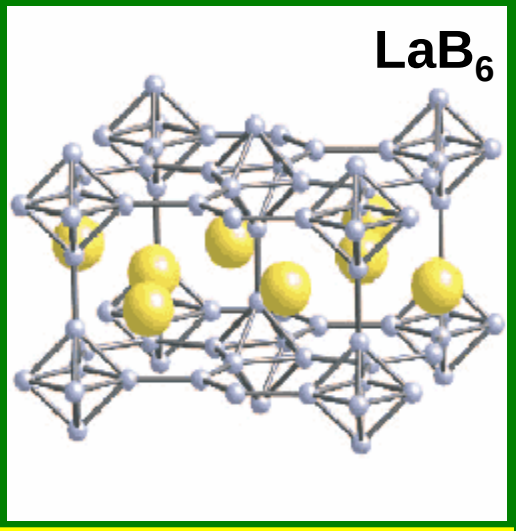
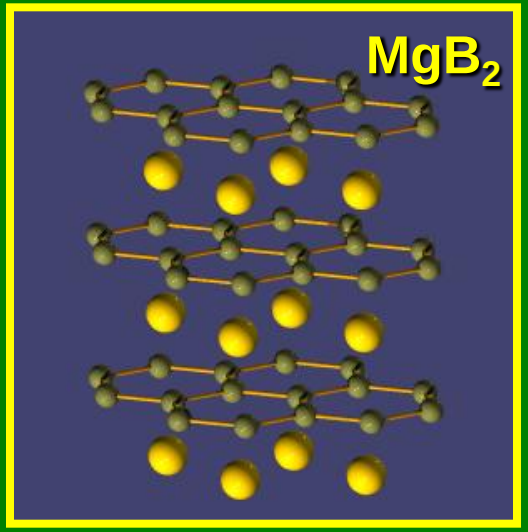
Crystalline β-Boron
Widom et al., PRB 77, 064113 (2008)



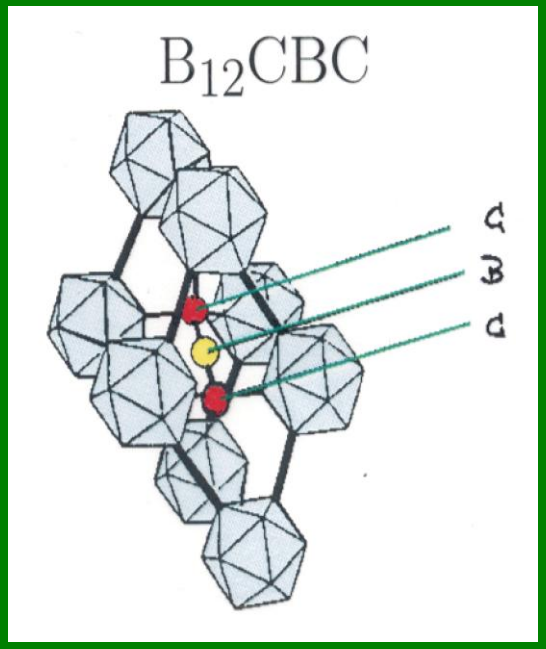
β-Boron viewed along the rhombohedral 111 axis

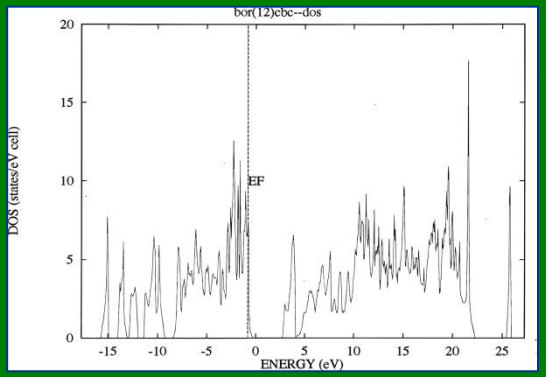
Metal-Hexaborides & Diboredes





Doped α-Boron,
Bylander & Kleinman PRB 43, 1487 (1991)





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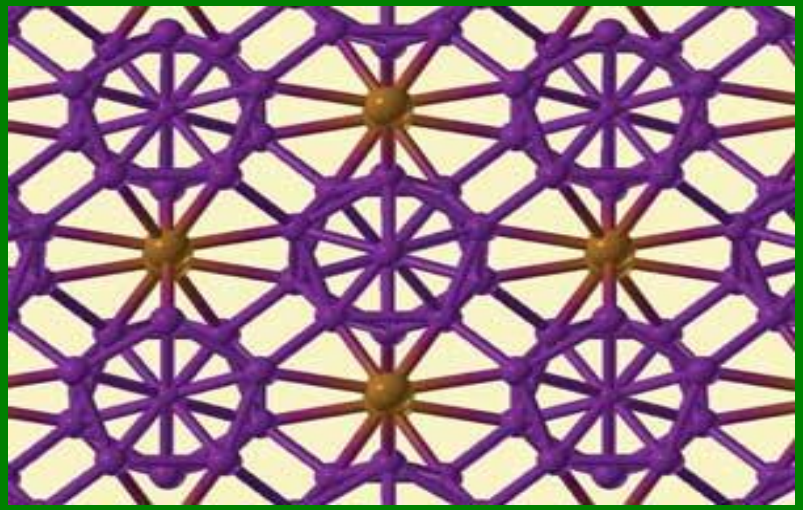
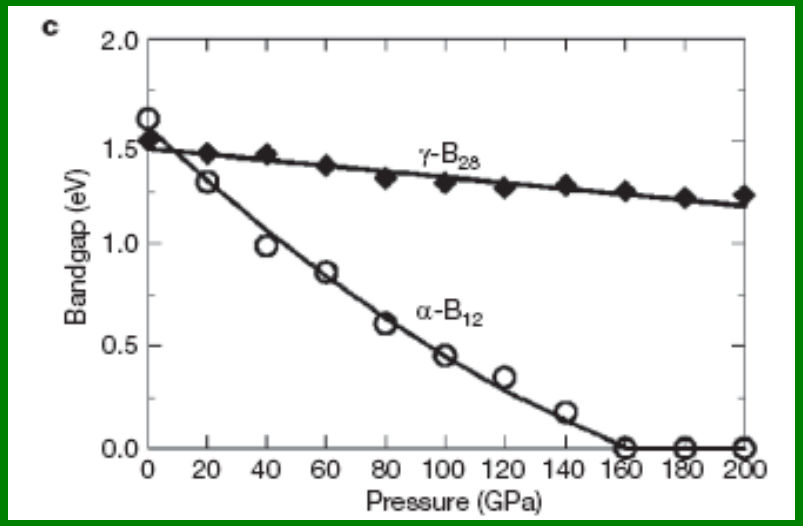
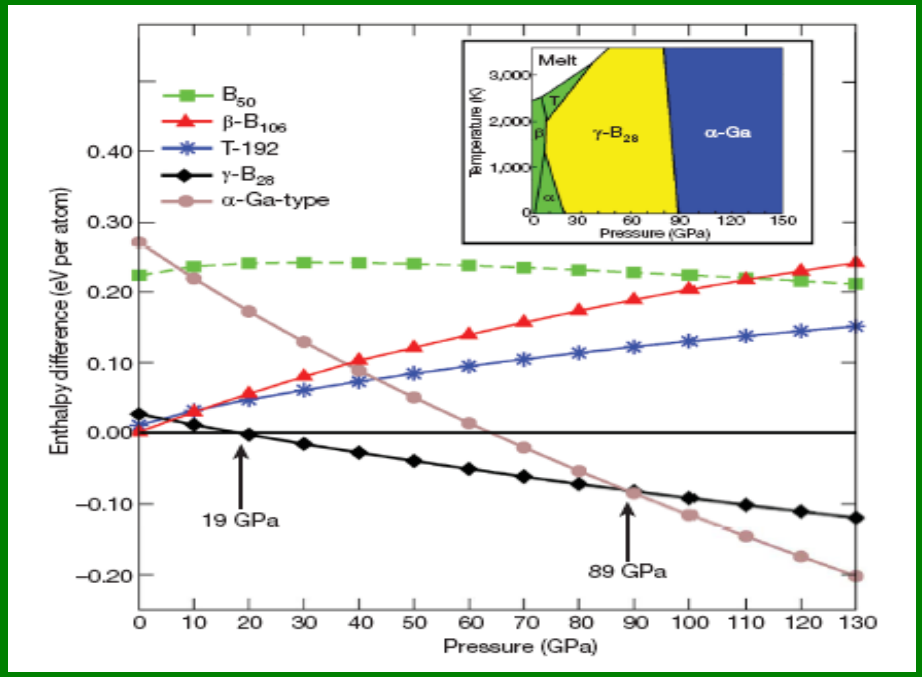
Novel Crystall: γ- Boron

A R Oganov et al, *Nature*, 2009, DOI:10.1038/nature07736







At 19 GPa α-B_{12} transforms to **γ-B_{28}**
At 89 GPa γ-B_{28} transforms to α-Ga
γ-B_{28} is at 200 GPa an insulator with a bandgap of 1.25 **eV**

Mass Spectra of Boron Clusters

Hanley, Whitten and Anderson JPC 92, 8503, 1988

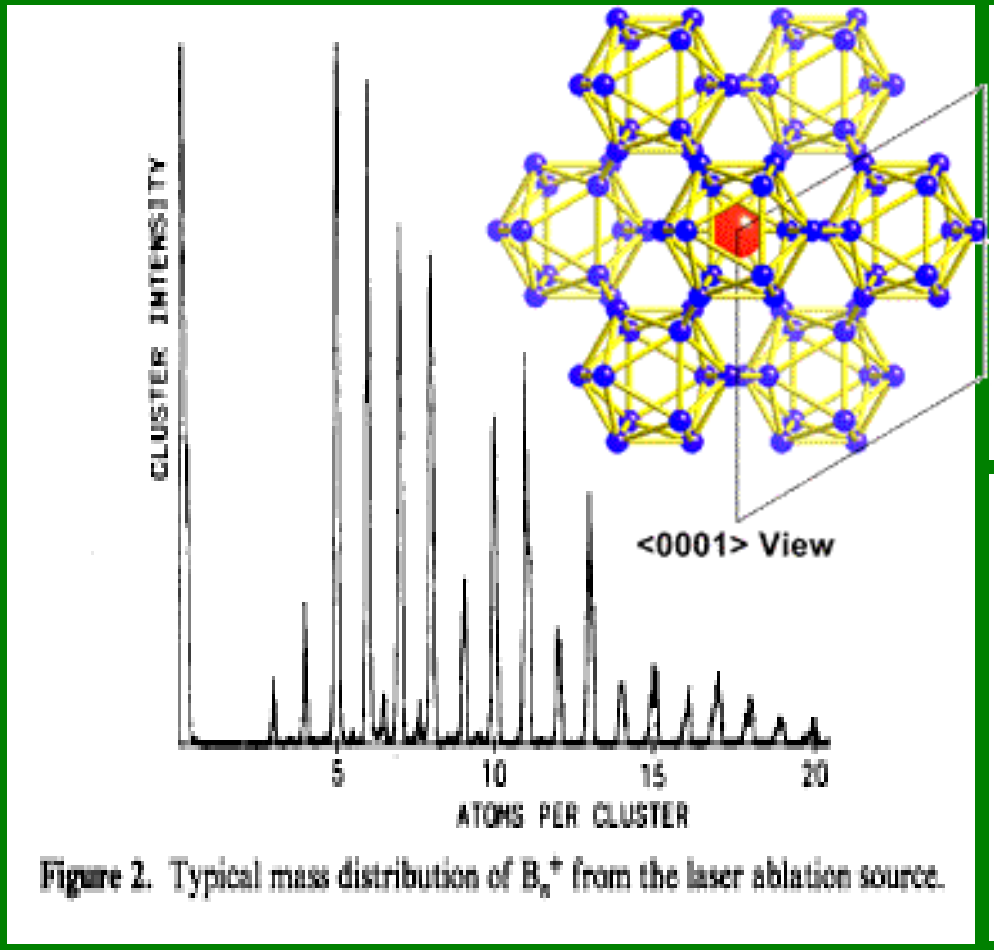
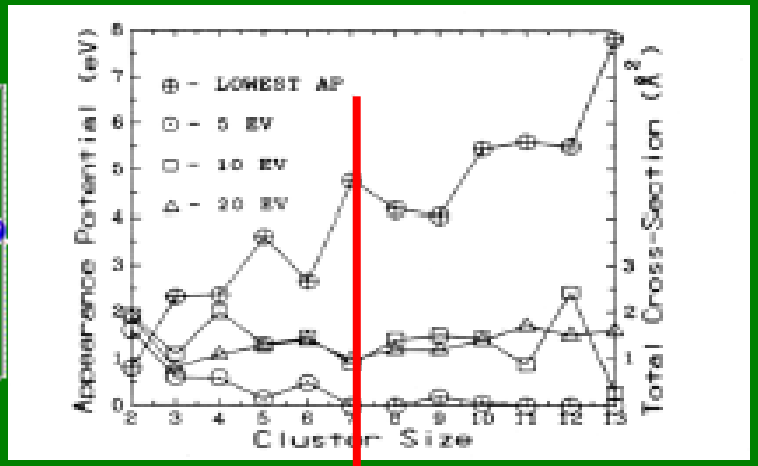
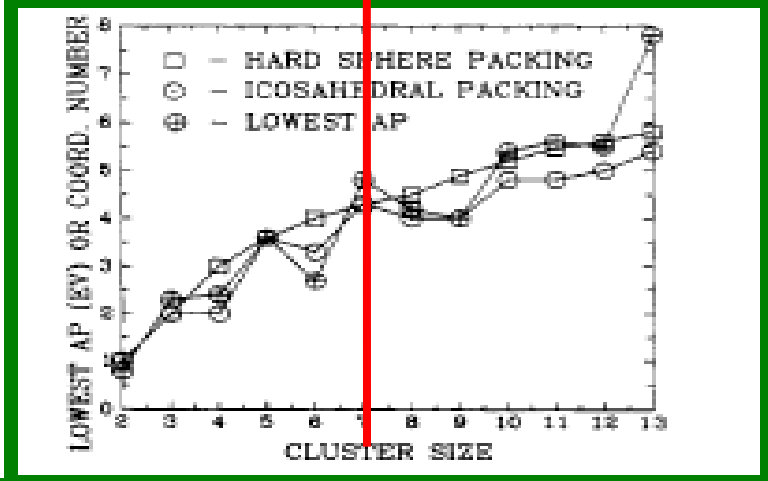


Figure 2. Typical mass distribution of B_n^+ from the laser ablation source.





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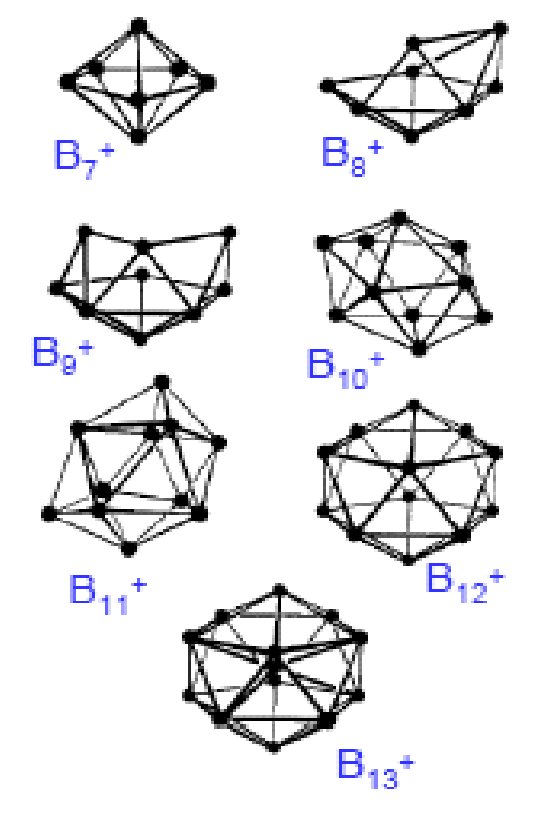
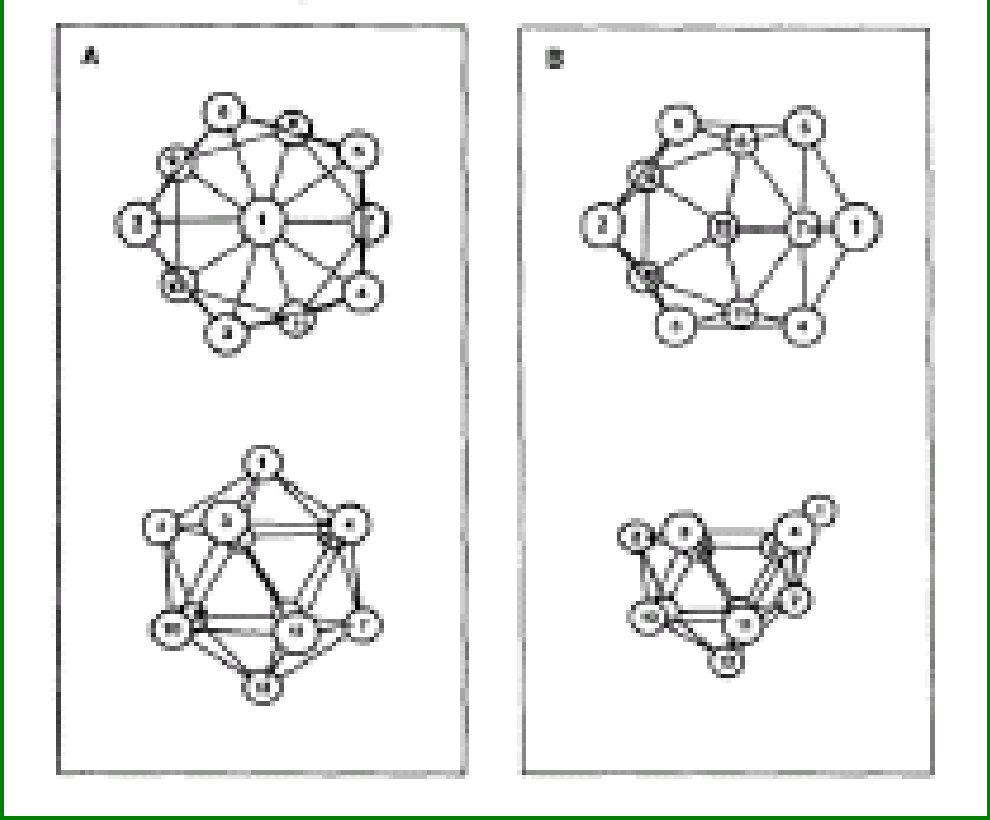
3D Boron Clusters

Anderson et al., *J. Phys. Chem.* 91, 5161, (1987) and 92, 5803 (1988)

Kawaı & Weare, J. *Chem. Phys.*, 95, 115 1 (1991)





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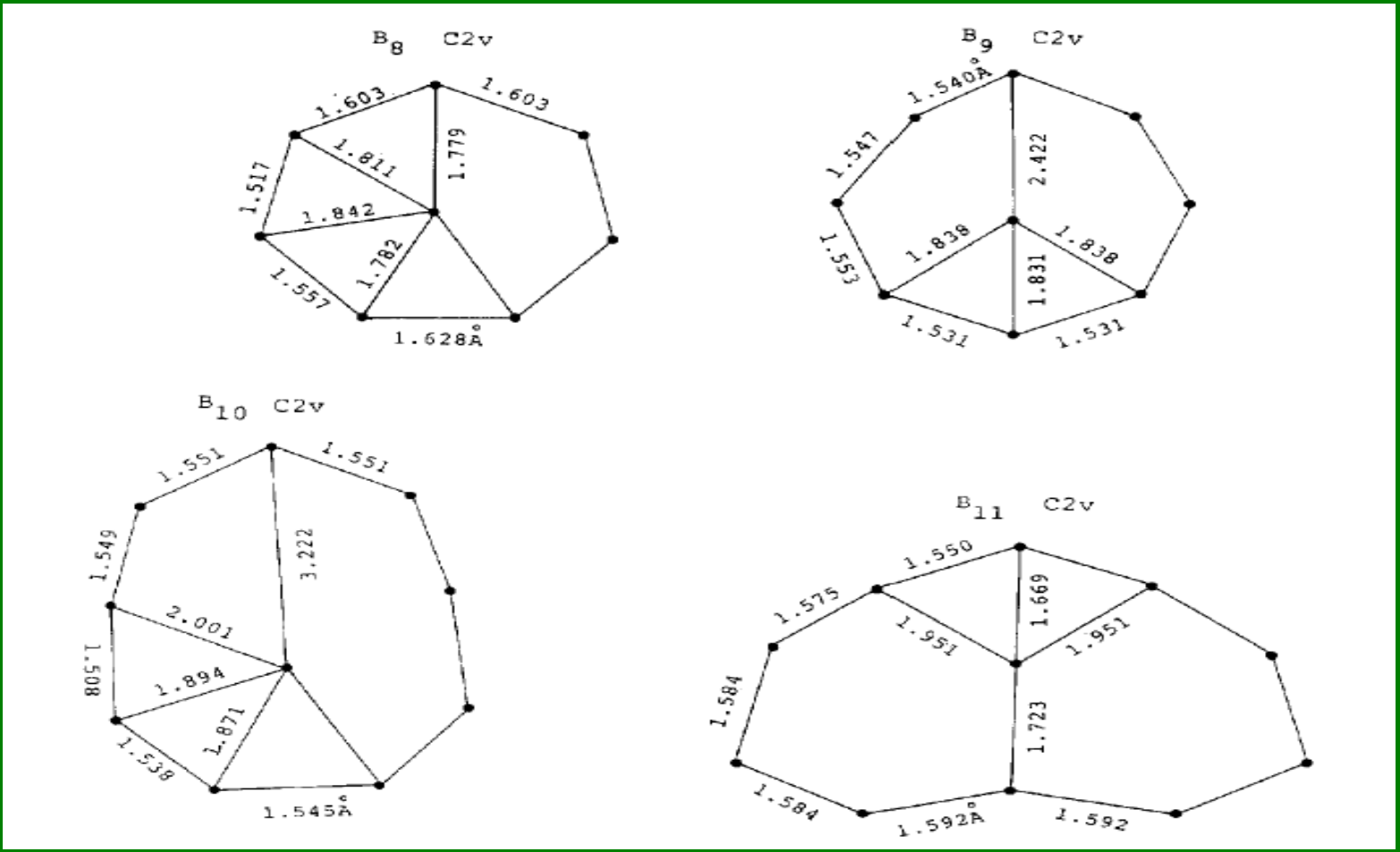
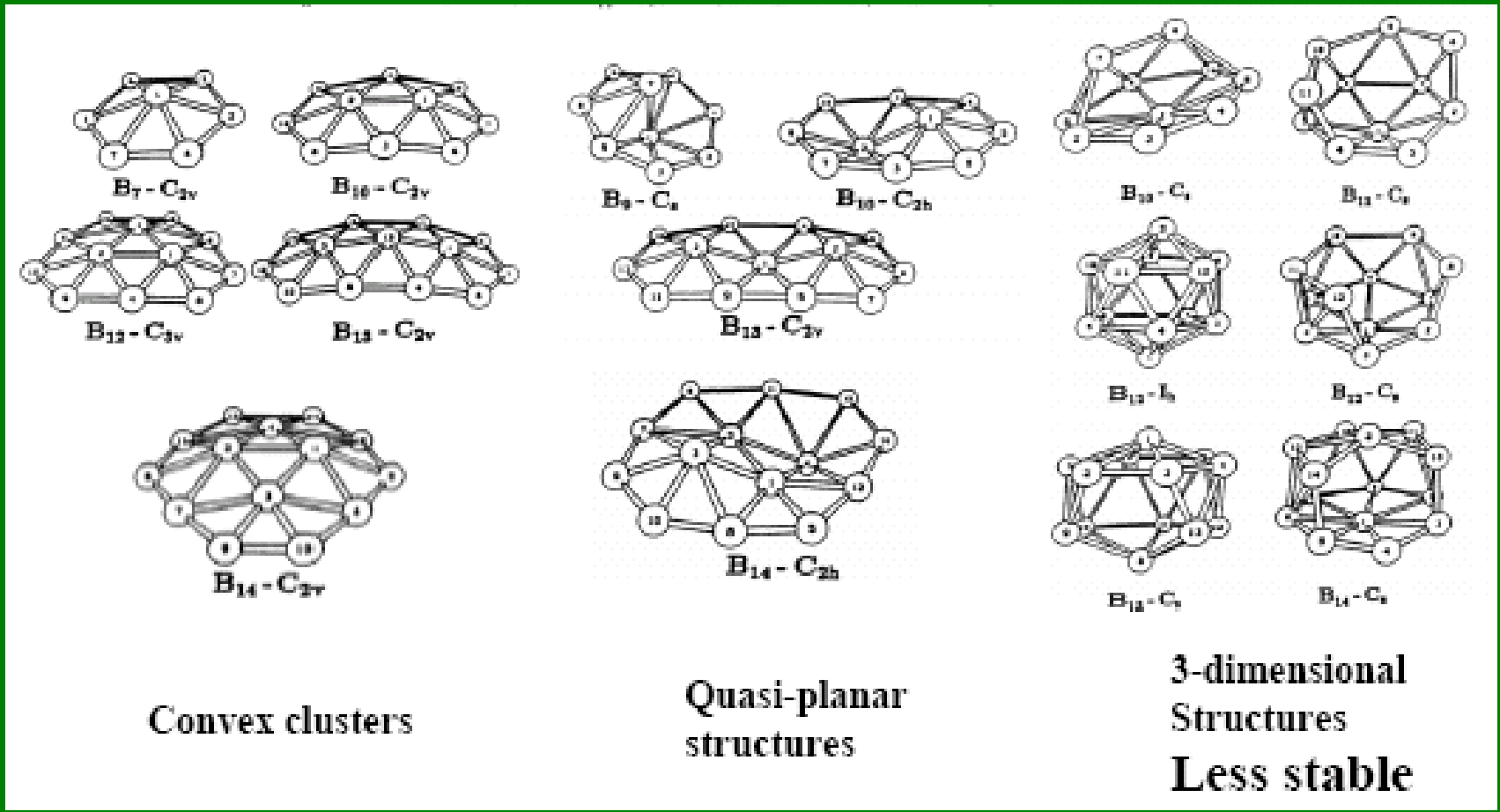
2D Boron Clusters

Kato & Yamashita, *Chem. Phys. Lett.* 190, 362 (1992)

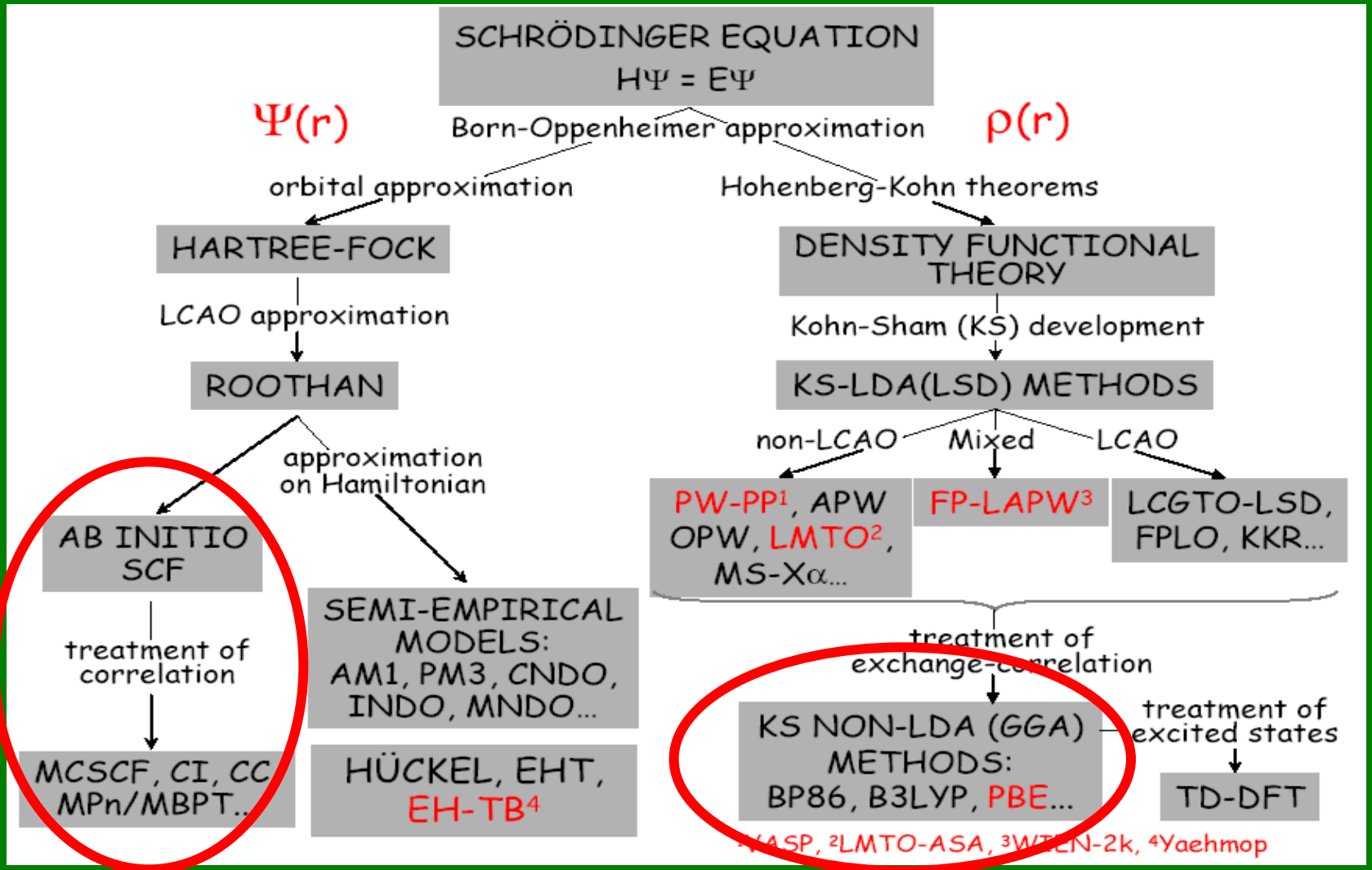


Prediction of Quasi-planar Boron Clusters

Boustani, IJQC 52, 1081 (1994)



Theoretical Methods



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Novel Boron

CitationIndex 2008
Ihsan Boustani

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11	CPL	214, 381 ,1995
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23	CMS	11, 132, 1998
34	CPL	311, 21 , 1999
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10	IJQC	78,131, 2000
15	JCP	113, 3814 ,2000
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7	CPL	339, 362, 2001
22	PRB	64, 125422, 2001

Clusters ,Sheets & Nanotubes

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Fowler	JPC A 104, 397, 2000
Cao	JP. Cond. M. 13, 5065, 2000
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PRL, Nature, JACS, Nano Letters, PRB …

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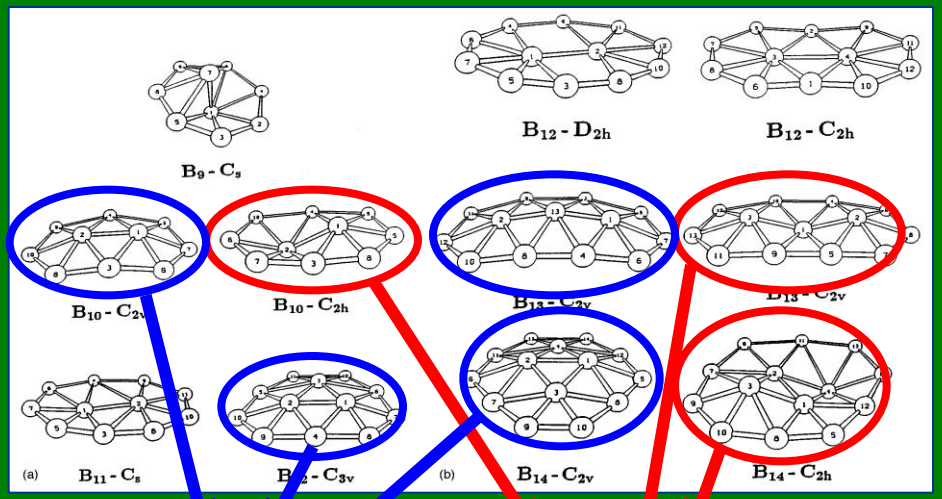
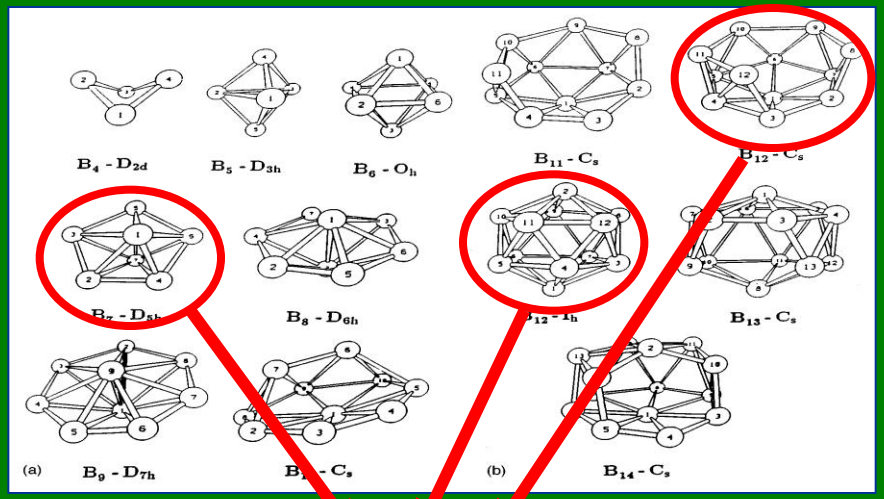
Prediction of Quasi-planar Boron Clusters

Boustani, IJQC 52, 1081 (1994)

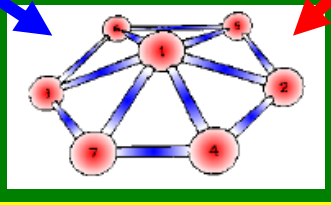
2D Clusters

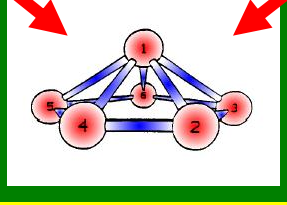


3D Clusters

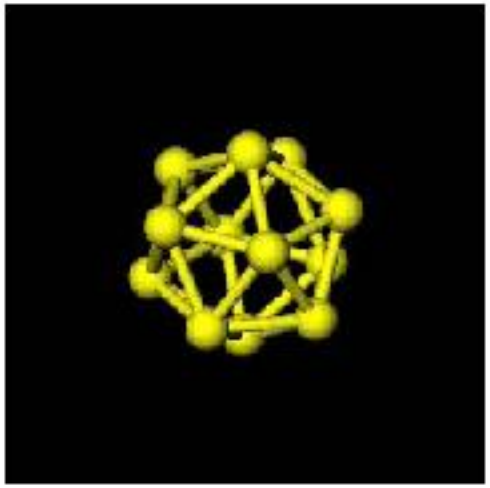


Convex **Quasiplanar** **(Open) Spheres**





Hexagonal Pyramide **Pentagonal Pyramide**



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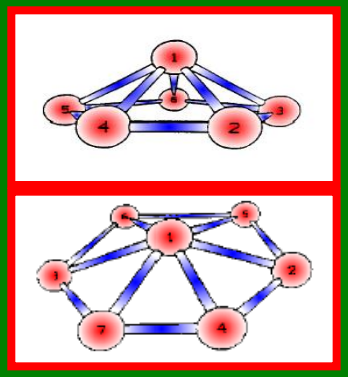
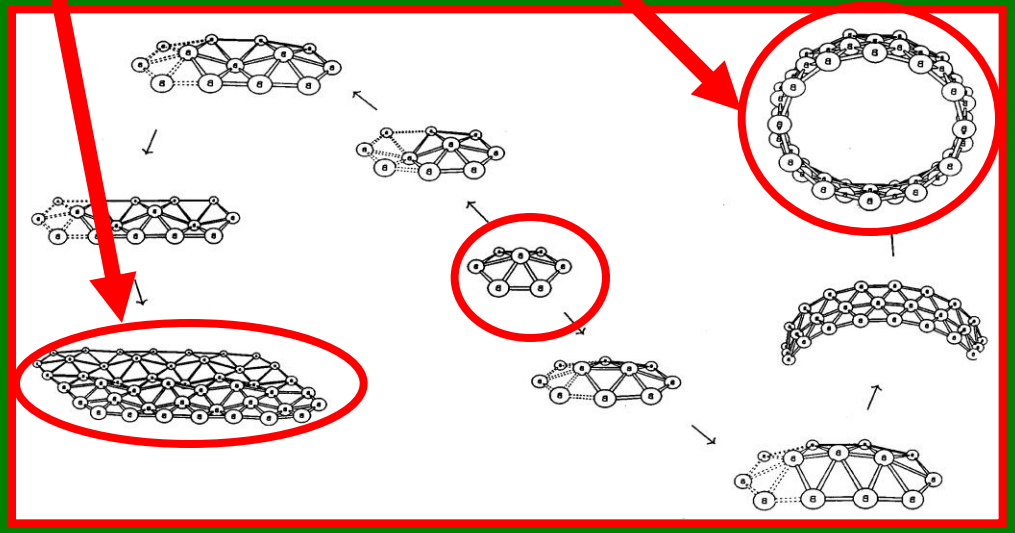
The Aufbau Principle

Boustani, CPL 240, 135 (1995), PRB 55, 16426 (1997)

Highly stable *Boron Clusters* and *Spheres* *can be constructed from two basic units* : B_6 & B_7, while *Boron Sheets & Nanotubes* *only from one basic units* : B_7



The Aufbau starts by consecutively adding atoms to B_7 forming new *hexagonal pyramids generating Sheets or Nanotubes.*



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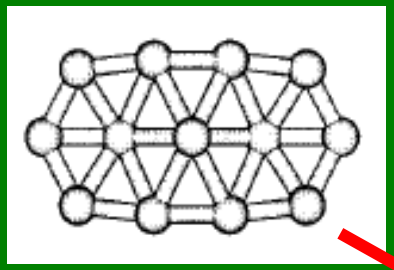
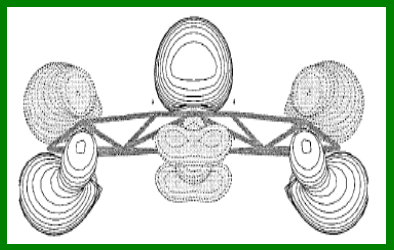
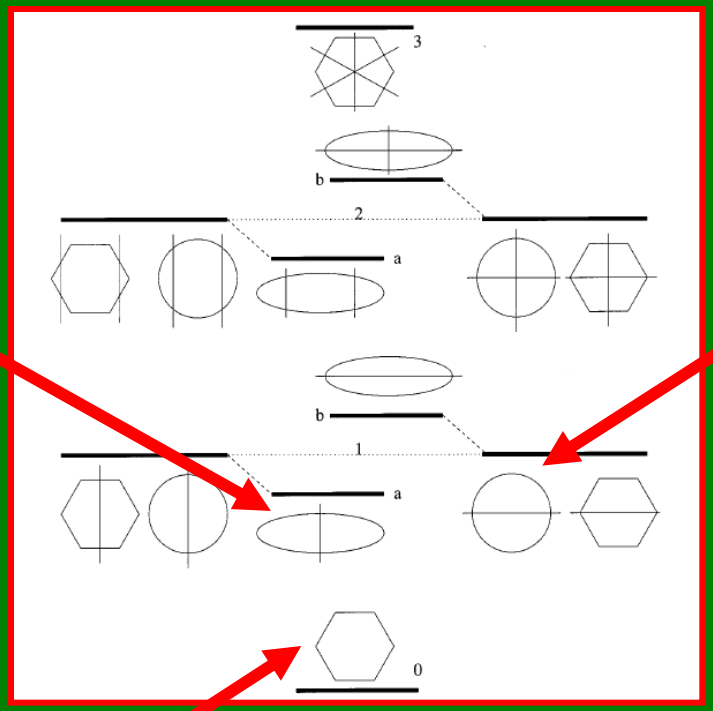
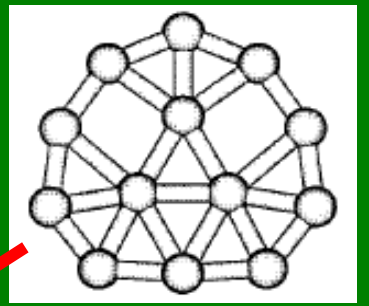
Theoretical Confirmation I
Curiously Stable Quasiplanar B_{13}^+

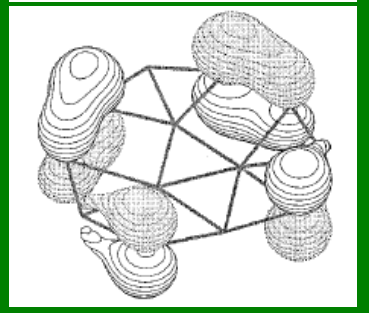
Fowler & Ugalde, JPC A 104, 394 (2000)











Similar to Benzene, Cationic B_{13} is Aromatic

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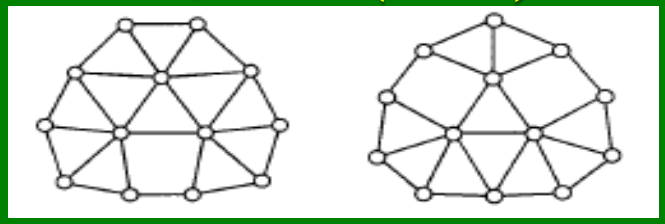
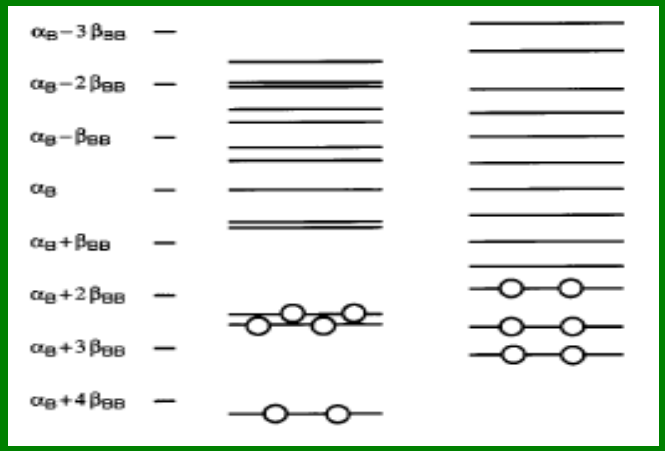
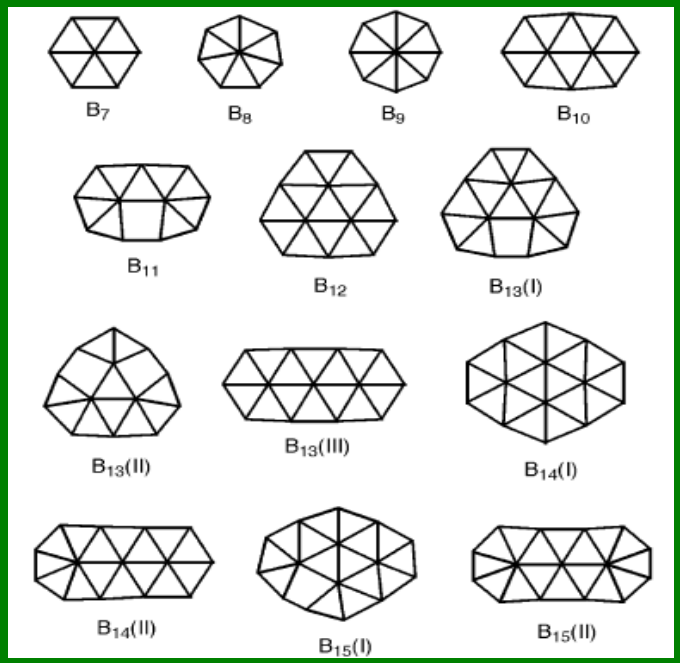
Theoretical Confirmation II of Quasiplanar Clusters

J. Aihara, JPC A 105, 5486 (2001)





J. Aihara, JACS 127, 13324 (2005)



π-MOs with six π electrons

Aromaticity of Planar Clusters is confirmed

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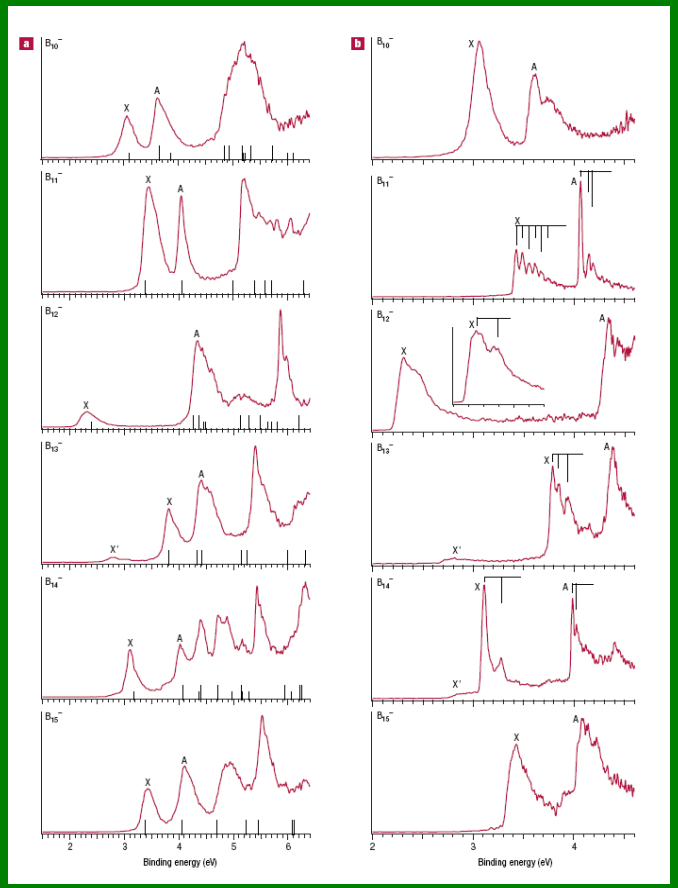
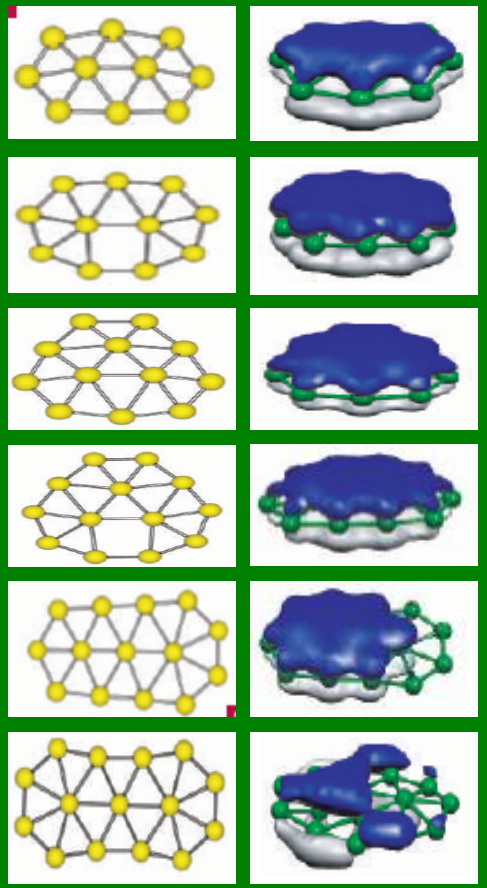
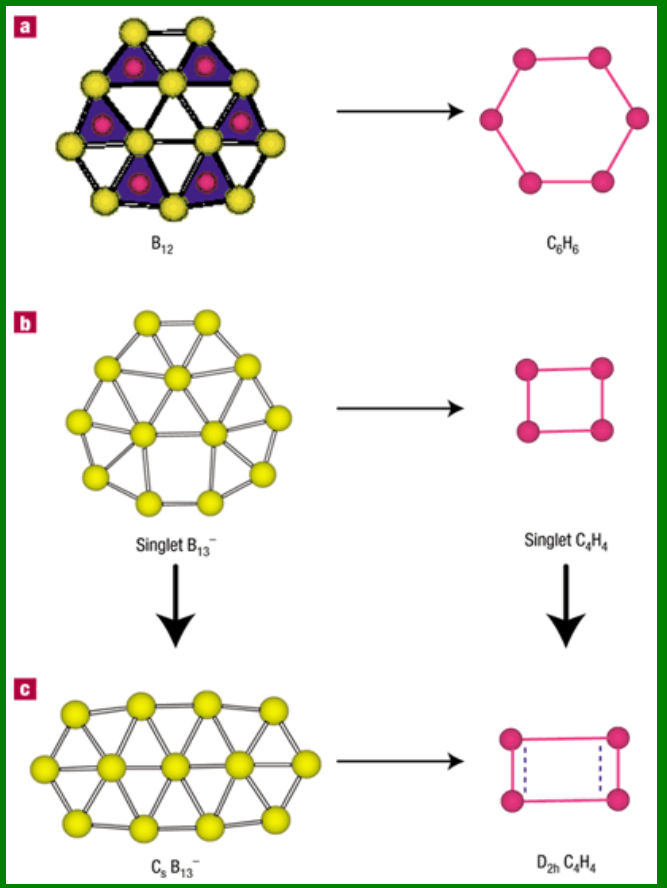
Experimental Confirmation of Quasiplanarity I

LS Wang et al. Nature Mat. 2, 827 (2003)







Vertical Electron Detachment | B_n Clusters | □-MOs | Aromatic Boron Clusters

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Experimental Confirmation of Quasiplanarity II

Oger et al., Angew. Chem. Int. Ed. 46, 8503 –8506 (2007)

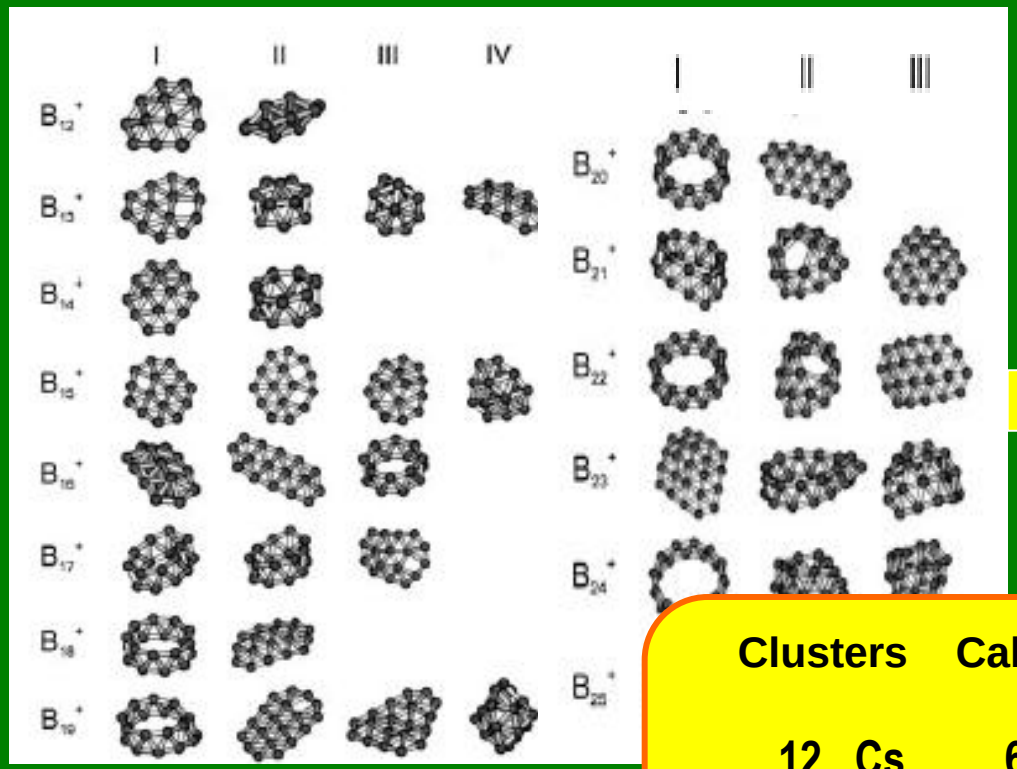

Table 2: Comparison of experimental and calculated cross sections.[a]

Cluster size	Number	Symmetry/ state label	ΔE [eV]	Ω_{calcd} [Å^2]	Ω_{expt} [Å^2]
12	I	$C_s/^2A''$	0	62.8*	63.6 ± 1.9
	II	$D_{2h}/^2A_u$	0.48	58.6	
13	I	C_{2v}	0	66.7*	66.7 ± 0.9
	II	C_{3v}	0.84	58.7	
	III	C_{3v}	0.89	59.5	
	IV	C_s	1.04	66.9	
22	I	$C_{2h}/^2B_u$	0	89.1	83.2 ± 1.4
	II	$C_1/^2A$	[illegible]	81.7*	
	III	$C_2/^2A$	1.13	90.2	
23	I		0	91.4	84.9 ± 1.8
			0.48	90.7	
			0.89	84.6*	
				95.9*	94.9 ± 2.9
			[illegible]03	80.0	
			[illegible]31	80.7	

Collision Cross Sections

Clusters	Calculated	Collision Cross Sections
12 Cs	62.8	63.6 ± 1.9
13 C2v	66.7	66.7 ± 0.9
14 C2v	68.3	69.0 ± 1.8
15 Cs	72.1	69.4 ± 2.6

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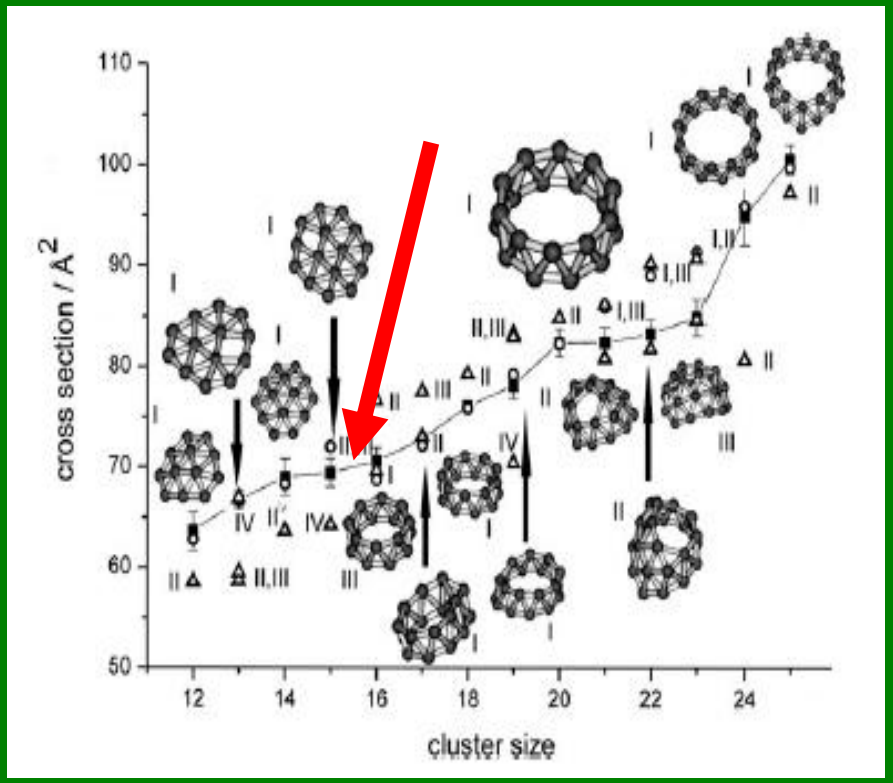
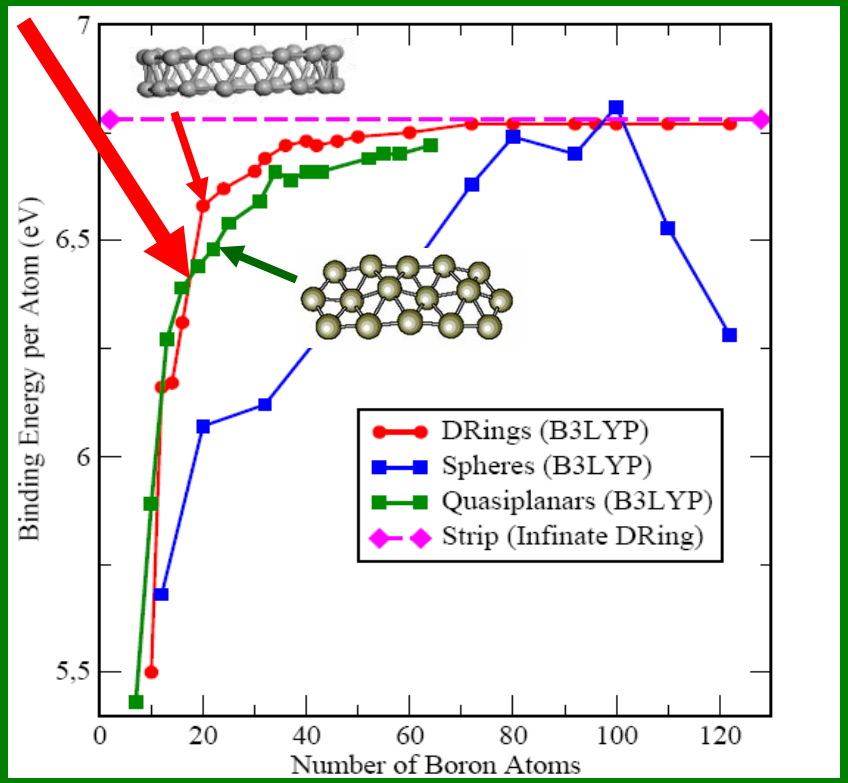
Bergische Universität Wuppertal, Germany

Transition from Quasiplanar to Cylindrical Structure

Oger et al., Angew. Chem. Int. Ed.
46, 8503 –8506 (2007)



Pandey & Boustani
J. Phys., submitted (2008)



Transition between Quasi-Planar and Cylindrical Structures at B_{16}

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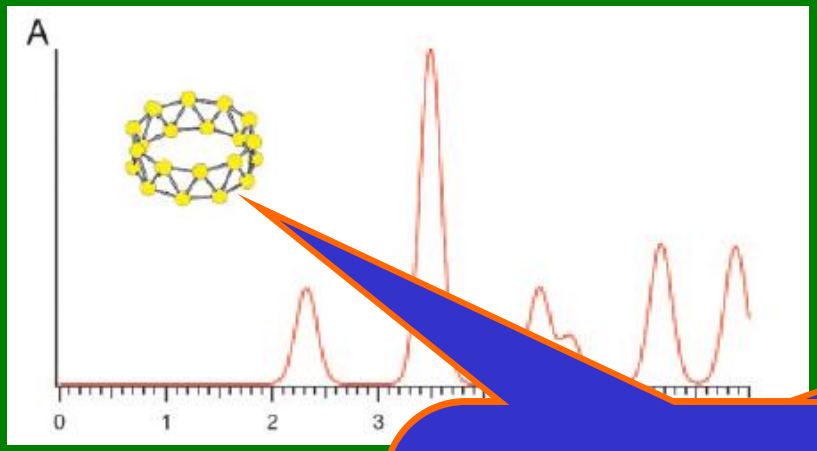
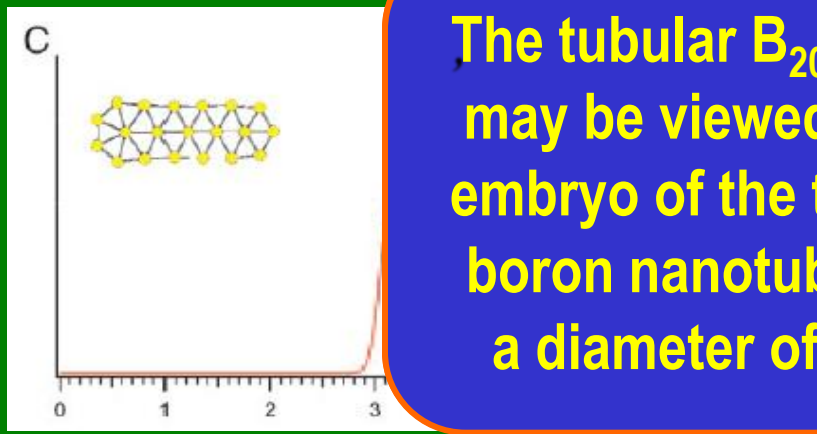
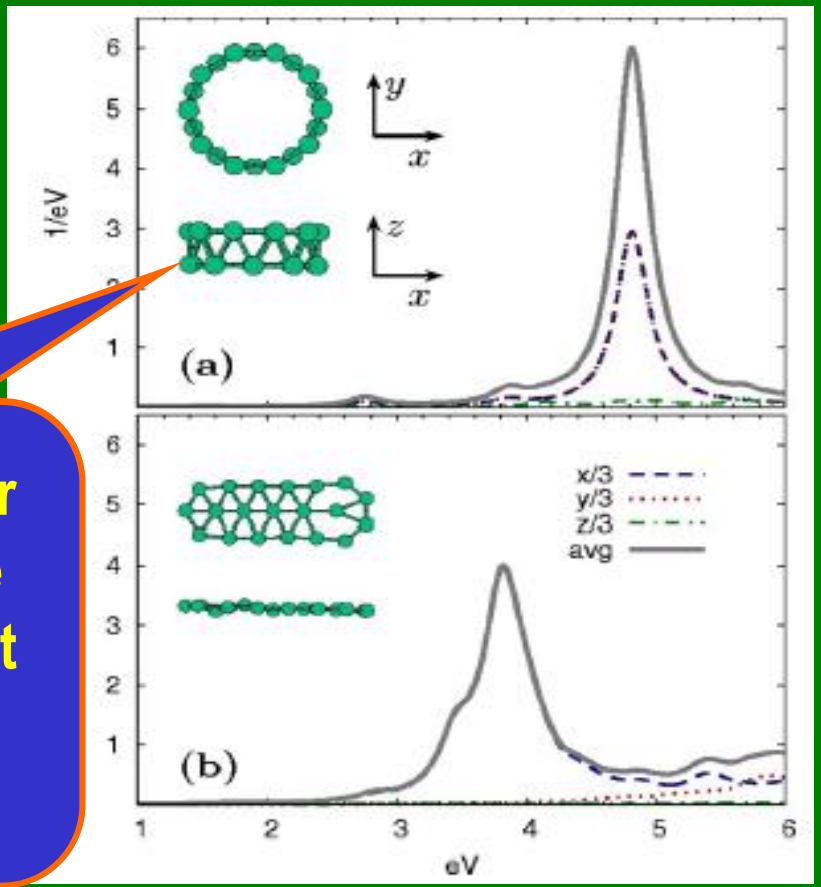
Transition from Quasiplanar to Cylindrical Structure II

B_{20} as the embryo of SWBNTs
Kiran et al., PNAS 102, 964 (2005)

Structural Transition via Optical Absorption
Marques & Botti, JCP 123, 014310 (2005)







The tubular B_{20} cluster may be viewed as the embryo of the thinnest boron nanotube, with a diameter of 5.2 Å.

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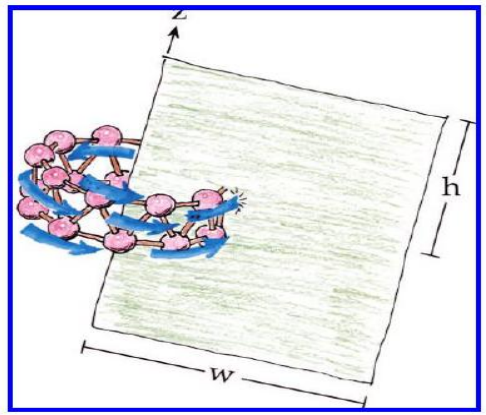
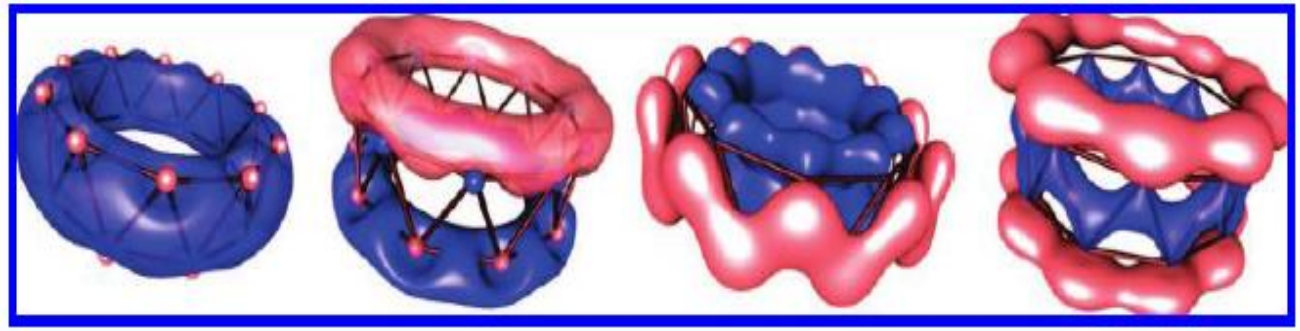
On the Strong Ring Currents in B20 and neighboring Boron Toroids

M. P. Johansson, J. Phys. Chem. C 113, 524 (2009)





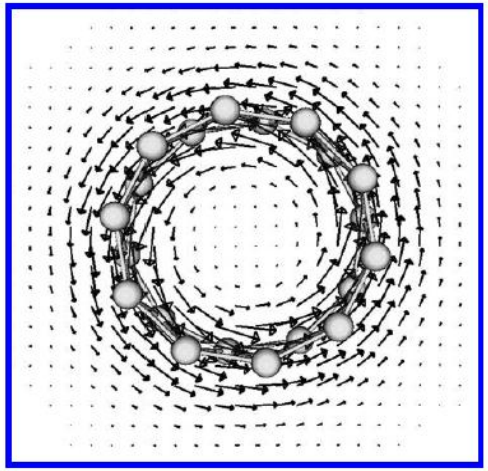
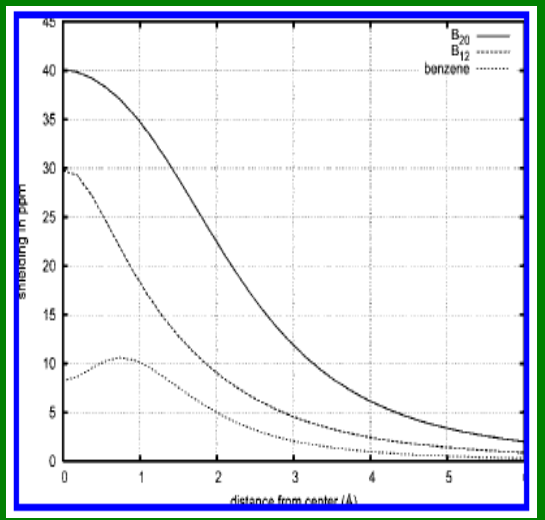


TABLE 2: Integrated Induced Currents for Selected Molecules in nA/T[a]

	sym	total current	diamagnetic	paramagnetic	NICS
B_{16}	D_{8d}	31	33	−1	−33
B_{20}	D_{10d}	42	43	−1	−40
B_{24}	D_{12d}	50	51	−1	−35
B_{18}	C_{2h}	−117	11	−128	+62
B_{22}	C_i	−121	8	−130	+90
B_{12}	C_{3v}	25	25	0	−30
$C_{60}^{10+\,b}$	I_h	60	81	−21	−82
C_6H_6	D_{6h}	12	17	−5	−8



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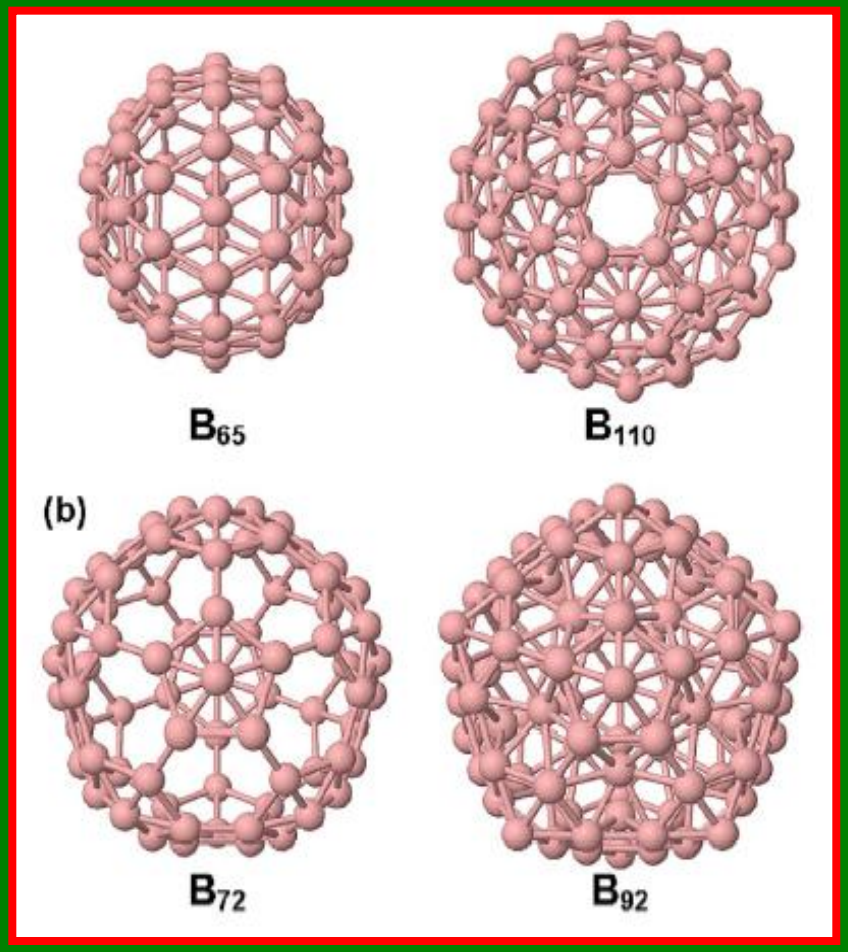
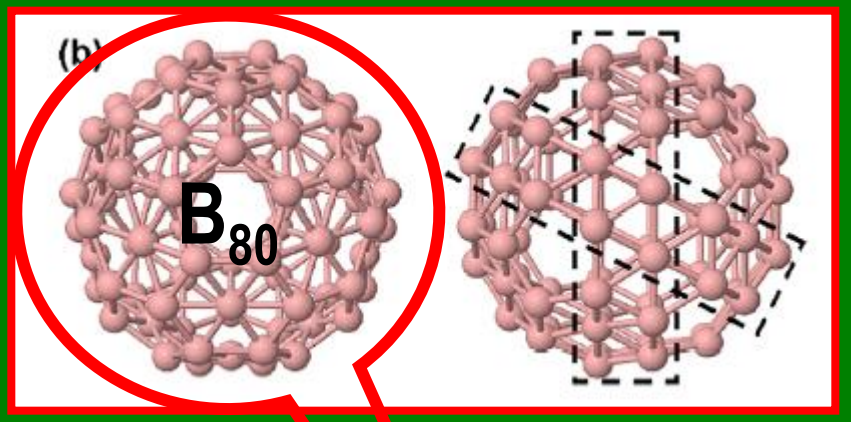
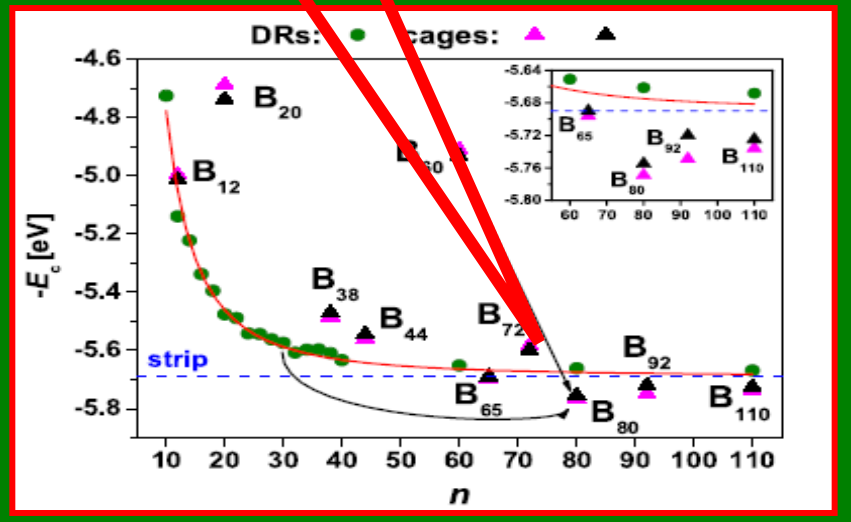
Boron Fullerenes

B. I. Yakobson et al., PRL 98, 166804 (2007)







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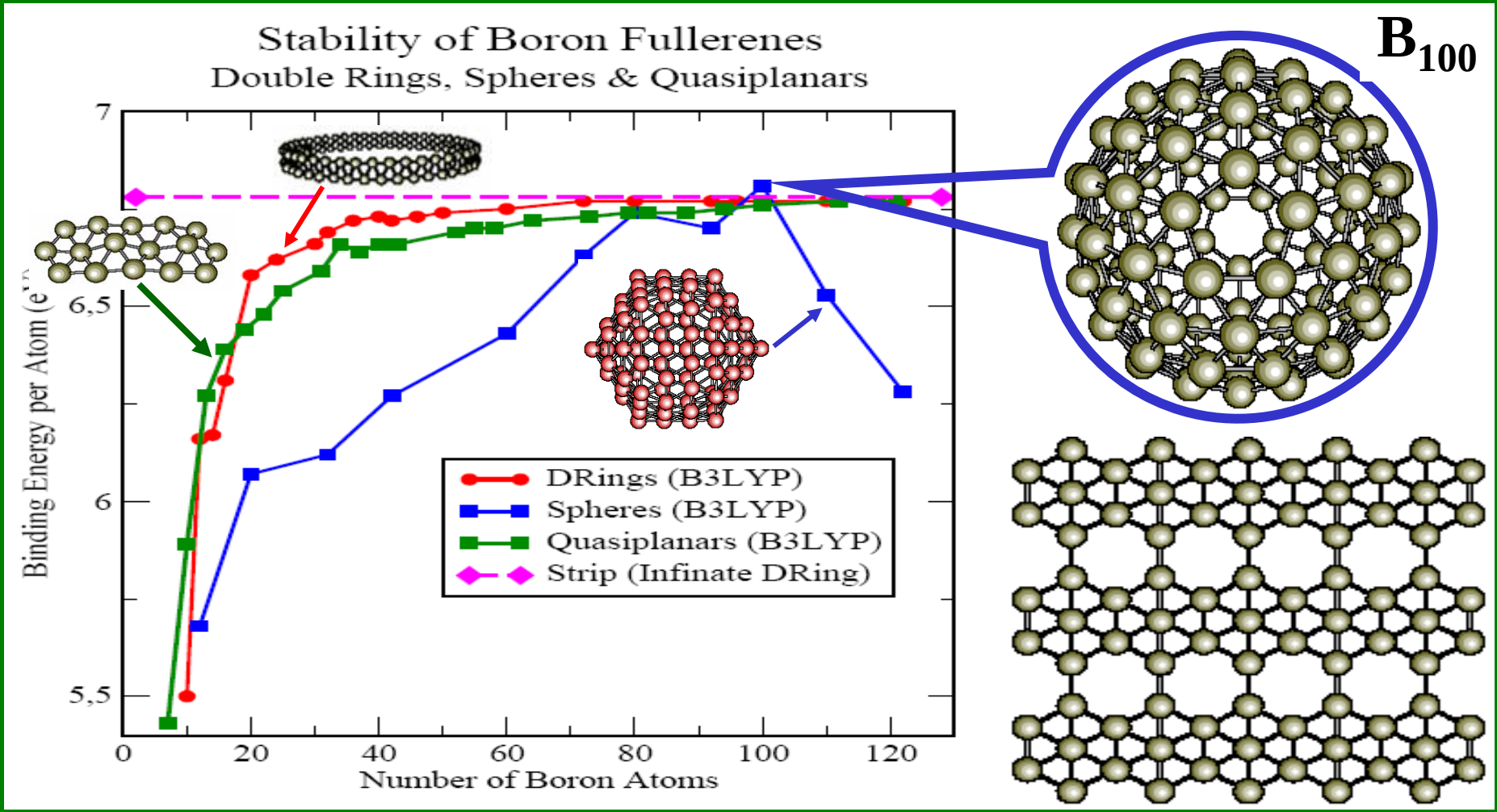
Boron Fullerene-like Nanospheres

Pandey & Boustani , J. Phys. Submitted (2008)



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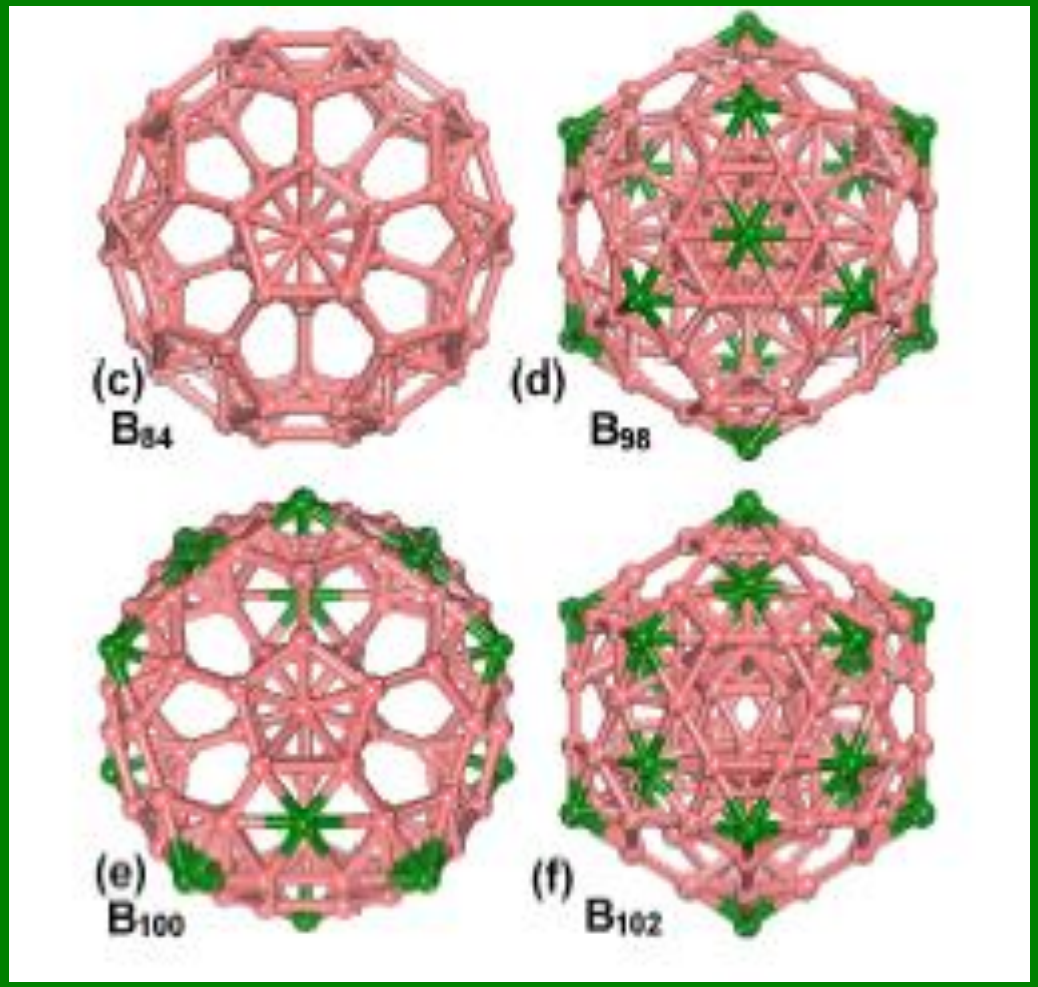
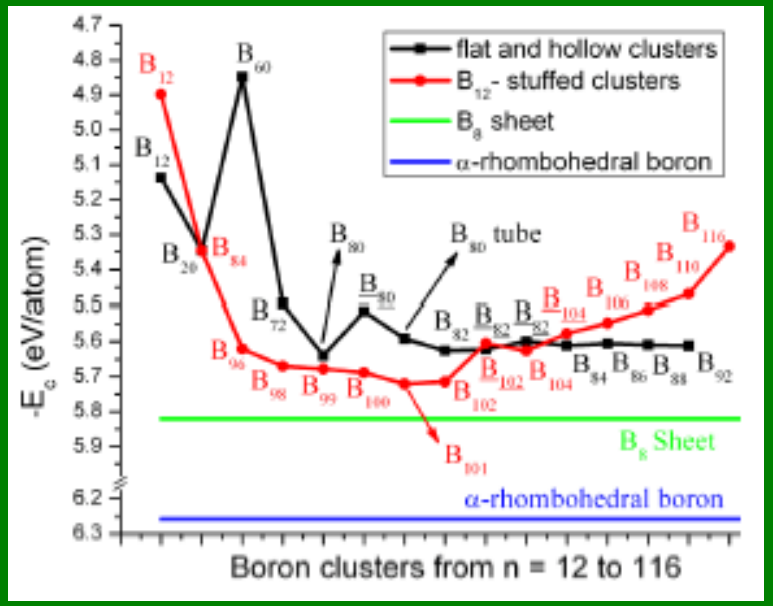
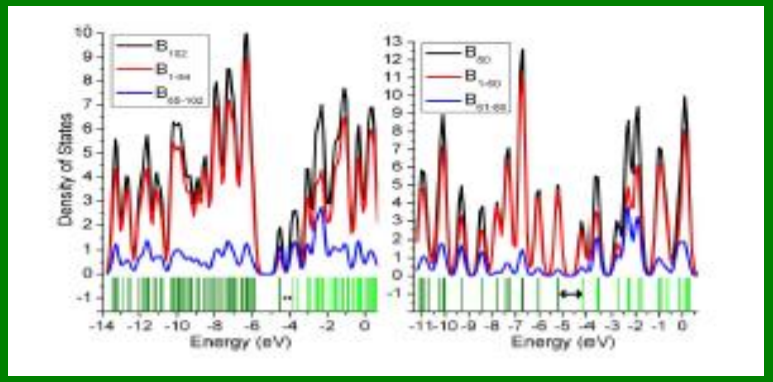
Stuffing Inproves the Stability of Fullerenelike Boron Clusters

Prased and Jemmis, PRL 100, 165504 (2008)

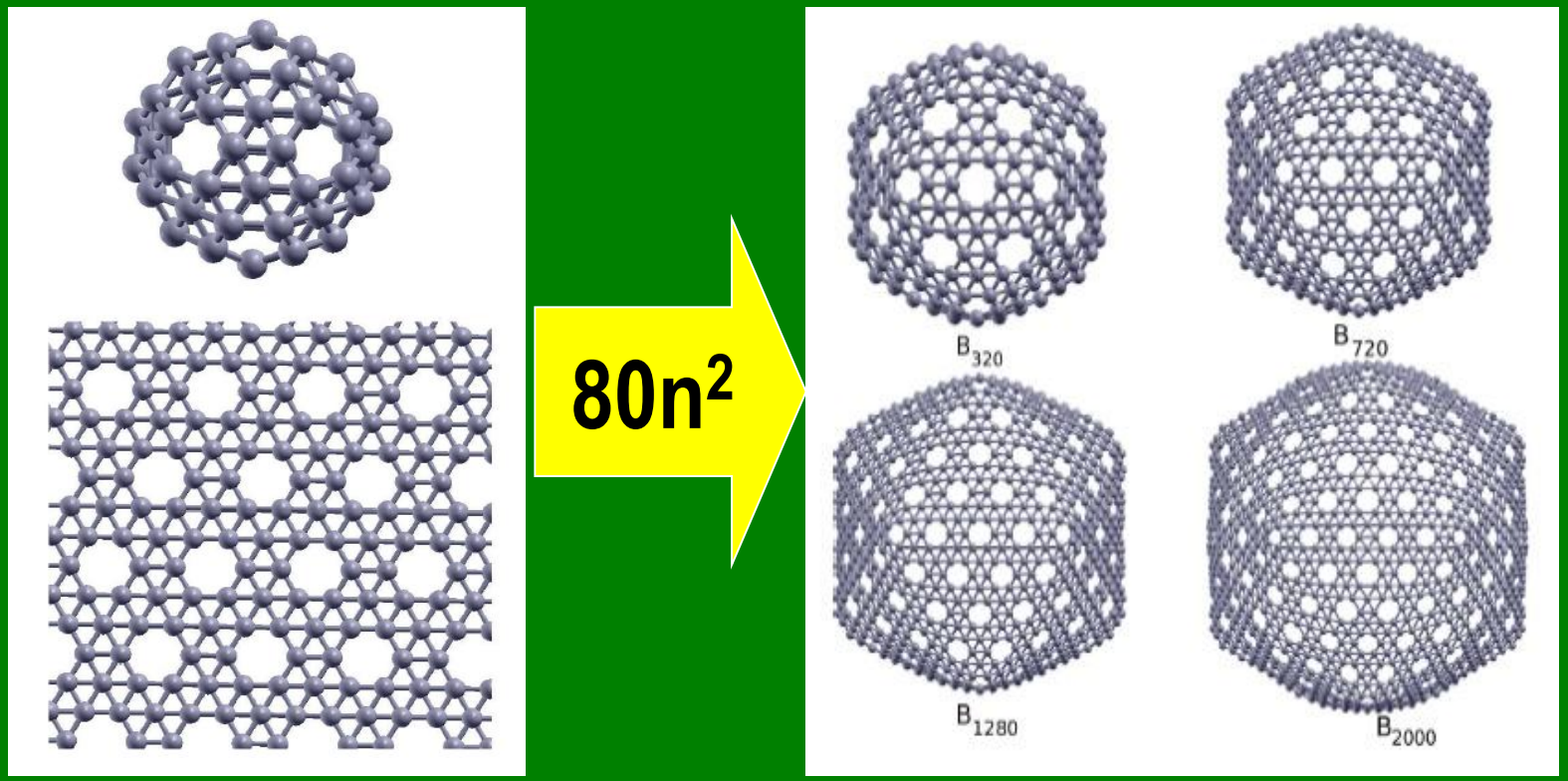






Boron fullerenes: from B_{80} to hole doped boron sheets

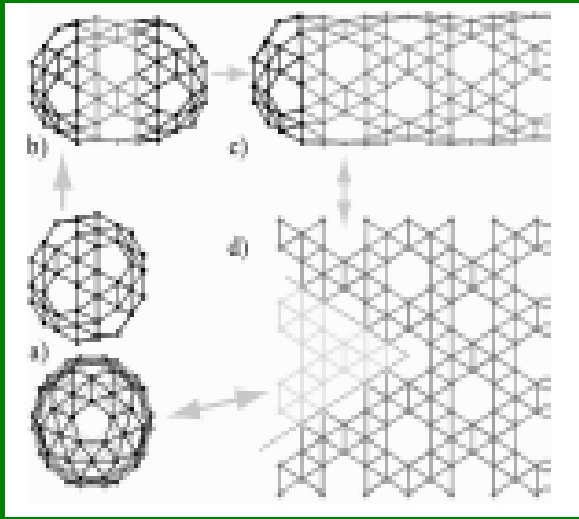
Amy Lui et al., PRB 79, 161403 (2009)

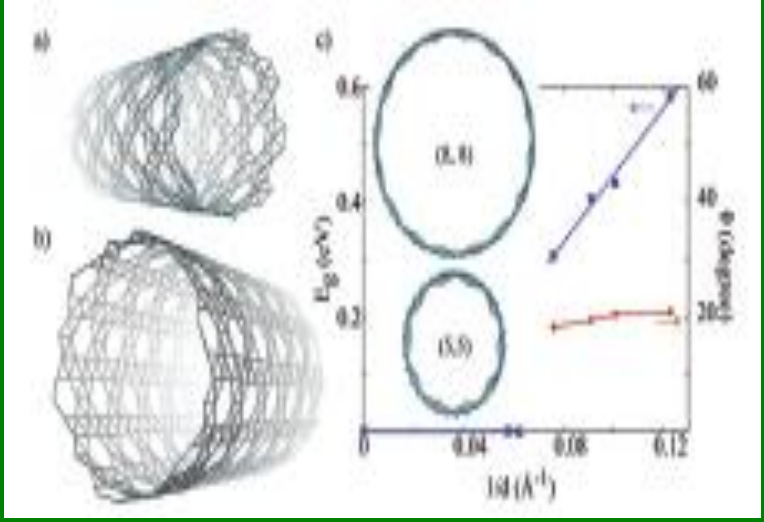


Boron Fullerenes become metallic around n= 4-5
Their $60n^2$ carbon cousins are semiconductors.

Probing Properties of Boron α-Tubes by *Ab Initio* Calculations

Yakobson et al., Nanoletters, 8, 1314 (2008)





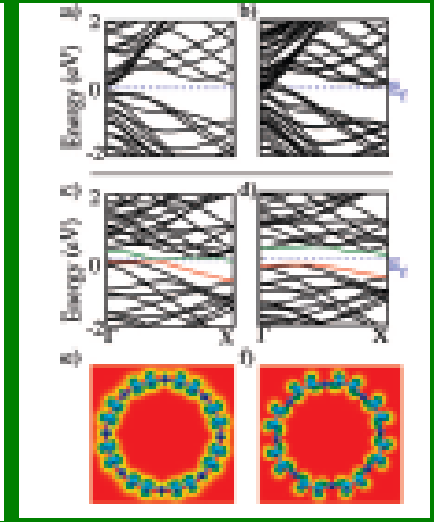


Table 1. Calculated Stiffness (C), Poission Ratio (ν), and Radial Breathing Mode Frequencies (f_{RBM}) of Boron α-Tubes

nanotubes	diameter (Å)	C (N/m)	ν	f_{RBM} (cm^{-1})
(5,5)	8.13	209.4	0.18	238.9
(9,0)	8.63	206.7	0.21	224.8
(6,6)	9.93	202.1	0.26	195.9
(12,0)	11.31	204.6	0.21	170.6
(7,7)	11.37	215.2	0.20	173.7
(8,8)	13.13	214.0	0.21	150.2
(18,0)	16.50	217.5	0.15	119.2

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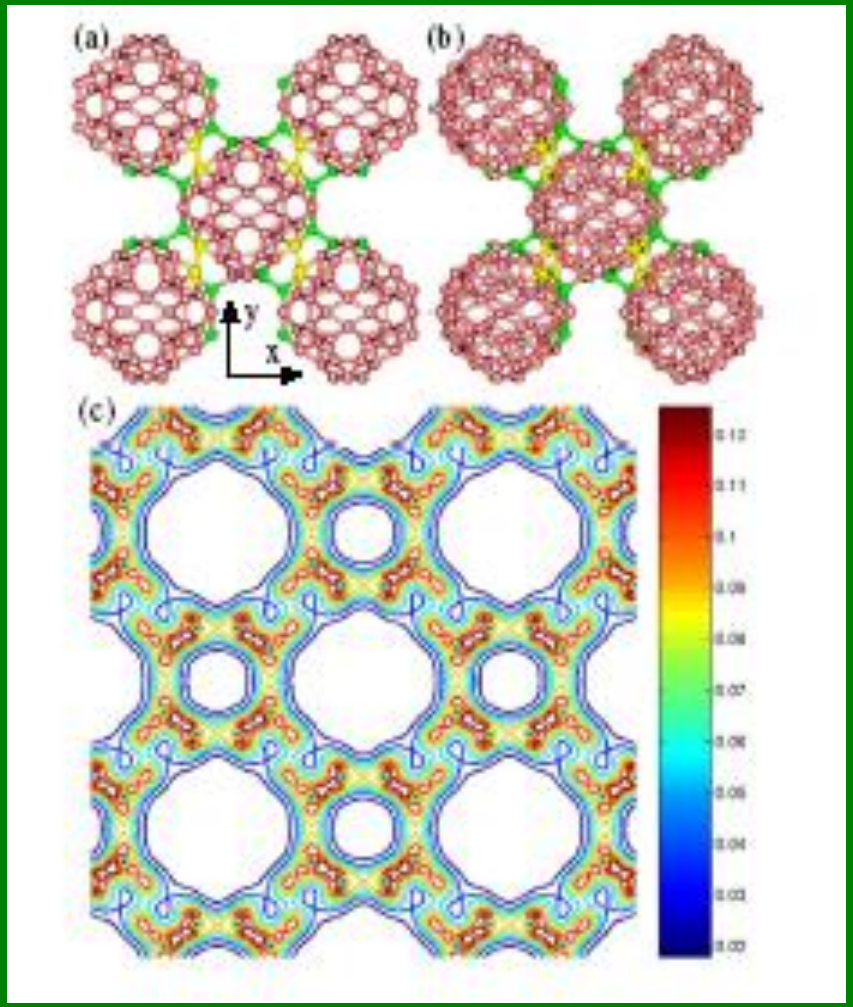
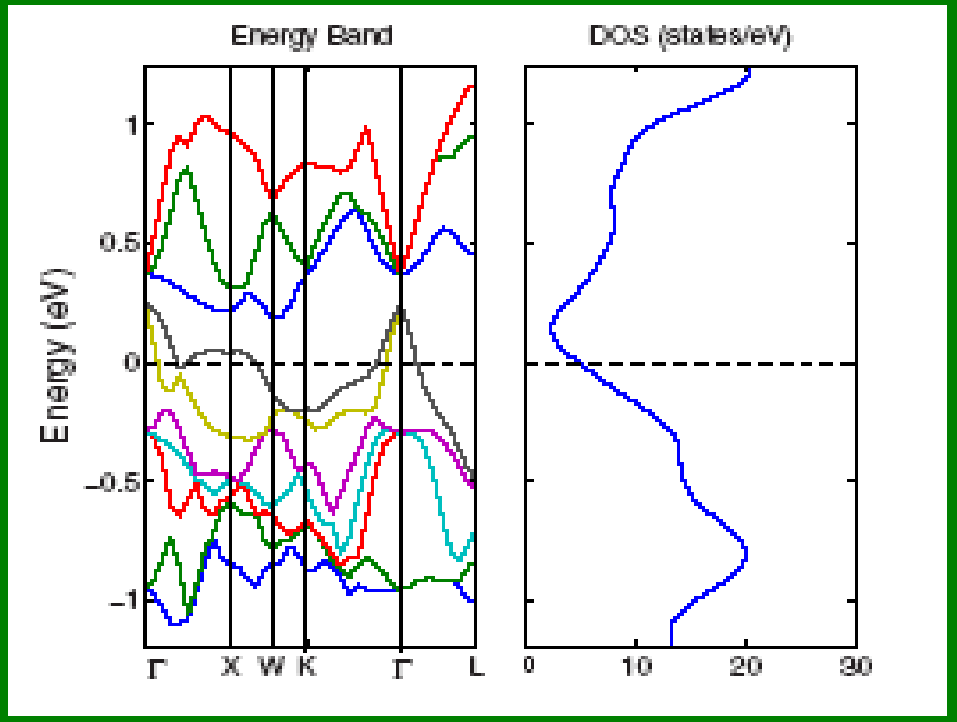
Face-centered-cubic B80 metal: Density Funktional Theory Calculations

Yan, Zheng, and Su, PRB 77, 224106 (2008)





The total energy of B_{80} fcc solid is 0.23 eV/atom lower than the isolated B_{80} fullerene

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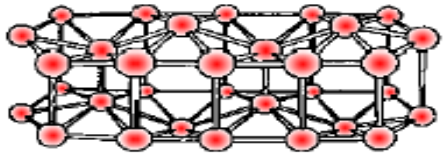
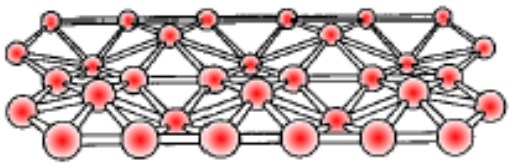
Boron Sheets

Boustani Surf. Sci., 1997
Kunstmann & Quandt 2008

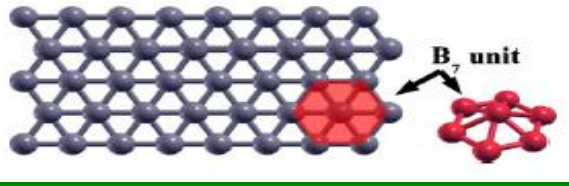
Double Layers



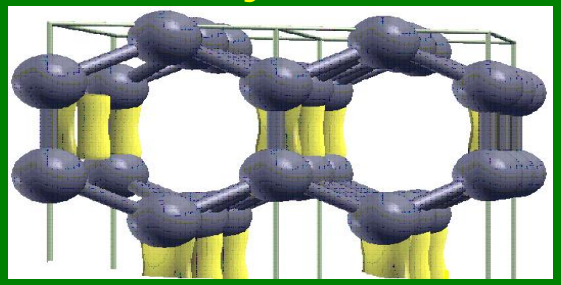
Single Layer

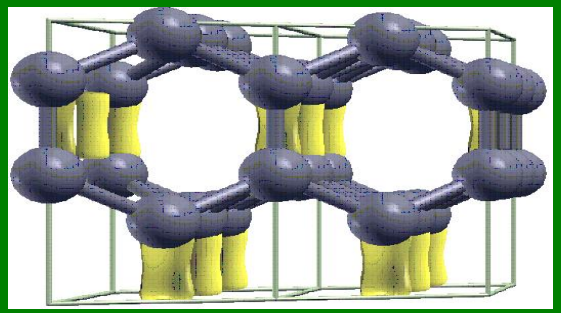


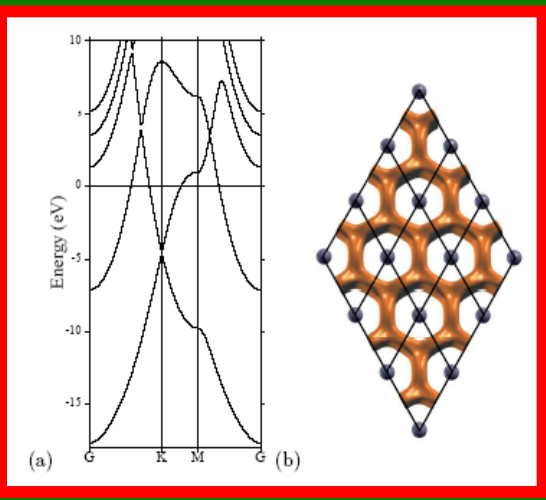
Infinite Sheet

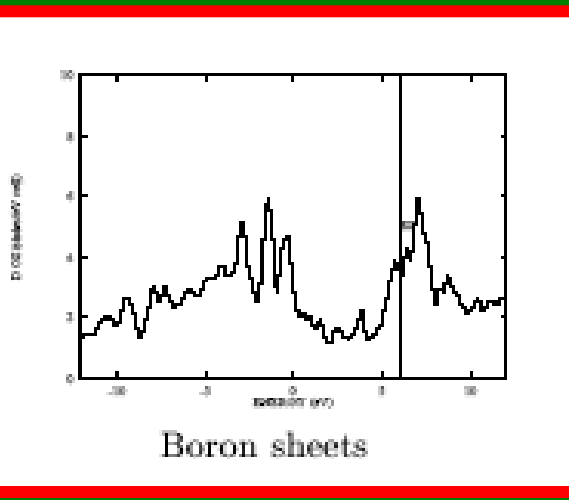


Multi Layers









Band Structure, Electron Density, DOS : metallic

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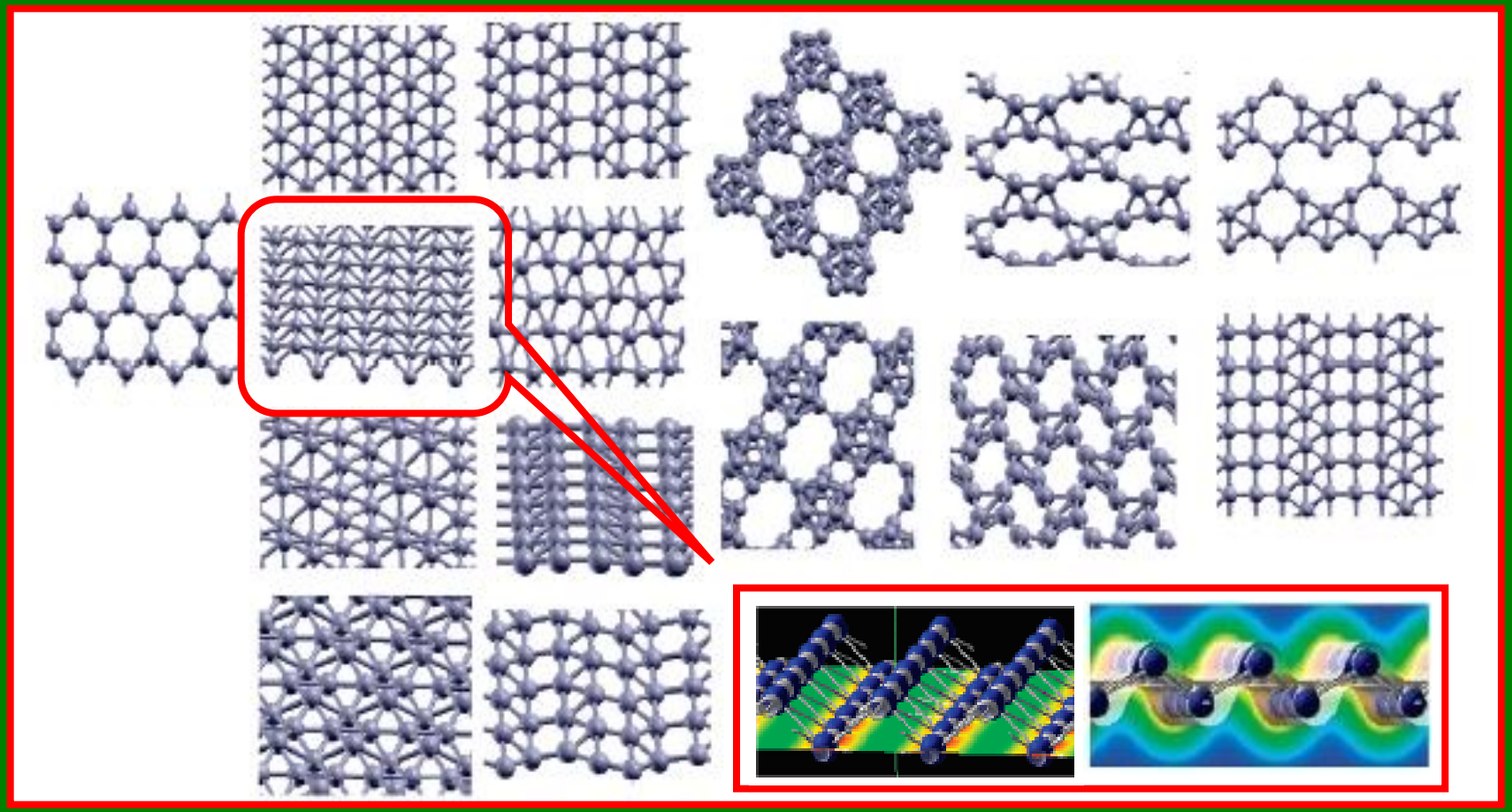
2D Boron Sheets

Lau & Pandey, JPC C, 111, 2906 (2007)



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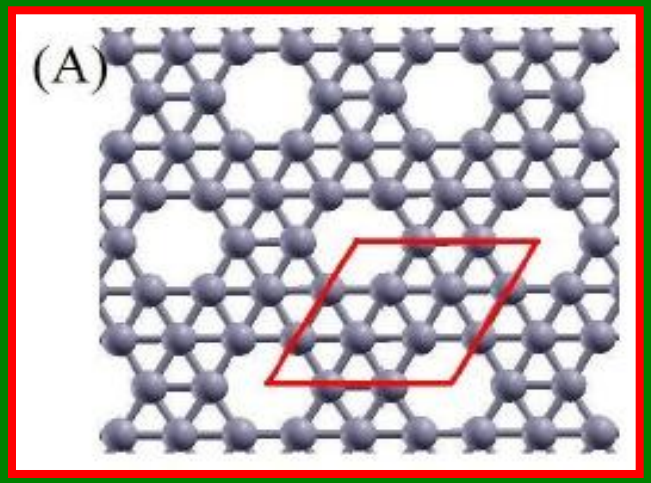
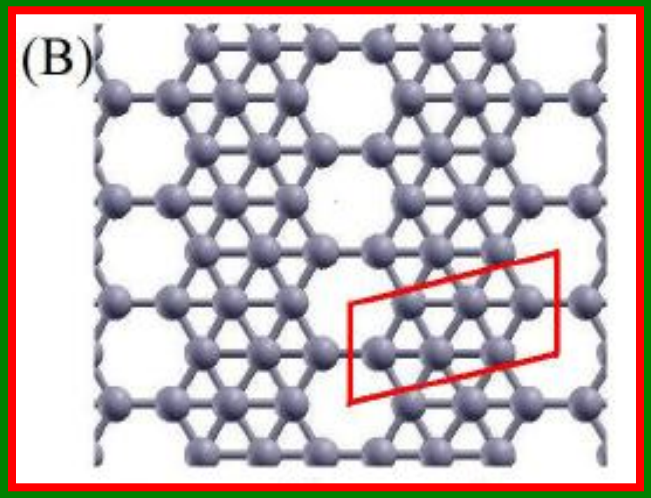
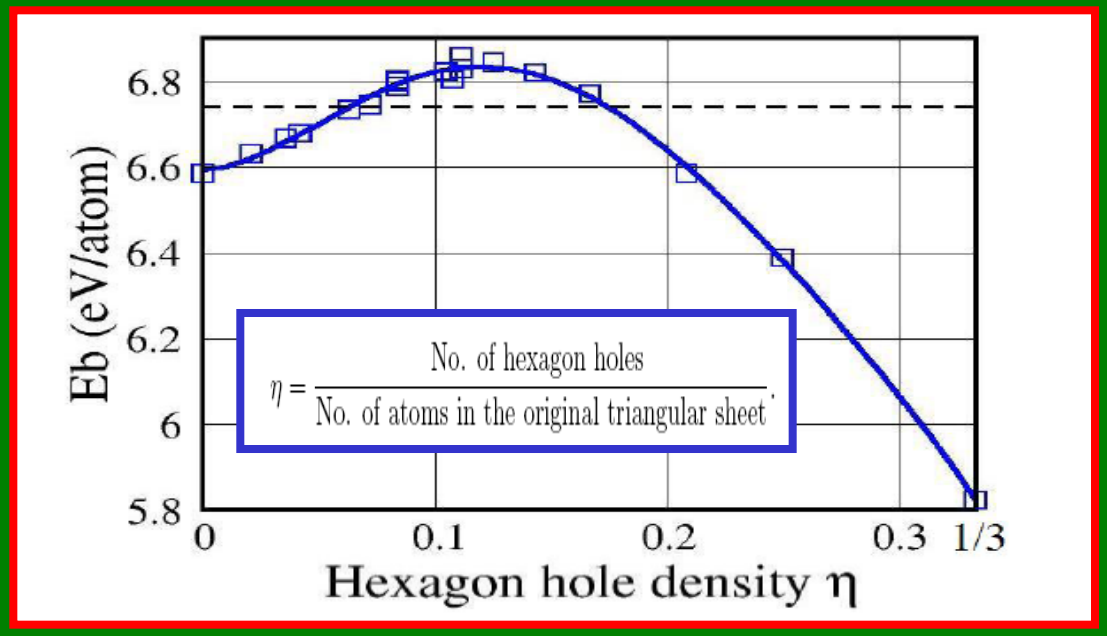
Bergische Universität Wuppertal, Germany

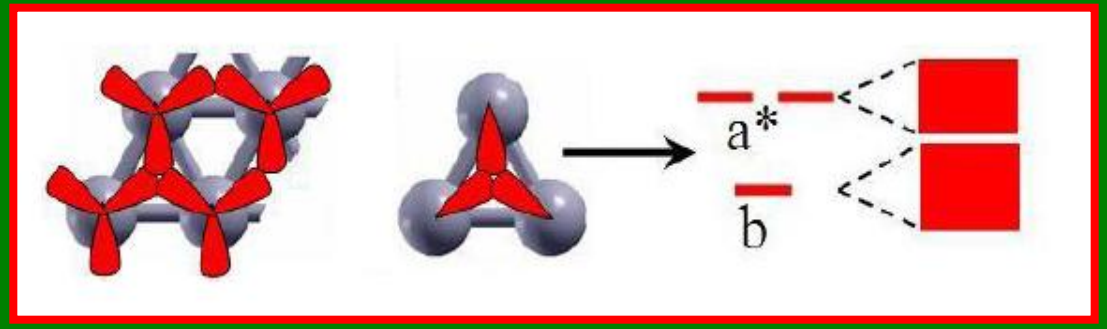
2D Boron Sheets with Hexagonal Motives

Tang & Ismail-Beigi, PRL, 99, 115501 (2007)









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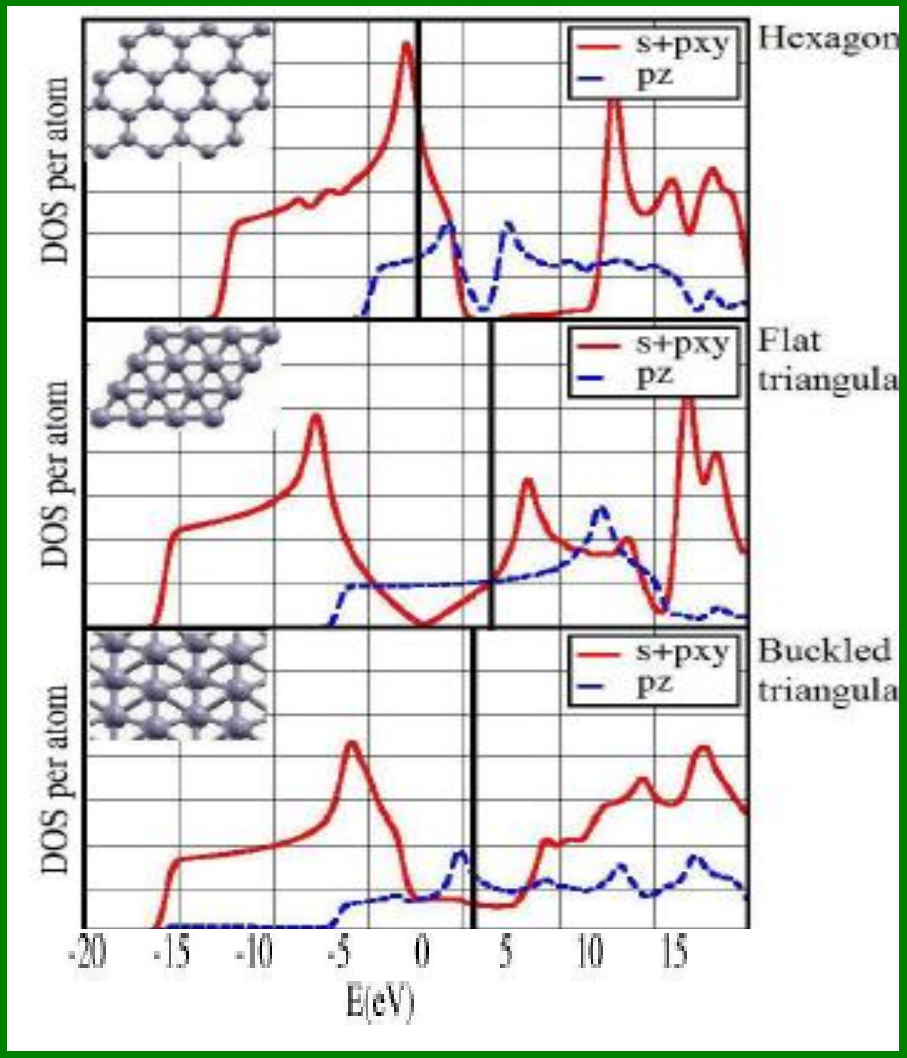
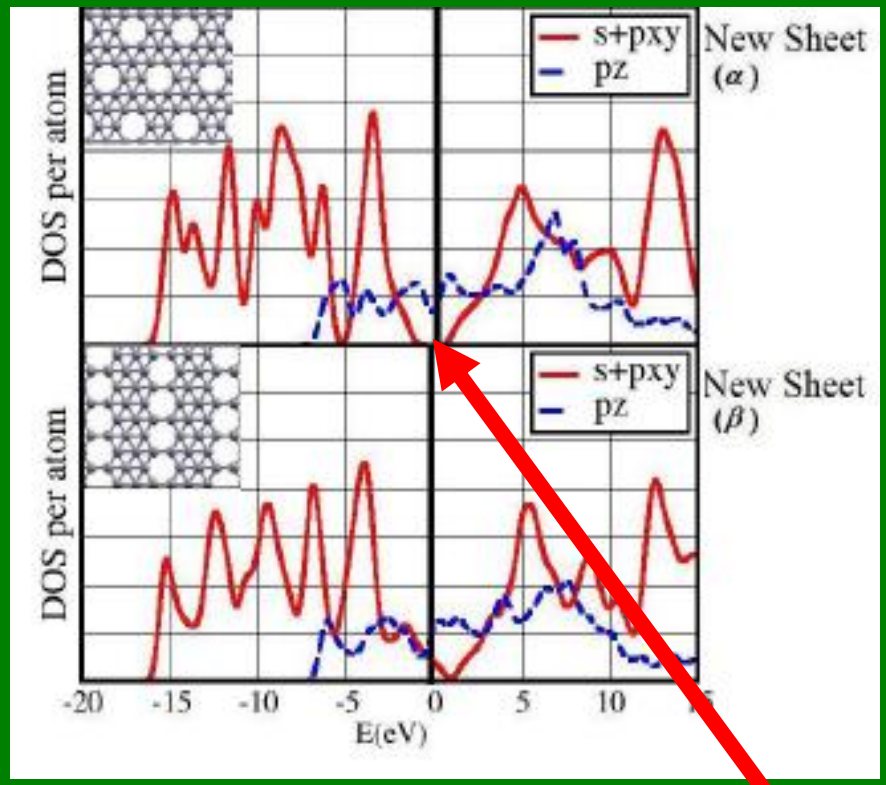
2D Boron Sheets with Hexagonal Motives

Tang & Ismail-Beigi, PRL, 99, 115501 (2007)





Highest stability occures when Ef places precisely at the zero-point of In-Plan PDOS filling all available in-plane bonding states and none of the anti-bonding ones.

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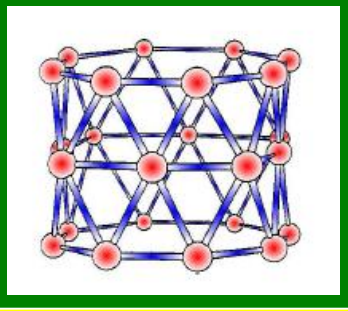
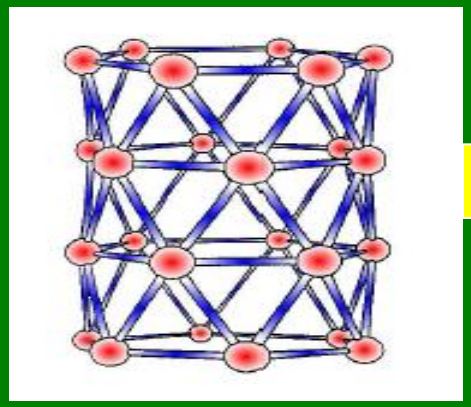
Single Wall Boron Nanotubes

Boustani & Quandt, EPL 1997, JCP 1999



24



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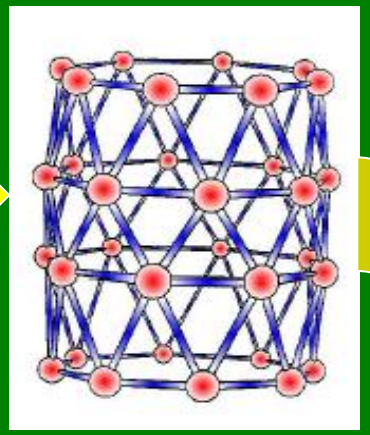

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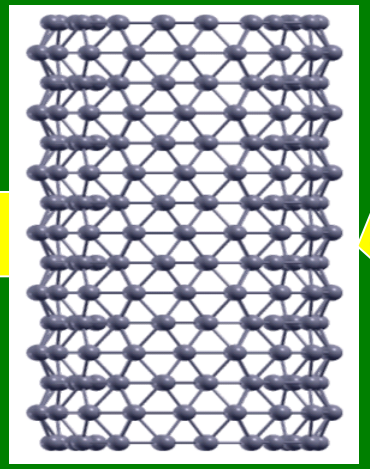

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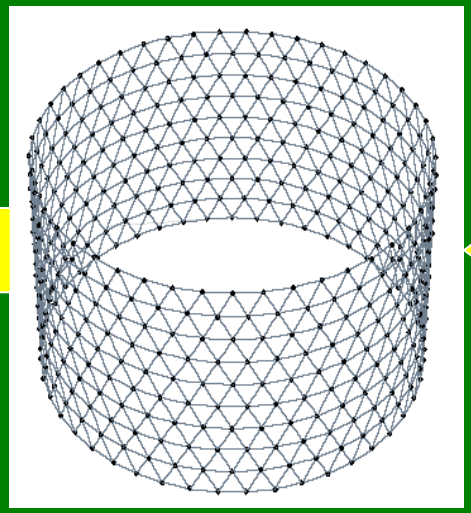
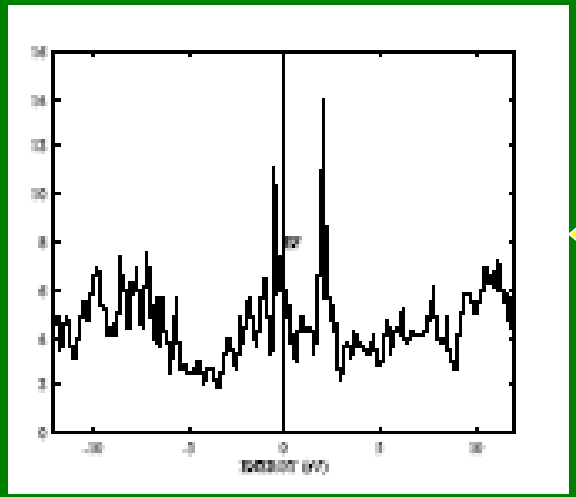


DOS



Metallic

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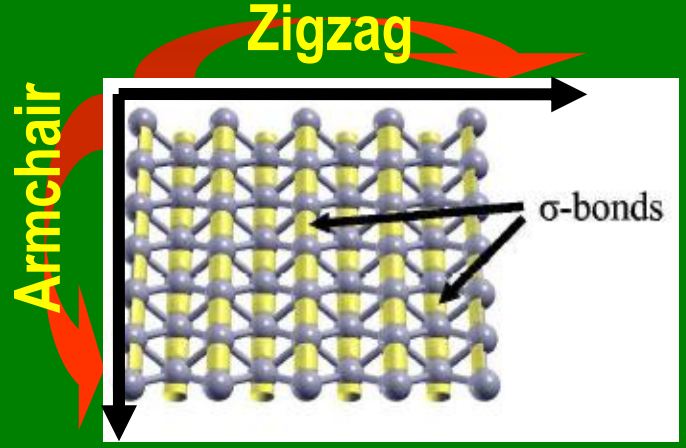
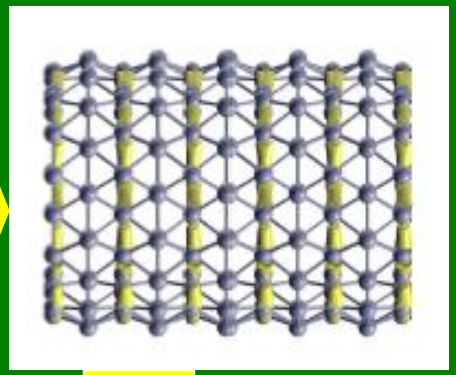
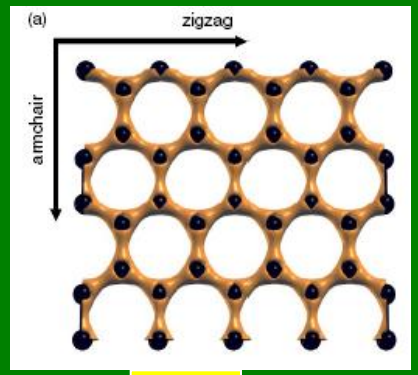
Control the Radius & Chirality of BNTs

Kunstmann, Quandt & Boustani, Nanotechnolgy 18, 155703 (2007)

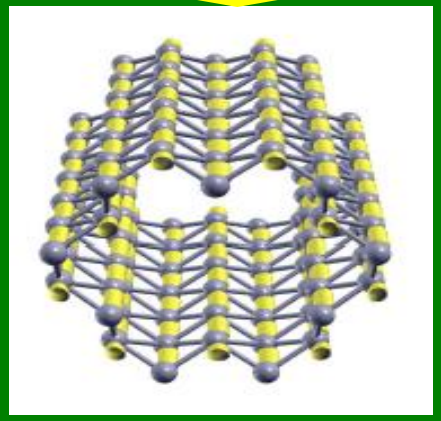


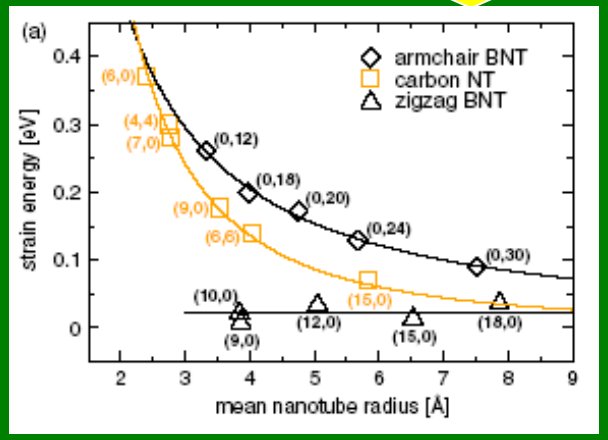
Armchair (0,N)

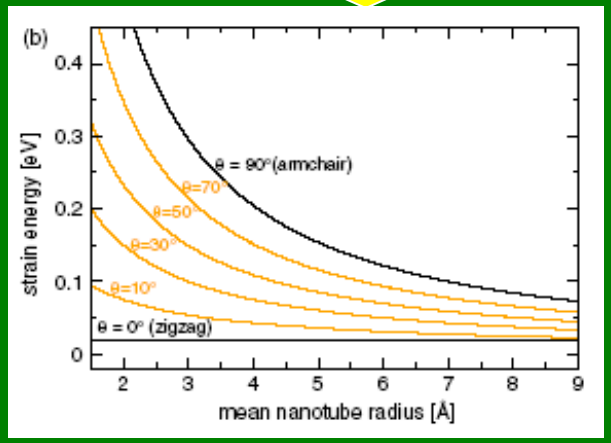




Zigzag (N,0)







Strain Energy

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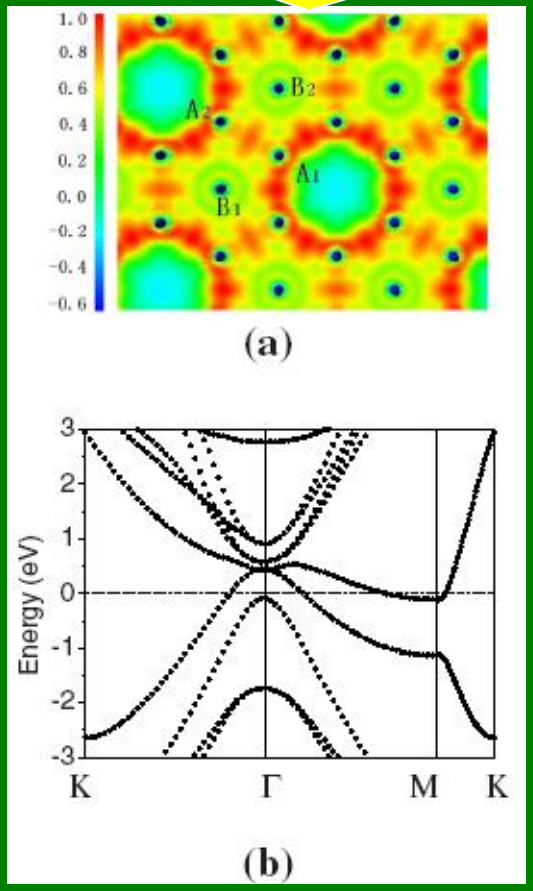
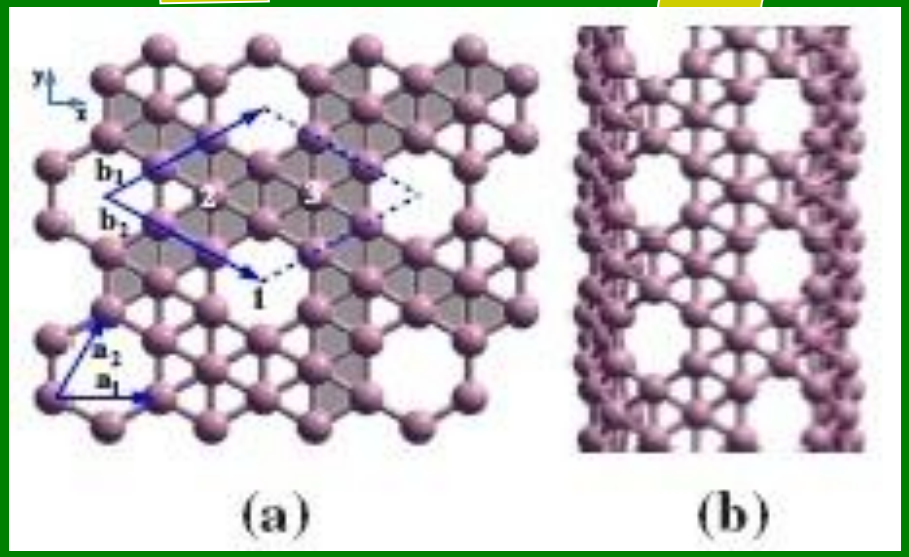
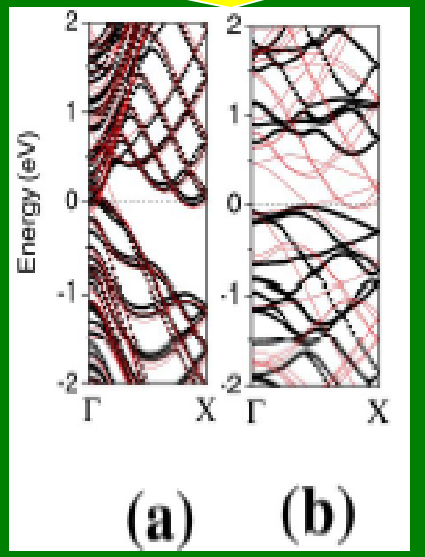
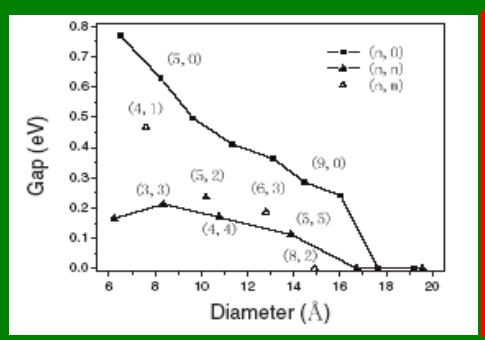
Ab initio Prediction of Boron Sheets and Nanotubes

X. Yang, Y. Ding, and J. Ni, PRB 77, 041402R (2008)









The boron sheet is a metal and the nanotubes can be either metals or semiconductors gap 0.1–0.8 eV dependent on diameter & chirality.

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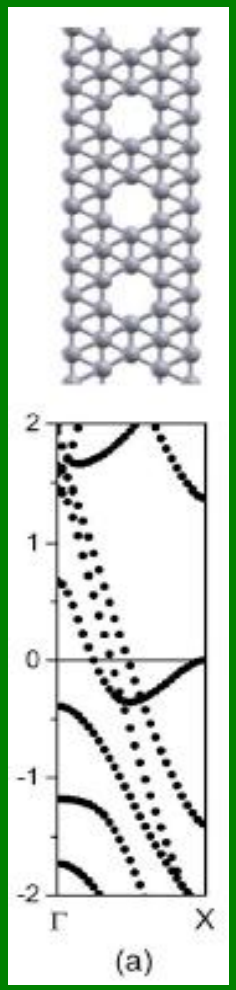
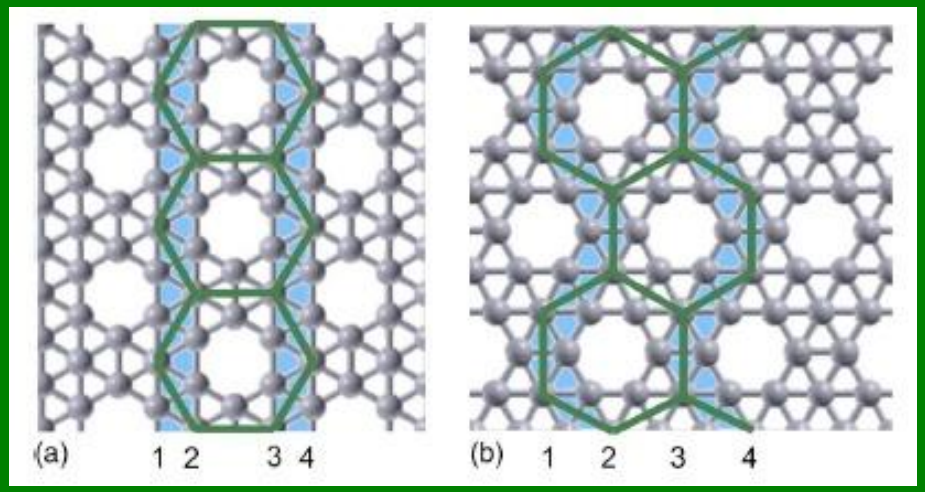
Bergische Universität Wuppertal, Germany

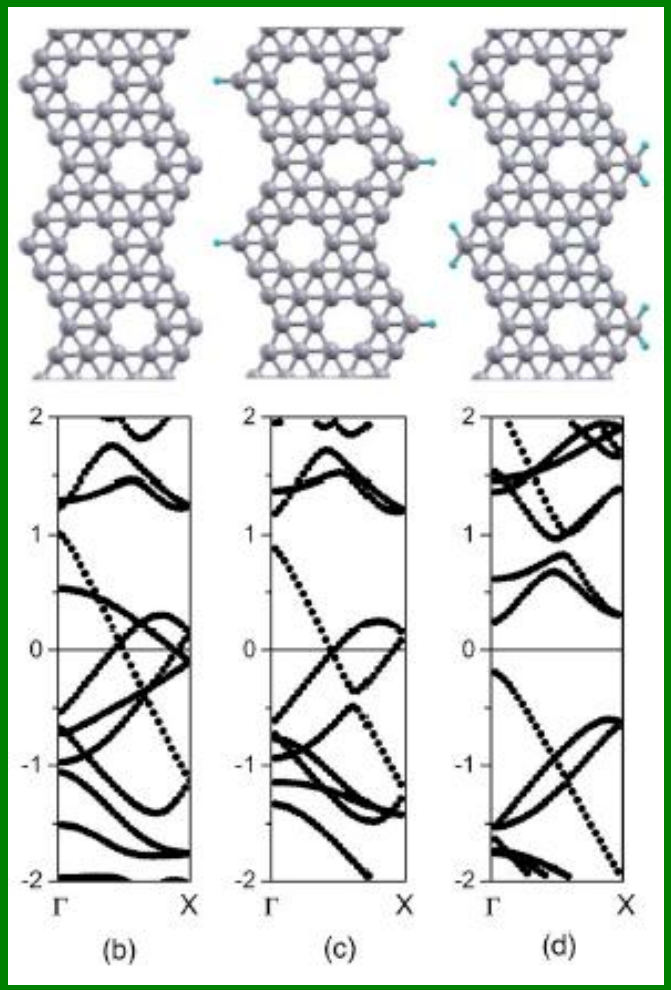
Electronic structures of boron nanoribbons

Y. Ding, X. Yang, and J. Ni, APL 93, 043107 (2008)





The boron nanoribbons with different edges are metals. The H-terminated nanoribbons are semi-conductors with a Band gap of 0.5 eV



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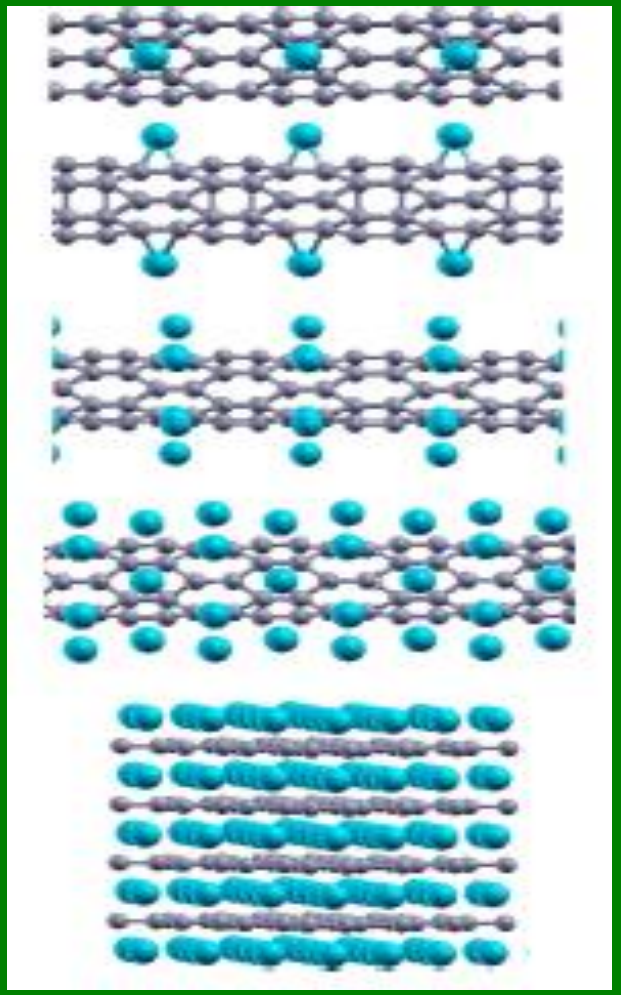
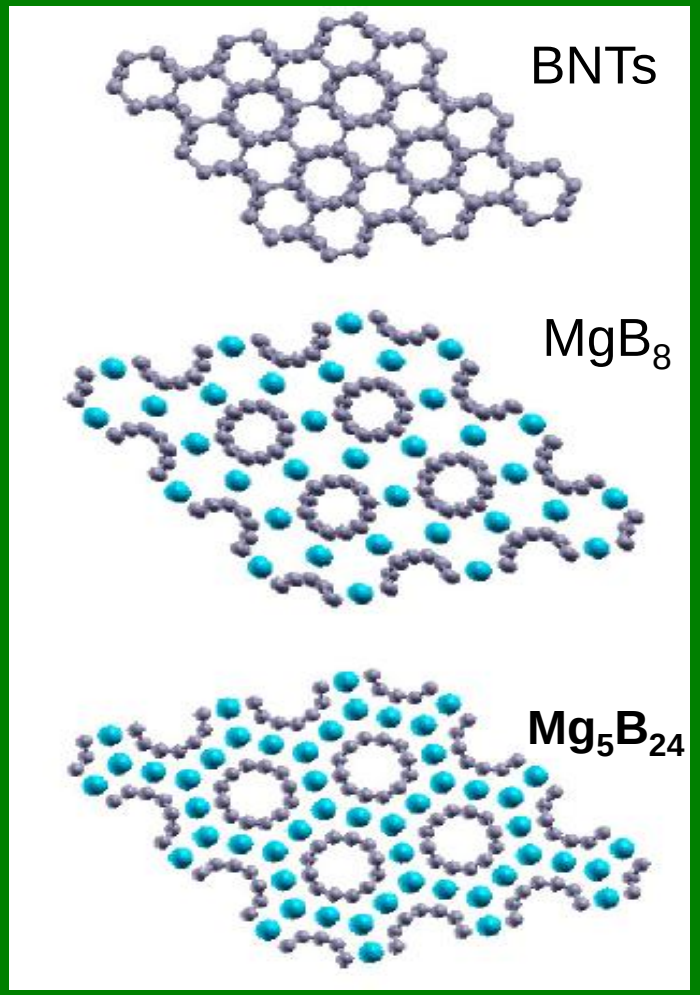
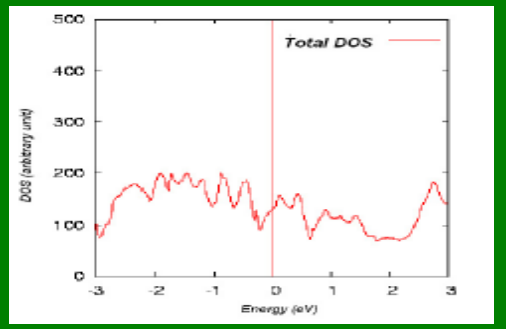
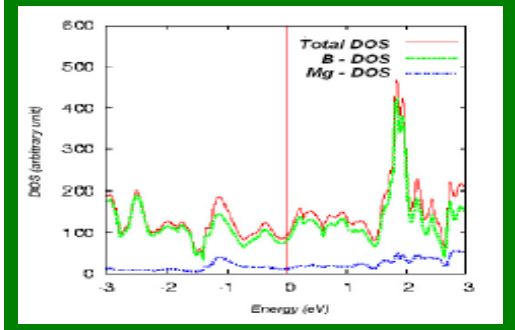
Structure and stability of Mg-intercalated boron nanotubes and crystalline bundles

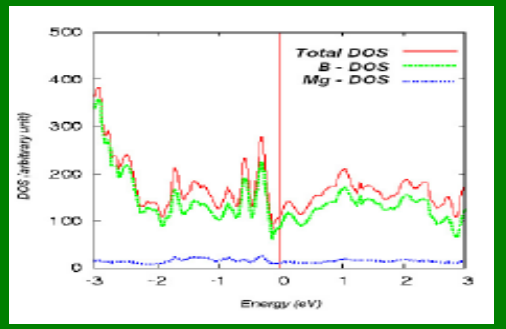
Lau, Orlando & Pandey, J. Phys.: Condens Matter 21, 045304 (2009)











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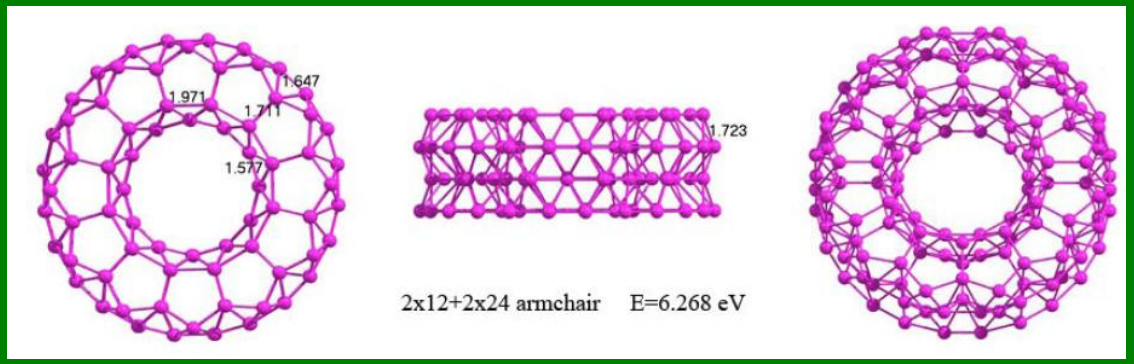
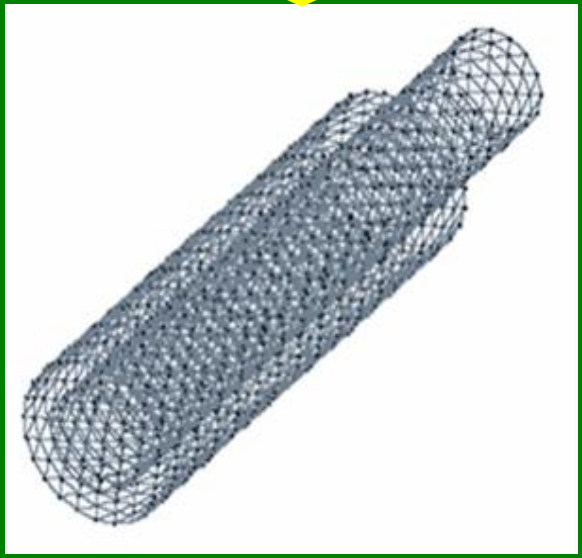
Double Wall Boron Nanotubes

Sebetci, Mete & Boustani , J. Phys. Chem. of Solids, 69, 2004 (2008)

- *Armchair (2x12+2x24)*





- *Zigzag (4x12+4x24)*

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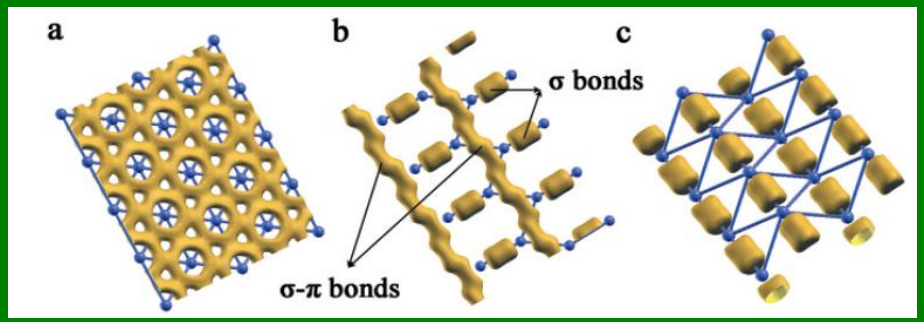
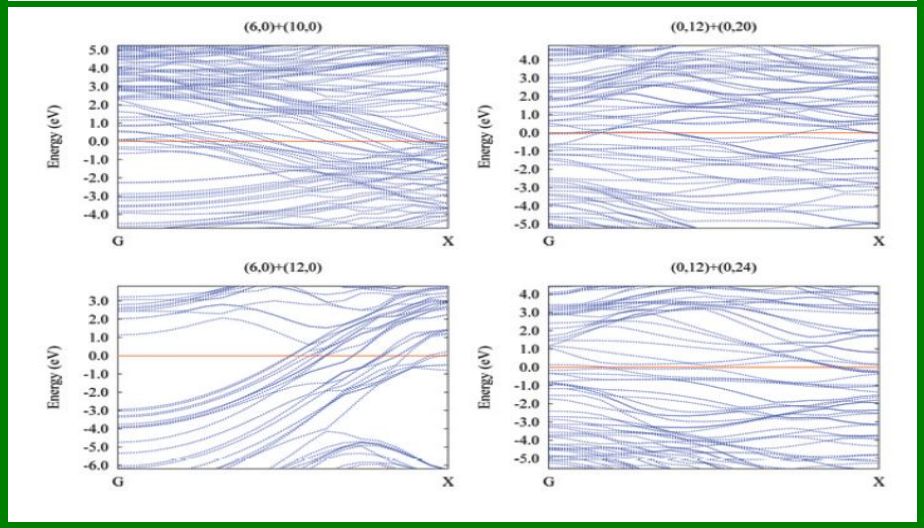
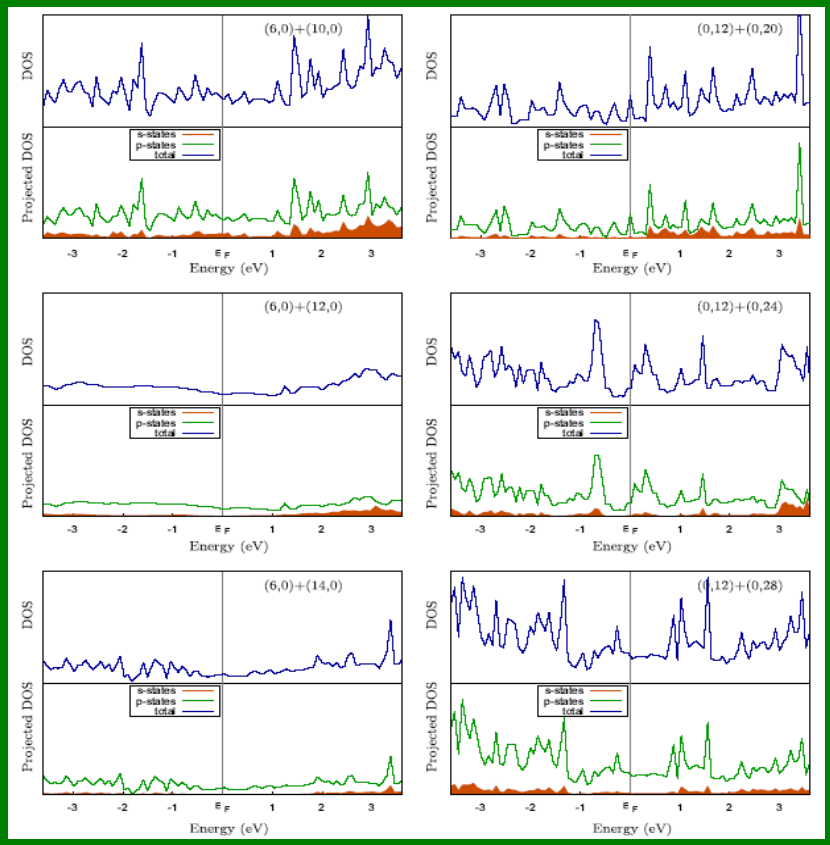
Double Wall Boron Nanotubes

Sebetci, Mete & Boustani , J. Phys. & Chem. of Solids, 69, 2004 (2008)







Band structure and density of states DOS of s-band and p-bands of zigzag and armchair DWBNTs

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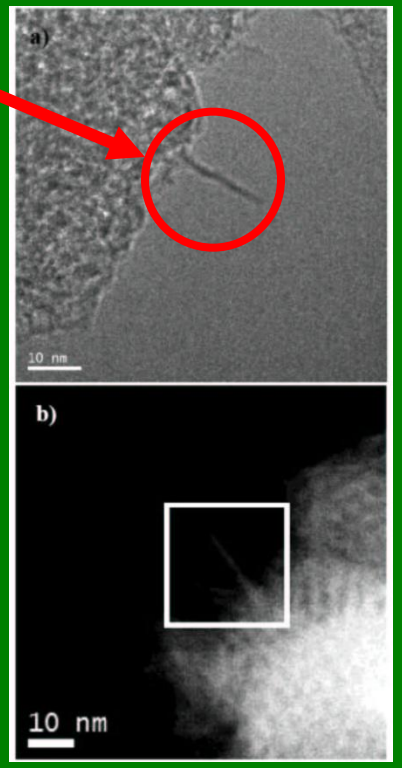
Experimental Confirmation of Single-Walled Boron Nanotubes

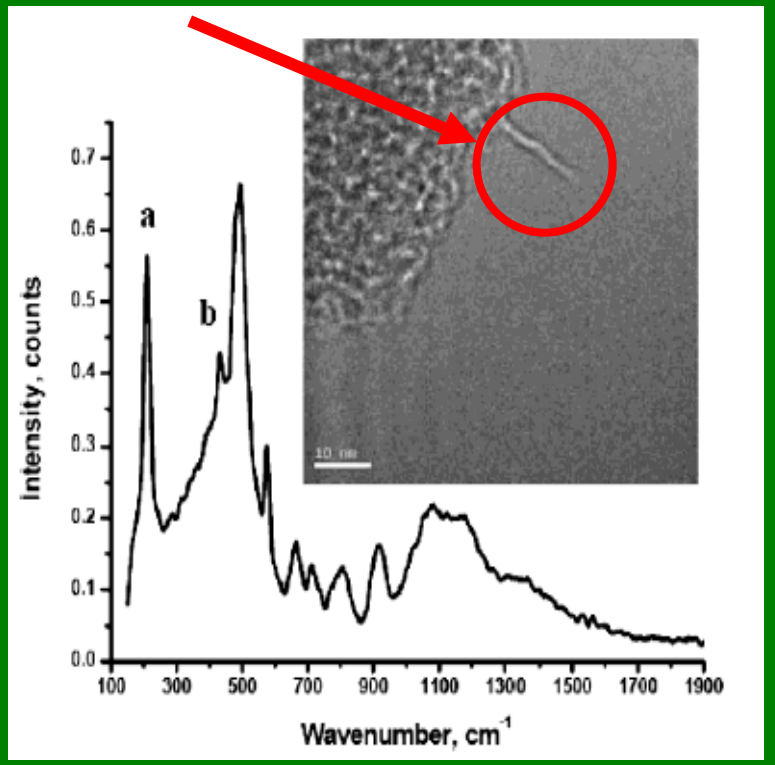
Theory : *Boustani & Quandt, Europhys. Lett. 39, 527 (1997)*

Gindulyte, Lipscomb & Massa, Inorg. Chem. 37, 6544 (1998)

Experiment :

D. Ciuparu, R.F. Klie, Y. Zhu & L. Pfefferle, J. Phys. Chem. B 108, 3967 (2004)





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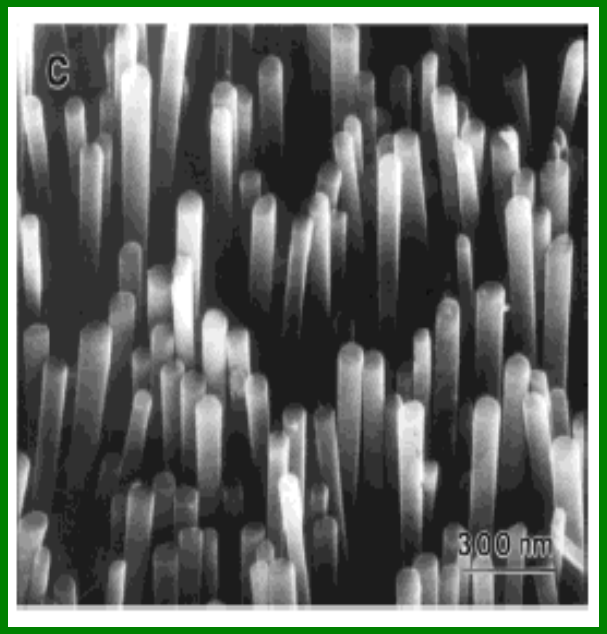
Experimental Developments of boron Nanostructures I

Theory
Boustani & Quandt et al.
JCP 110,3176 (1999)

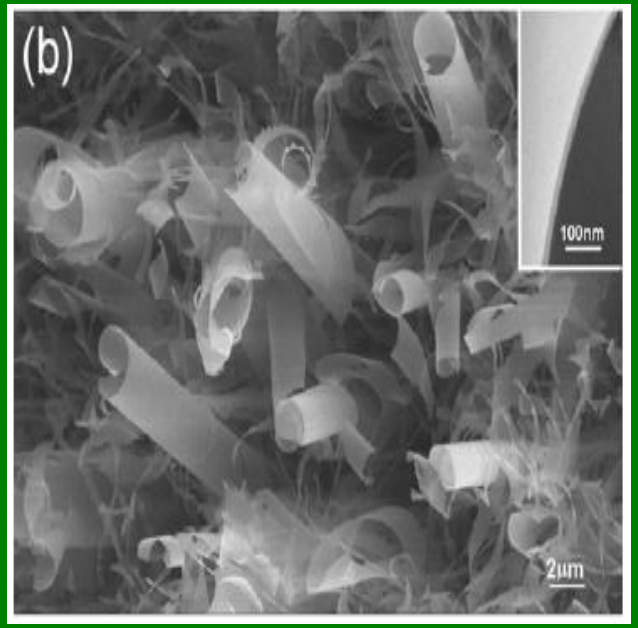
Nanowires
Cao et al. Adv. Mat.
13, 1701 (2001)

Nanoribbons
Ruoff et al. Nano Lett.
124, 4564 (2002)

Experiment



Nanobelts
Kimura et al. J. Vac. Sci.
B 23, 2510 (2005)



Nanorods
Otten et al. JACS
124, 4564 (2002)

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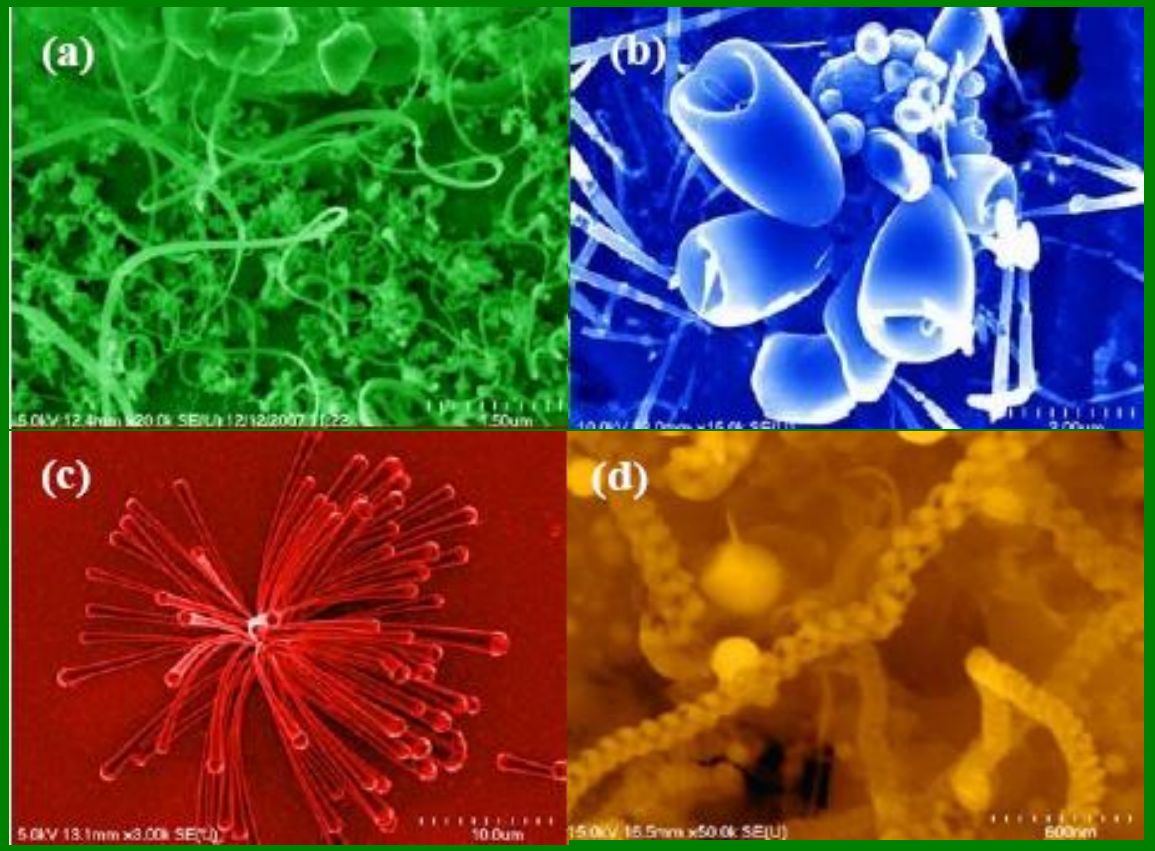
Experimental Developments of boron Nanostructures II

Yoke Khin Yap, Michigan TechnicaL University (MTU), 2008

- Nanobelts
- Nanocups
- Nanobats
- Nanoyarns



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Potential Applications

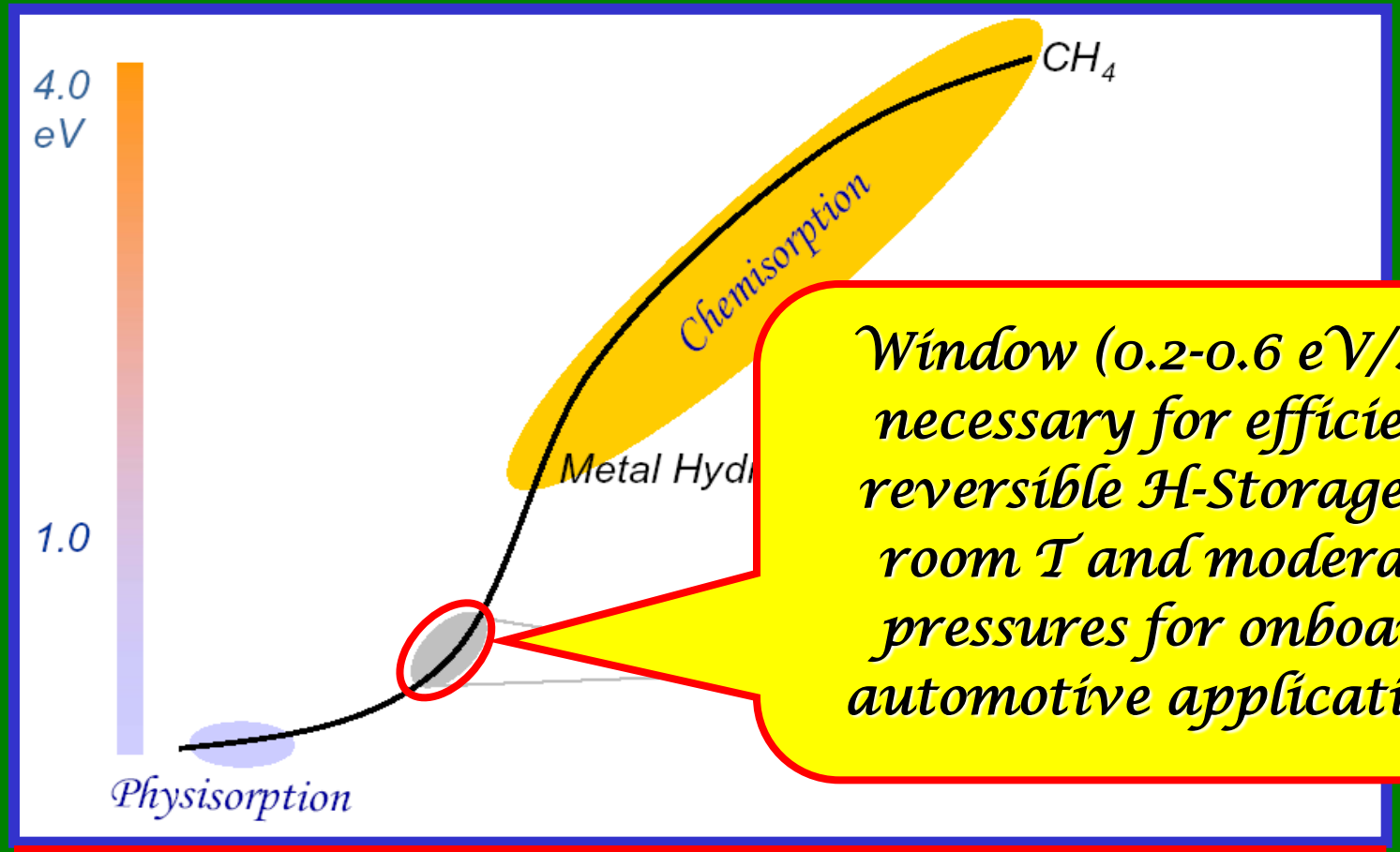
Boron Clusters :
Boron Chemistry
Hydrogen Storage
Propulsion & Energetic
Embedding & Implantation

Boron Sheets and Nanotubes :
Semiconductors
Nanotechnology
Superconductors
Neutron Absorber, Fieldemission

Doped α-Boron
Thermoelectric Devices
Coating & Ceramics
High-Temperature Devices
Electro-Optics & Corrosion

Boron Cages (Nanotubes !):
Liquid Crystals
Inorganic Chemistry
Nuclear Medicine (BNCT)

Hydrogen Storage



Materials needed for hydrogen storage are chemically non-dissociatively binding hydrogen molecules

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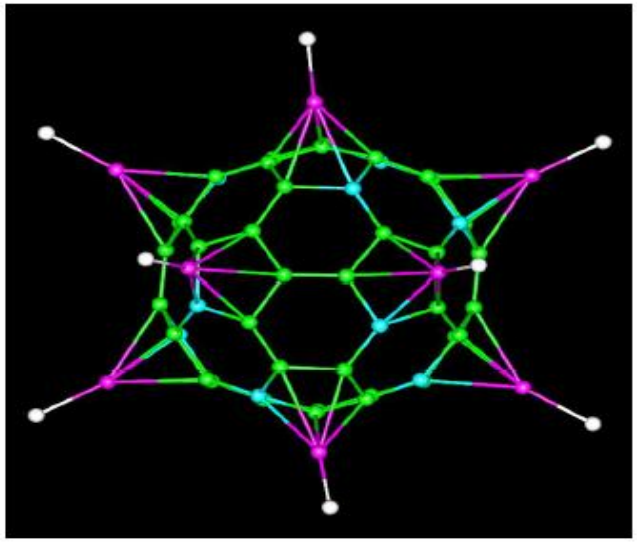
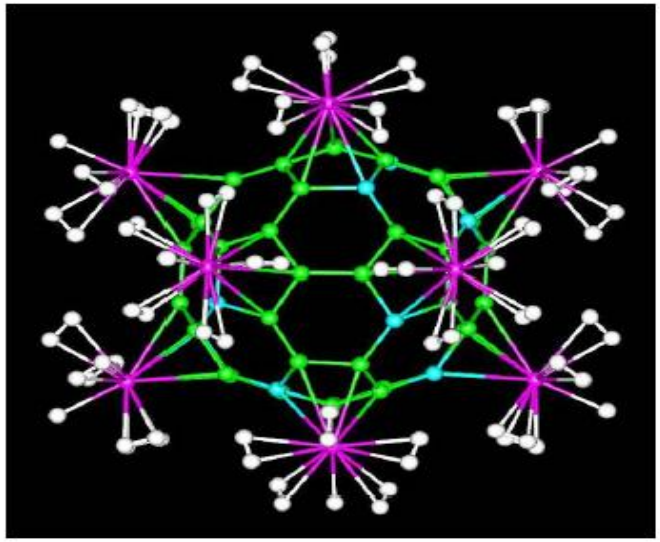
Bergische Universität Wuppertal, Germany

Hydrogen Storage I

H-Storage in Novel Organometallic Buckyballs

Zhao et al., PRL 94, 155504 (2005)





$$C_{48}B_{12}[ScH]_{12} \xrightleftharpoons{60H_2} C_{48}B_{12}[ScH(H_2)_5]_{12}$$

One more electron is transferred from each Sc atom to the corresponding pentagon, which enhances both the Sc-C46B12 binding and the hydrogen storage capacity.

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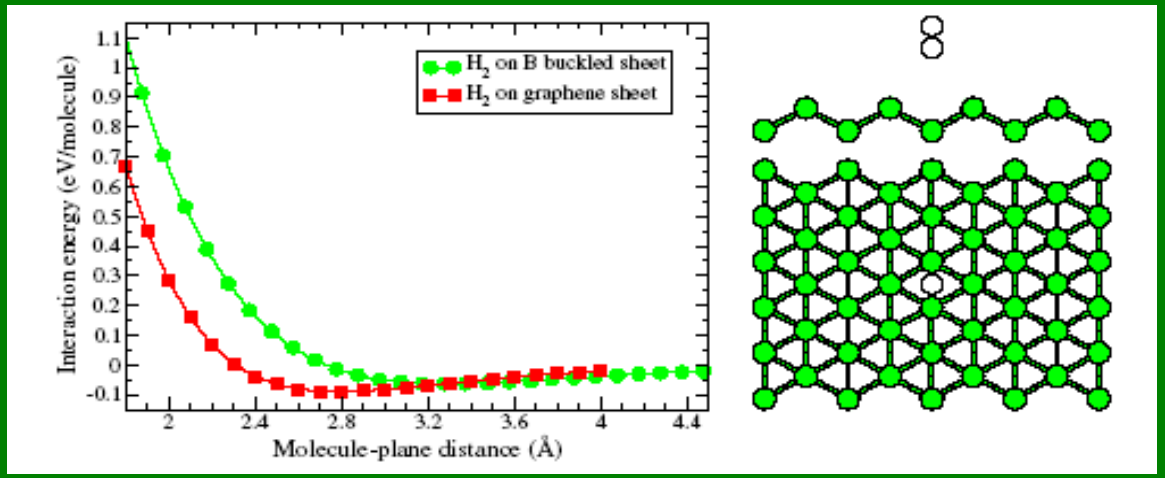
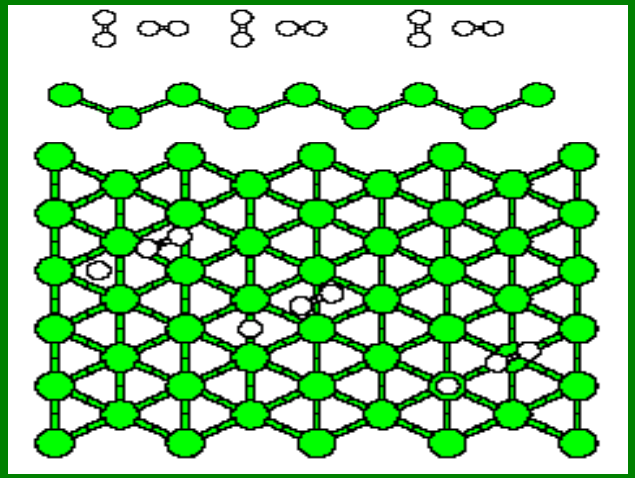
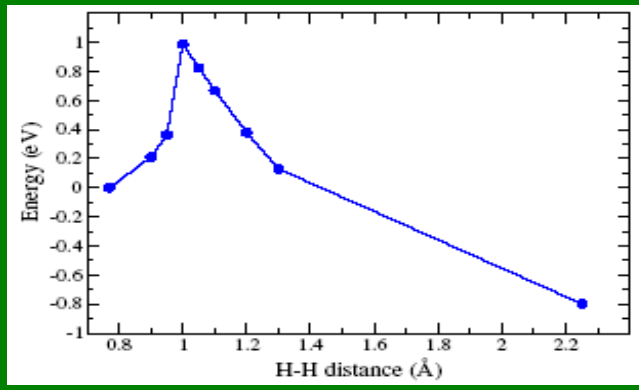
Hydrogen Storage II

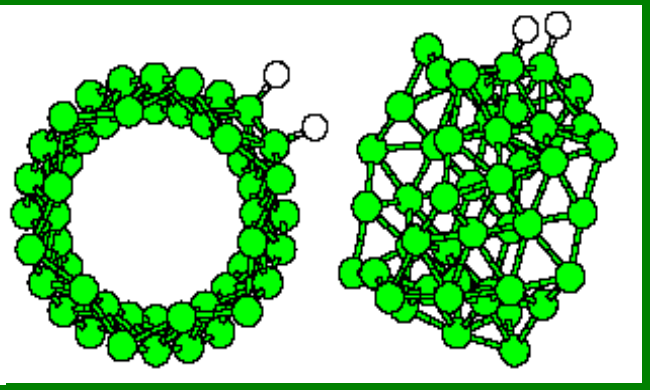
Physisorption on Boron Sheets and Nanotubes

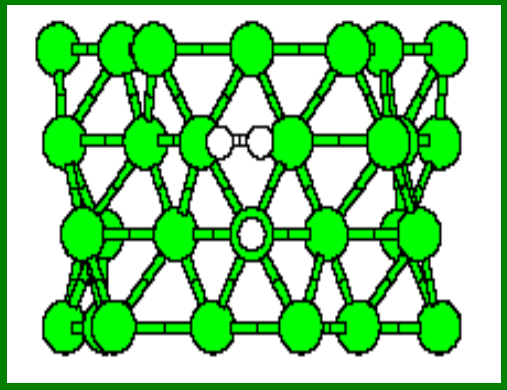
Cabria, Lopez and Alonso, Nanotechnology 17, 778 (2006)



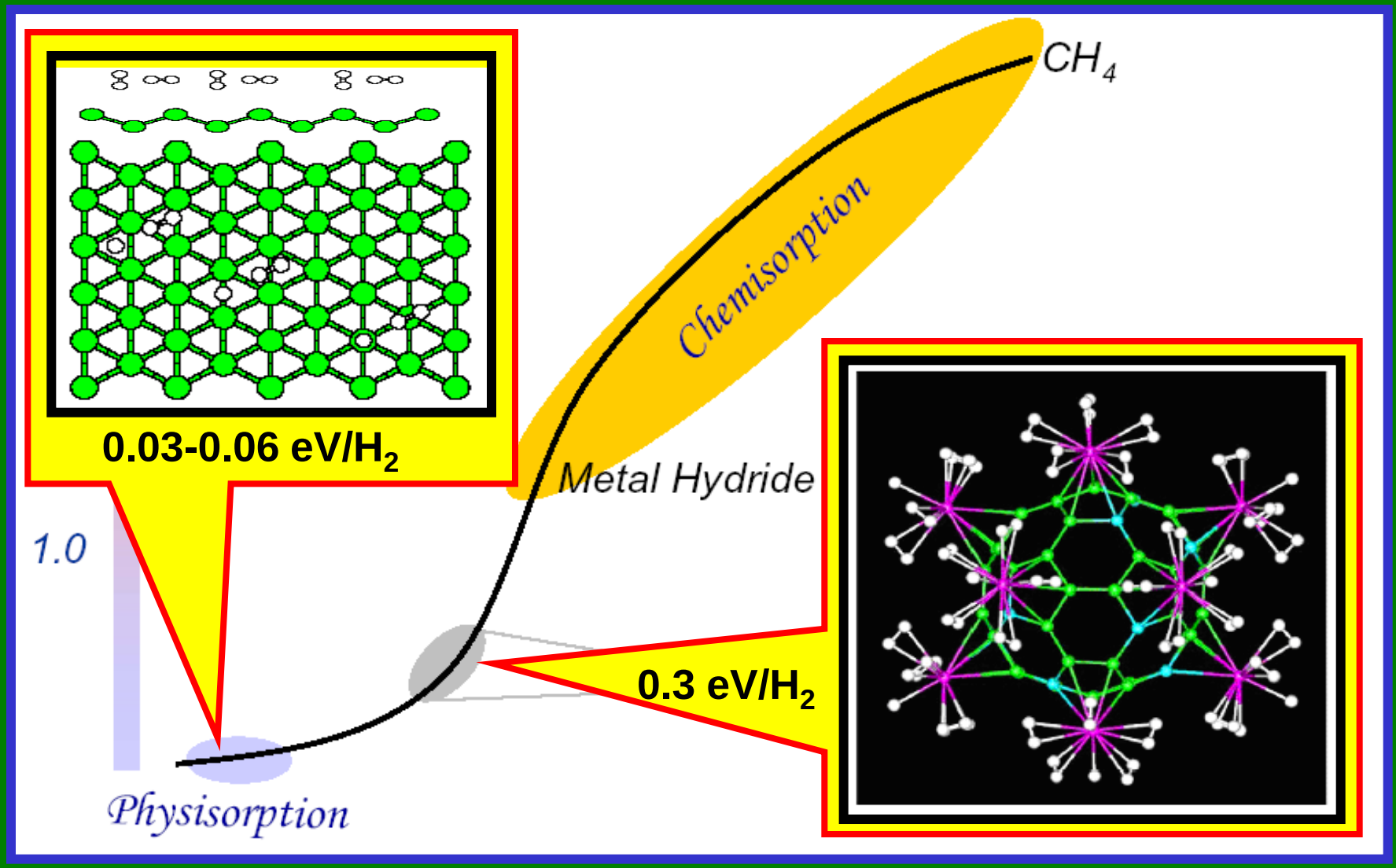






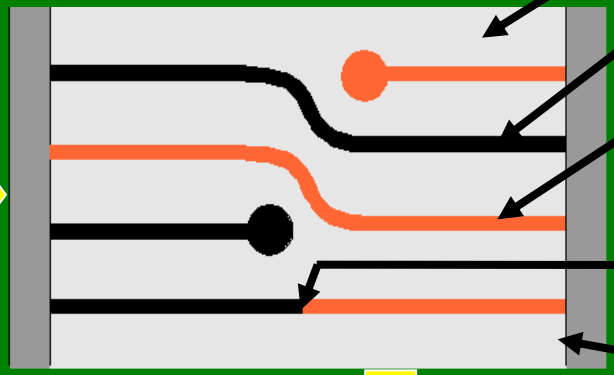


Hydrogen Storage

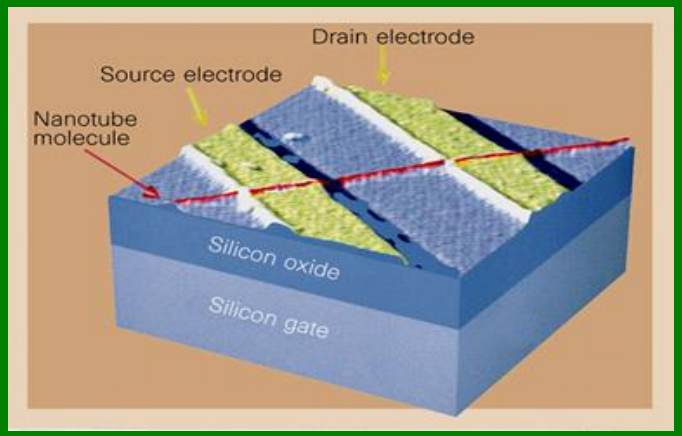


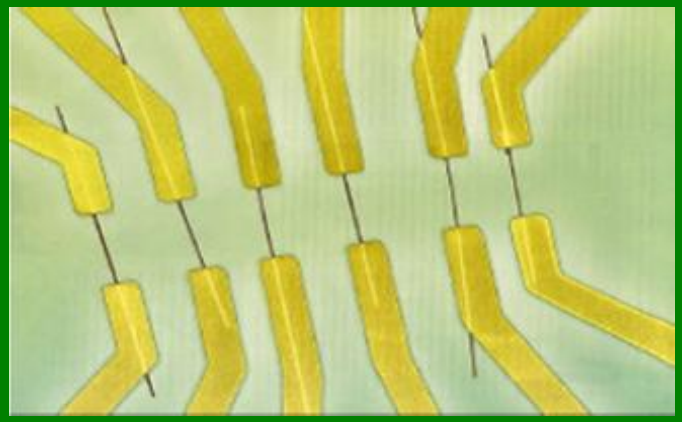
Nanotechnology

- Nanotubular Network



- Basic Layout for nanodevices





Nanowires, 5-10nm diameter

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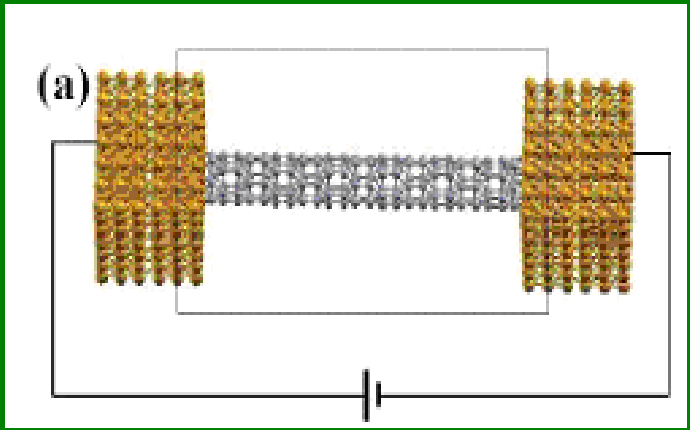
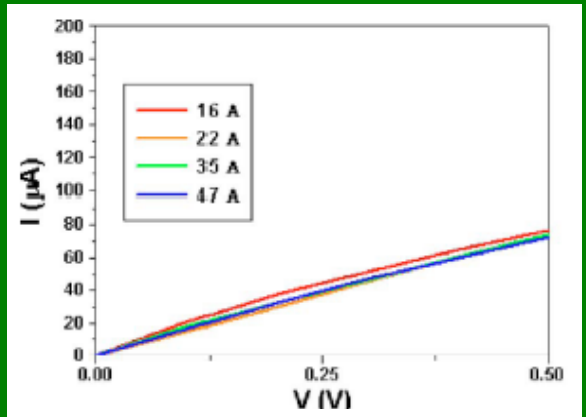
Electron Transport in Boron Nanotubes

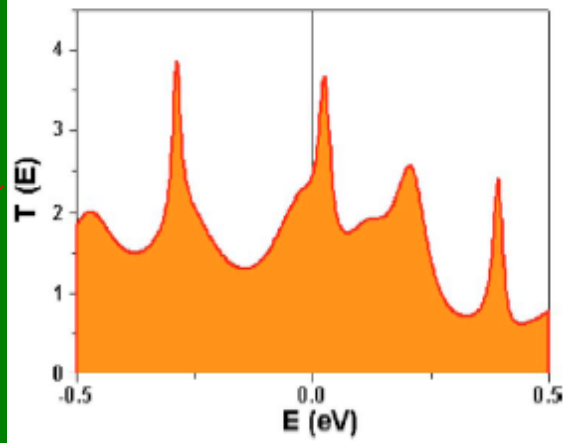
Lau & Pandey, et al., Appl. Phys. Lett., 88, 212111 (2006).

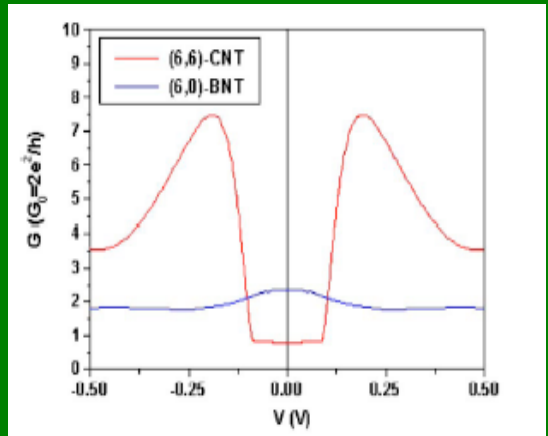


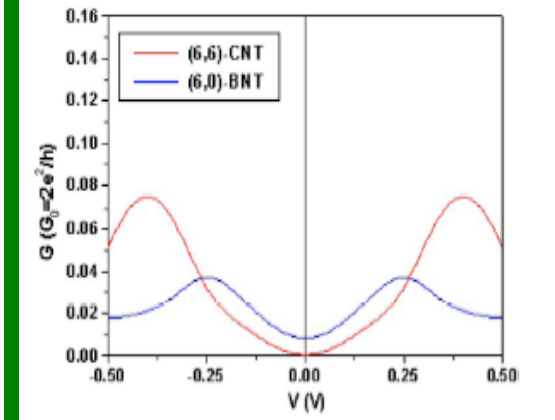
Schematic model of (6,0) SWBNT between two gold electrods

I-V characteristics and the transmission spectra of the system.









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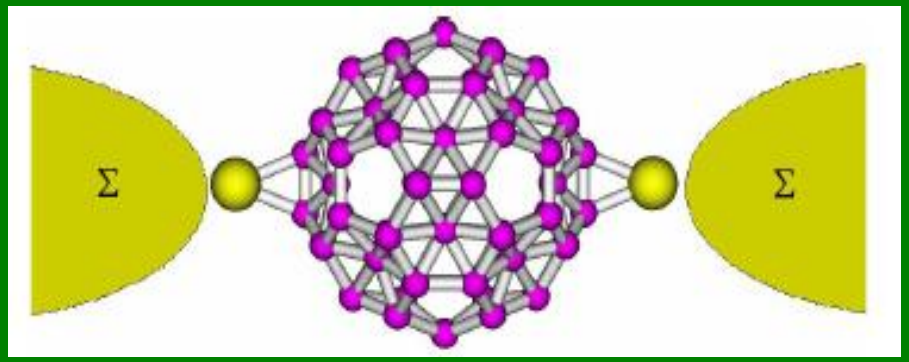
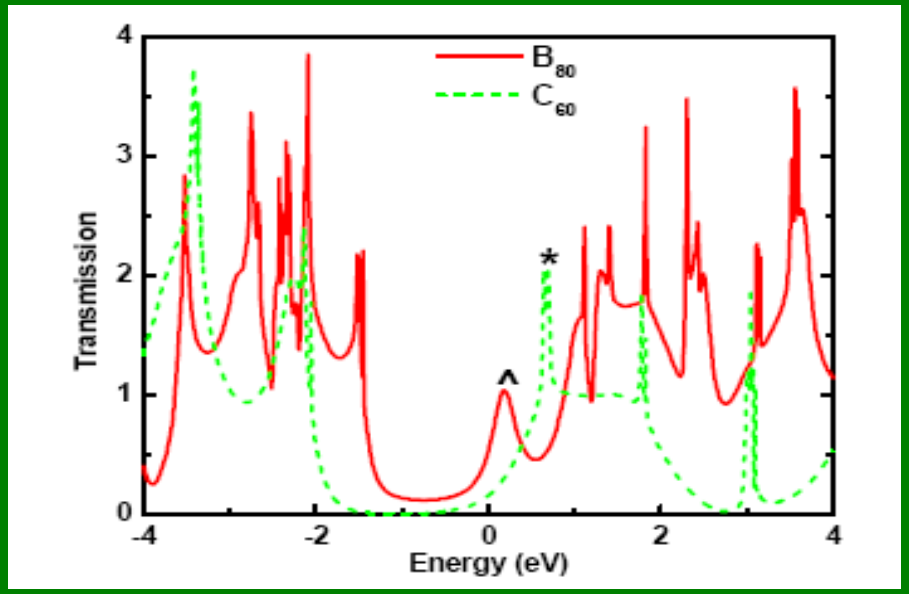
Bergische Universität Wuppertal, Germany

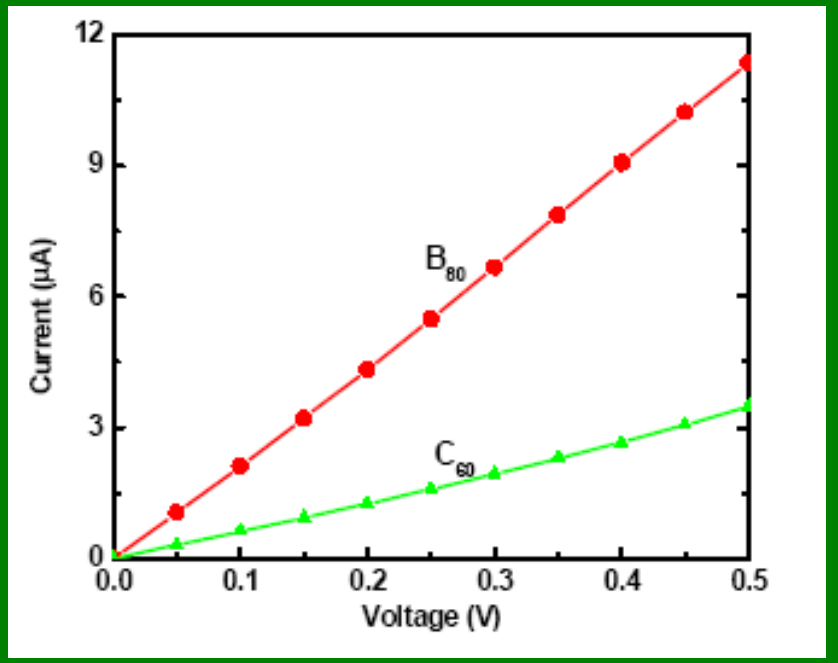
Elektron Transport in Boron Fullerenes

H. Hi, R. Pandey, and I. Boustani, IEEE (2008).



Schematic model of B_{80} Sphere between two gold electrods





Current-voltage curves for B_{80} and C_{60} molecular systems.

Conclusions

- We established a new fullerene-like researchfield called *Boron Nanomaterials*.
- Theory is able to predict nanostructures and the experimentally observed boron clusters and nanotubes are the best evidence.
- The planarity (aromaticitiy) of small boron clusters is *unique* between all atomic clusters known up to date.
- Boron Nanomaterials have (in opposite to carbon) potential applications in nanotechnology & medicine.

What is missing!

- **Theory :** Mech., Optical, Therm. and Electronic Properties, the Nature of 2e-3c Bonds, and the Aromaticity of the Most Boron Nanostructures, Simulation of Proteins@Natotubes!
- Chemical Reaction of Boron Nanostructures with small molecules (H_2, O_2, HF, CO, CO_2 ...) → H-Storage, Sensoric !
- **Experiment :** Synthesis and Production of Boron Nanotubes & Fullerenes → New Synthesis-Methods are required
- Development the Chemistry of Boron Clusters & Fullerenes → Benefit of the Planarity and Aromaticity.
- Synthesis and Production of Boron Nanosheets & Thinfilms. → Does exist a Boron-Graphene or New Boron Phases!
- Can BNanoflakes&Sheets replace expensive *c-BN*-Coating!
- Synthesis of Boron Nanomaterials for BNCT.
- Thermoelectric & Magnetic BNTs (Doping with TM & RE)

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P. Liebermann

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- *Nato Linkage Grant 972010*
- *Donostia Int. Physics Center*
- *Junta de Castilla y Leon*

Thank you for your attention