Computational Design and Modeling in Nanotechnology

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Physics and Applied physics

Nanomanufacturing Center of Excellence

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What we can do

Fundamentals

- ➤ Theoretical Prediction
- ➤ Understanding of Unknown Phenomena
- ➤ We investigate:
  - – Electronic properties
  - – Transport properties
  - – Thermal properties
 - – Mechanical properties
  - – Optical properties

Applications

- ➤ Device Design
  - – Memory devices
  - – Hydrogen storage
  - – Nanosensors

- ➤ Modeling & Simulations
  - – Device modeling
 - – Detection schemes
  - – Device response time

"Bucky-Shuttle" Memory Device
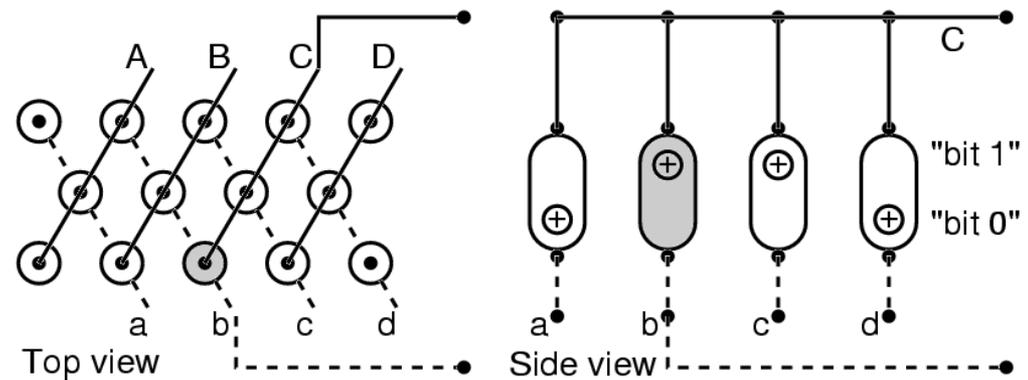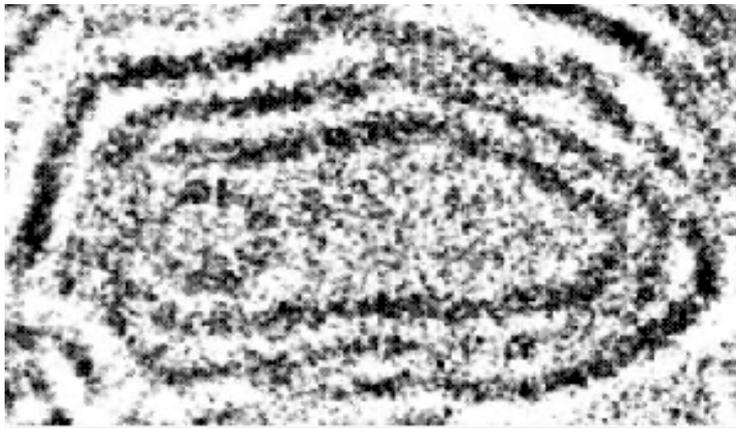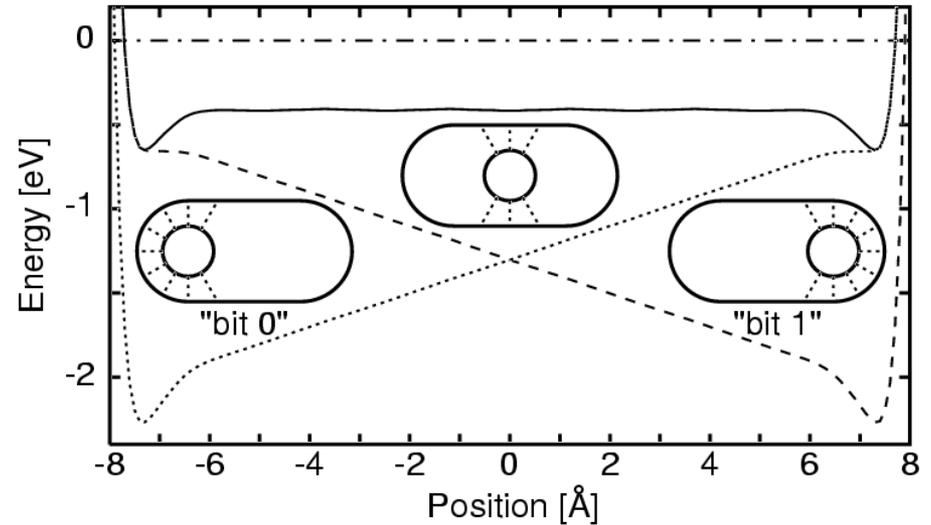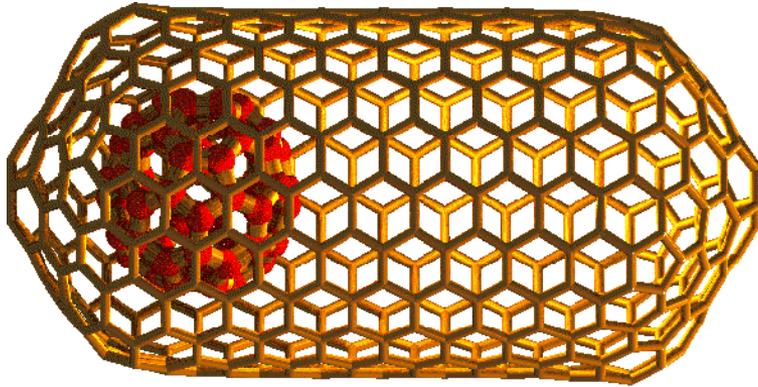
[PRL **82**, 1470 (1999); US patent # US6,473,351]

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Hydrogen Storage

1 H 100%								
3 Li 14%	4 Be 22%	5 B 28%	6 C 33%	7 N 21%	8 O 12%	9 F 5.3%		
11 Na 4.5%	12 Mg 8.3%	13 Al 11%	14 Si 14%	15 P 9.7%	16 S 6.2%	17 Cl 2.8%		

H₂ storage

H₂ production ↔ **Fuel cell**

Target: **6 Weight % of Hydrogen by 2010**
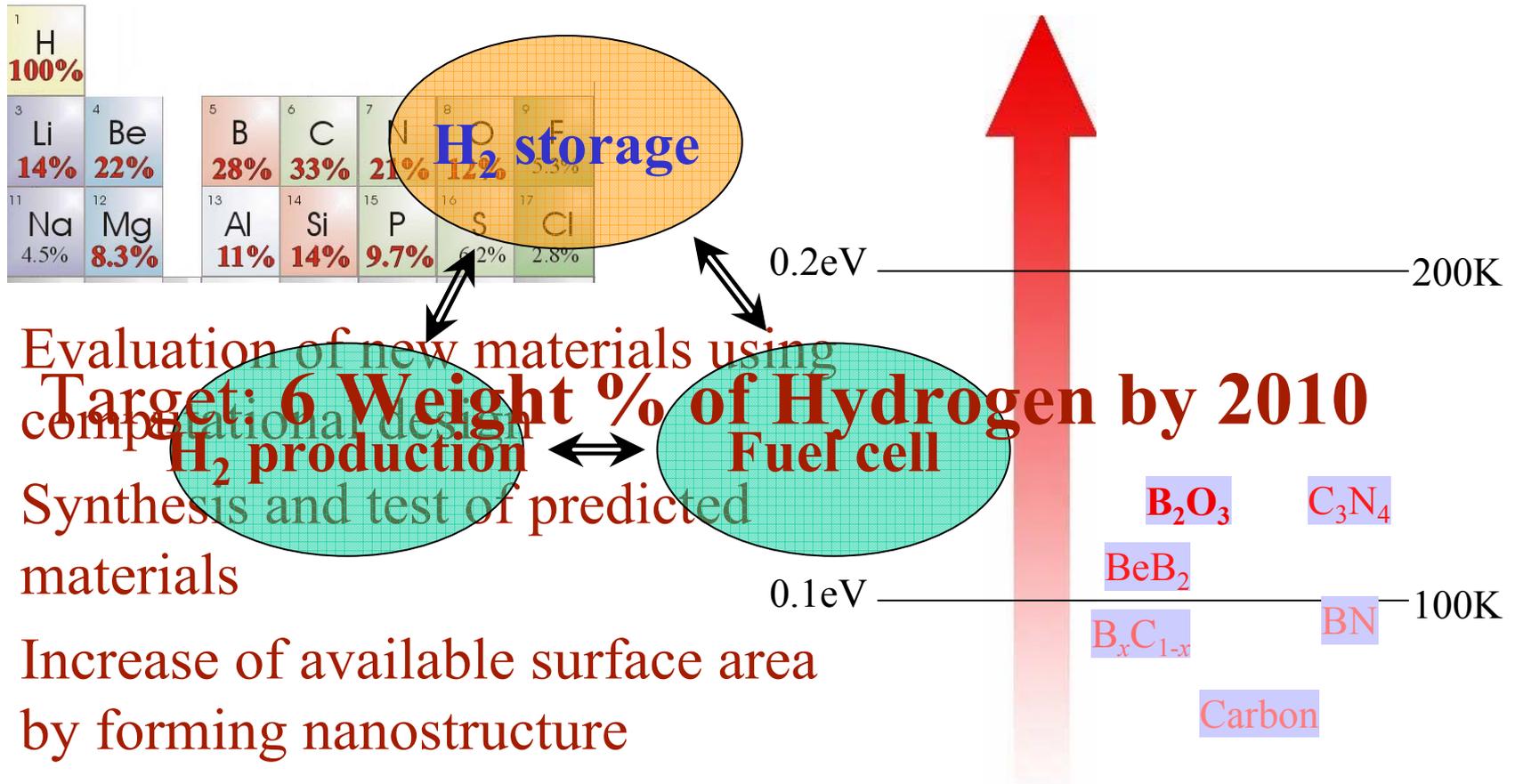
➢ Evaluation of new materials using computational design

➢ Synthesis and test of predicted materials

➢ Increase of available surface area by forming nanostructure

0.2eV ——————— 200K

0.1eV ——————— 100K

B₂O₃   C₃N₄

BeB₂

BₓC₁₋ₓ   BN

Carbon

[PRB **69**,245407 (2004); Solid State Commun. **129**, 769 (2004); PRB **71**, 035408 (2005);   US Patents #6,672,077; #6,834,508; #6,991,773]

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Gas Adsorption on NTs: Sensors
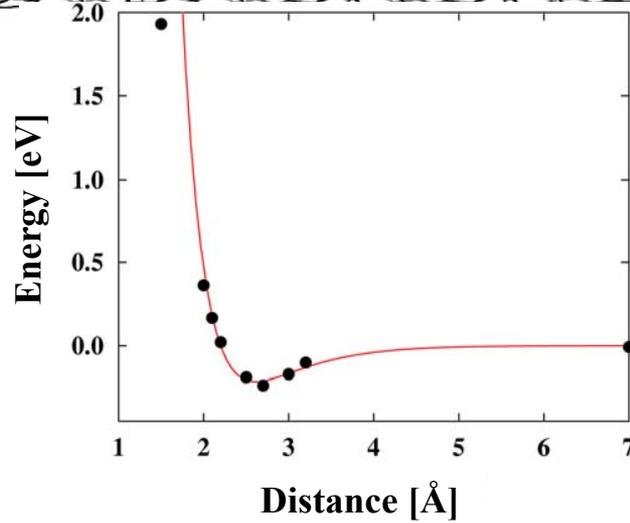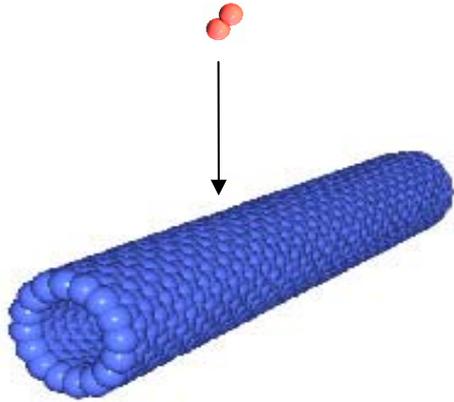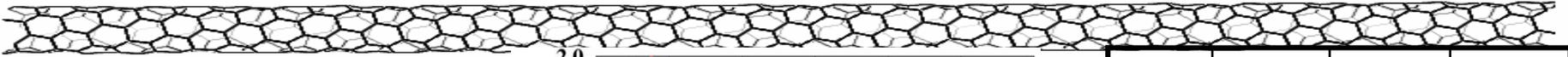
Gas	Calc. [eV]	Expt. [eV]	$\Delta q[e]$
O_2	0.12		+0.1
H_2	0.065	0.06	+0.01
NH_3	0.25	0.25	−0.02
NO_2	0.43	0.4	+0.2
CH_4	0.13	0.126	
SO_2	0.4		+0.3
O_3	0.3		+0.1
CO_2	0.27		

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