

Small is Beautiful

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Which is the smallest object that
you have *seen* so far?

Which is the smallest object that
you have *seen* so far?

Macroscopic : visible to the naked eye

Which is the smallest object that you *know*?

Which is the smallest object that you *know*?

Microscopic : Not visible to the naked eye



That is a fantasy!!

That is a fantasy!!

*Here is a REAL example of
miniaturization*

256 MB = 256×10^6 Bytes

16 GB = 16×10^9 Bytes

a byte is a unit of computer memory

It is miniaturized (reduced in size) with enhanced capacity

Miniaturization: Reduce the size without changing the property!

1971: Intel Transistor count 2,300 with area 12 sq. mm

2016: Intel Transistor count 7,200,000,000 within area of
456 sq. mm

In last 45 years size of a transistor has
reduced drastically

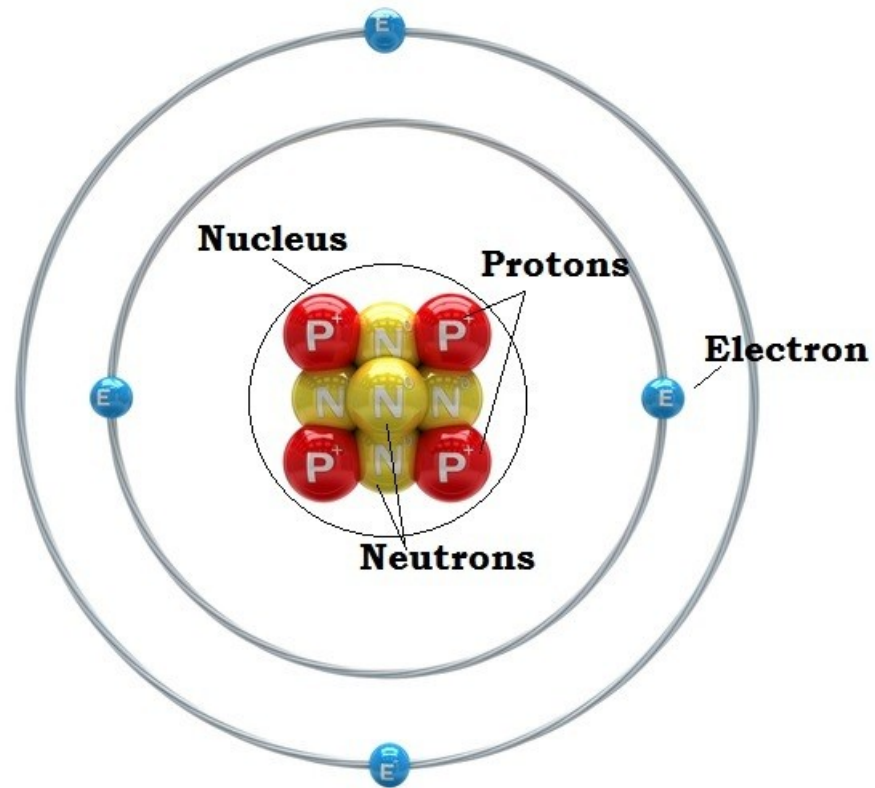
Reduce the size without
changing the property!

There is limit to this
miniaturization!!

Why?

What is *everything* made up of?

Inside an atom



Periodic Table of the Elements

Period	Periodic Table of the Elements																			
	1 IA 1A	2 IIA 2A		3-10 IIIB-10B										11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A
1	1 H Hydrogen 1s ¹																	2 He Helium 1s ²		
2	3 Li Lithium [He]2s ¹	4 Be Beryllium [He]2s ²											5 B Boron [He]2s ² 2p ¹	6 C Carbon [He]2s ² 2p ²	7 N Nitrogen [He]2s ² 2p ³	8 O Oxygen [He]2s ² 2p ⁴	9 F Fluorine [He]2s ² 2p ⁵	10 Ne Neon [He]2s ² 2p ⁶		
3	11 Na Sodium [Ne]3s ¹	12 Mg Magnesium [Ne]3s ²	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 9	10 VIII 10	11 IB 1B	12 IIB 2B	13 Al Aluminum [Ne]3s ² 3p ¹	14 Si Silicon [Ne]3s ² 3p ²	15 P Phosphorus [Ne]3s ² 3p ³	16 S Sulfur [Ne]3s ² 3p ⁴	17 Cl Chlorine [Ne]3s ² 3p ⁵	18 Ar Argon [Ne]3s ² 3p ⁶		
4	19 K Potassium [Ar]4s ¹	20 Ca Calcium [Ar]4s ²	21 Sc Scandium [Ar]3d ¹ 4s ²	22 Ti Titanium [Ar]3d ² 4s ²	23 V Vanadium [Ar]3d ³ 4s ²	24 Cr Chromium 2.8 13 2 [Ar]3d ⁵ 4s ¹	25 Mn Manganese 2.8 13 2 [Ar]3d ⁵ 4s ²	26 Fe Iron 2.8 13 2 [Ar]3d ⁶ 4s ²	27 Co Cobalt 2.8 13 2 [Ar]3d ⁷ 4s ²	28 Ni Nickel 2.8 13 2 [Ar]3d ⁸ 4s ²	29 Cu Copper 2.8 18 1 [Ar]3d ¹⁰ 4s ¹	30 Zn Zinc 2.8 18 2 [Ar]3d ¹⁰ 4s ²	31 Ga Gallium 2.8 18 3 [Ar]3d ¹⁰ 4s ² 4p ¹	32 Ge Germanium 2.8 18 3 [Ar]3d ¹⁰ 4s ² 4p ²	33 As Arsenic 2.8 18 3 [Ar]3d ¹⁰ 4s ² 4p ³	34 Se Selenium 2.8 18 4 [Ar]3d ¹⁰ 4s ² 4p ⁴	35 Br Bromine 2.8 18 5 [Ar]3d ¹⁰ 4s ² 4p ⁵	36 Kr Krypton 2.8 18 6 [Ar]3d ¹⁰ 4s ² 4p ⁶		
5	37 Rb Rubidium 2.8 18 18 1 [Kr]5s ¹	38 Sr Strontium 2.8 18 18 2 [Kr]5s ²	39 Y Yttrium 2.8 18 18 2 [Kr]4d ¹ 5s ²	40 Zr Zirconium 2.8 18 10 2 [Kr]4d ² 5s ²	41 Nb Niobium 2.8 18 12 1 [Kr]4d ⁴ 5s ¹	42 Mo Molybdenum 2.8 18 13 1 [Kr]4d ⁵ 5s ¹	43 Tc Technetium 2.8 18 14 1 [Kr]4d ⁵ 5s ²	44 Ru Ruthenium 2.8 18 15 1 [Kr]4d ⁷ 5s ¹	45 Rh Rhodium 2.8 18 16 1 [Kr]4d ⁸ 5s ¹	46 Pd Palladium 2.8 18 18 [Kr]4d ¹⁰	47 Ag Silver 2.8 18 18 1 [Kr]4d ¹⁰ 5s ¹	48 Cd Cadmium 2.8 18 18 2 [Kr]4d ¹⁰ 5s ²	49 In Indium 2.8 18 18 3 [Kr]4d ¹⁰ 5s ² 5p ¹	50 Sn Tin 2.8 18 18 4 [Kr]4d ¹⁰ 5s ² 5p ²	51 Sb Antimony 2.8 18 18 5 [Kr]4d ¹⁰ 5s ² 5p ³	52 Te Tellurium 2.8 18 18 6 [Kr]4d ¹⁰ 5s ² 5p ⁴	53 I Iodine 2.8 18 18 7 [Kr]4d ¹⁰ 5s ² 5p ⁵	54 Xe Xenon 2.8 18 18 8 [Kr]4d ¹⁰ 5s ² 5p ⁶		
6	55 Cs Cesium 2.8 18 18 18 1 [Xe]6s ¹	56 Ba Barium 2.8 18 18 18 2 [Xe]6s ²	57-71 Lanthanide Series	72 Hf Hafnium 2.8 18 32 10 2 [Xe]4f ¹⁴ 5d ² 6s ²	73 Ta Tantalum 2.8 18 32 11 2 [Xe]4f ¹⁴ 5d ³ 6s ²	74 W Tungsten 2.8 18 32 12 2 [Xe]4f ¹⁴ 5d ⁴ 6s ²	75 Re Rhenium 2.8 18 32 13 2 [Xe]4f ¹⁴ 5d ⁵ 6s ²	76 Os Osmium 2.8 18 32 14 2 [Xe]4f ¹⁴ 5d ⁶ 6s ²	77 Ir Iridium 2.8 18 32 15 2 [Xe]4f ¹⁴ 5d ⁷ 6s ²	78 Pt Platinum 2.8 18 32 17 1 [Xe]4f ¹⁴ 5d ⁹ 6s ¹	79 Au Gold 2.8 18 32 18 1 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹	80 Hg Mercury 2.8 18 32 18 2 [Xe]4f ¹⁴ 5d ¹⁰ 6s ²	81 Tl Thallium 2.8 18 32 18 3 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ¹	82 Pb Lead 2.8 18 32 18 4 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ²	83 Bi Bismuth 2.8 18 32 18 5 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ³	84 Po Polonium 2.8 18 32 18 6 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁴	85 At Astatine 2.8 18 32 18 7 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁵	86 Rn Radon 2.8 18 32 18 8 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁶		
7	87 Fr Francium 2.8 18 32 18 18 1 [Rn]7s ¹	88 Ra Radium 2.8 18 32 18 18 2 [Rn]7s ²	89-103 Actinide Series	104 Rf Rutherfordium 2.8 18 32 18 10 2 [Rn]5f ¹⁴ 6d ² 7s ²	105 Db Dubnium 2.8 18 32 18 11 2 [Rn]5f ¹⁴ 6d ³ 7s ²	106 Sg Seaborgium 2.8 18 32 18 12 2 [Rn]5f ¹⁴ 6d ⁴ 7s ²	107 Bh Bohrium 2.8 18 32 18 13 2 [Rn]5f ¹⁴ 6d ⁵ 7s ²	108 Hs Hassium 2.8 18 32 18 14 2 [Rn]5f ¹⁴ 6d ⁶ 7s ²	109 Mt Meitnerium 2.8 18 32 18 15 2 [Rn]5f ¹⁴ 6d ⁷ 7s ²	110 Ds Darmstadtium 2.8 18 32 18 16 2 [Rn]5f ¹⁴ 6d ⁸ 7s ²	111 Rg Roentgenium 2.8 18 32 18 17 2 [Rn]5f ¹⁴ 6d ⁹ 7s ²	112 Cn Copernicium 2.8 18 32 18 18 2 [Rn]5f ¹⁴ 6d ¹⁰ 7s ²	113 Uut Ununtrium 2.8 18 32 18 18 3 [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ¹	114 Fl Flerovium 2.8 18 32 18 18 4 [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ²	115 Uup Ununpentium 2.8 18 32 18 18 5 [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ³	116 Lv Livermorium 2.8 18 32 18 18 6 [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁴	117 Uus Ununseptium 2.8 18 32 18 18 7 [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁵	118 Uuo Ununoctium 2.8 18 32 18 18 8 [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁶		

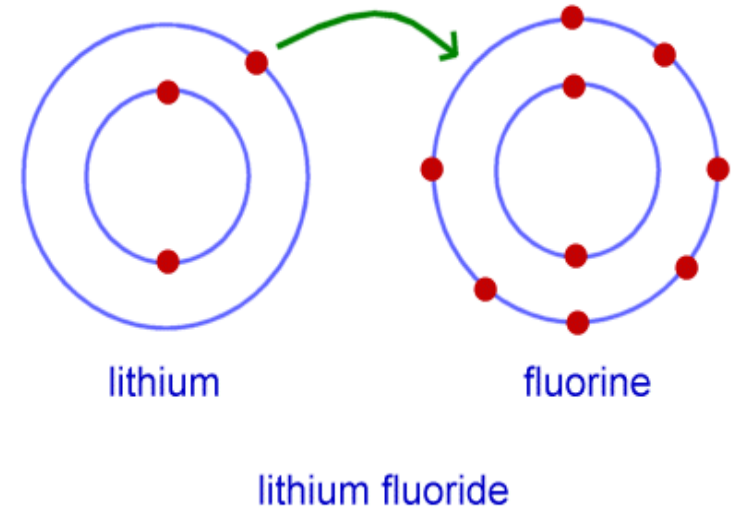
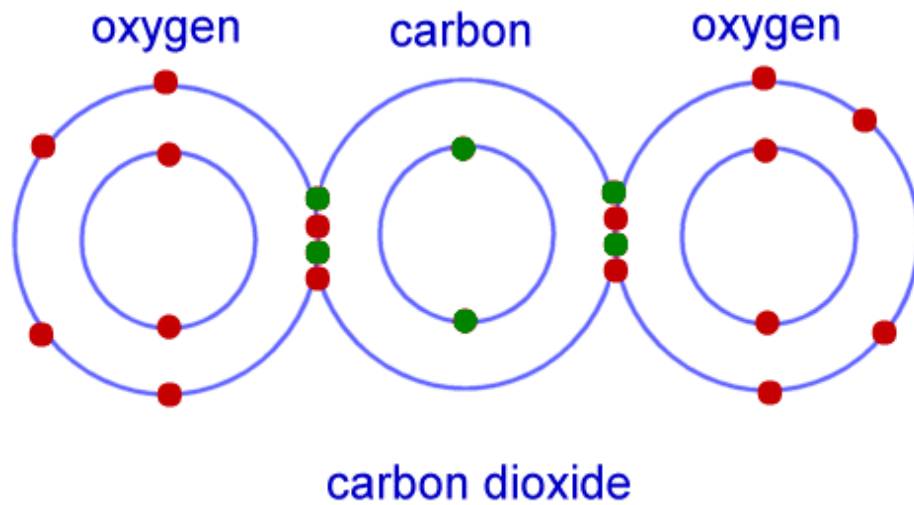
Atomic Number	Atomic Mass
Symbol Name	
Electron Shells	
Electron Configuration	

Element symbol represents state at room temperature.

Solid, Liquid or Gas

- Alkali Metal
- Alkaline Earth
- Transition Metal
- Basic Metal
- Metalloid
- Nonmetal
- Halogen
- Noble Gas
- Lanthanide
- Actinide

How the bonds are formed?



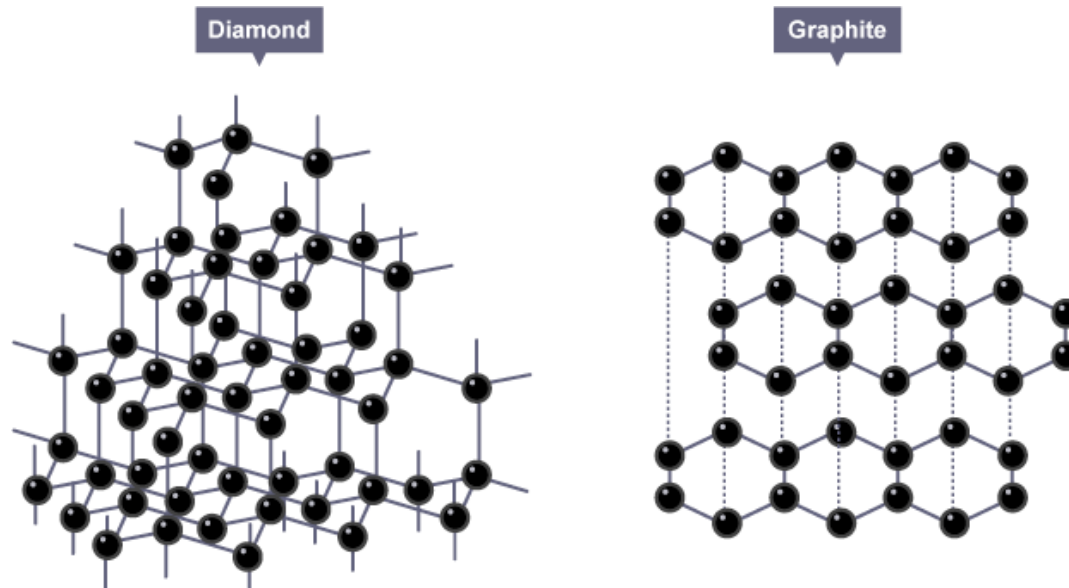
Electrons are shared
equally or unequally

Metals and Non-metals

Metals : electrons shared by all the atoms
non-directional bonds

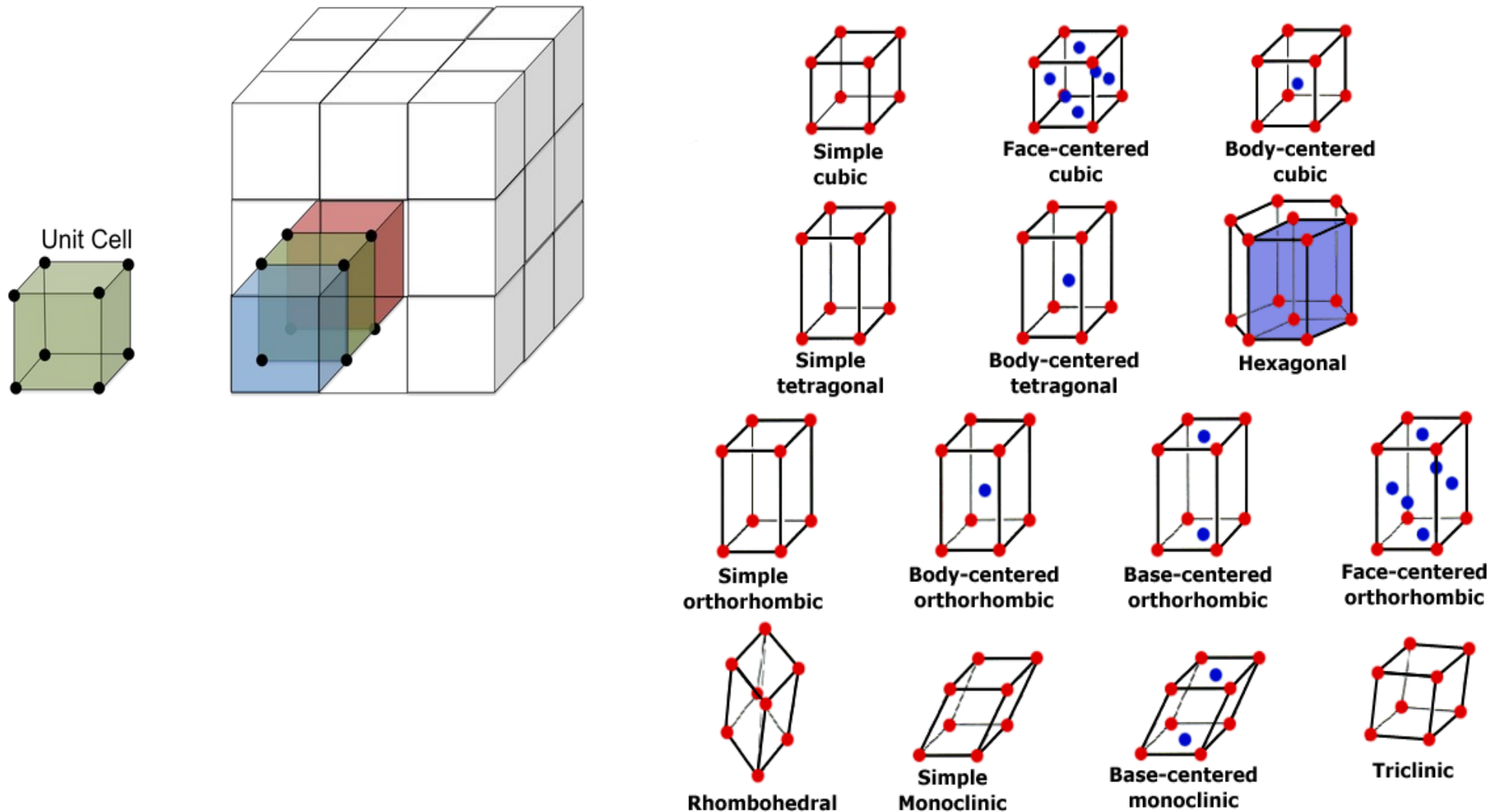
Non-metals: electrons are shared within
small group of atoms
Directional bonds

Carbon



Same element: Different structure: different bonding
drastically different properties!!

How atoms are arranged in a bulk?



What happens as the size reduces?

Atoms are no more organized in a periodic fashion

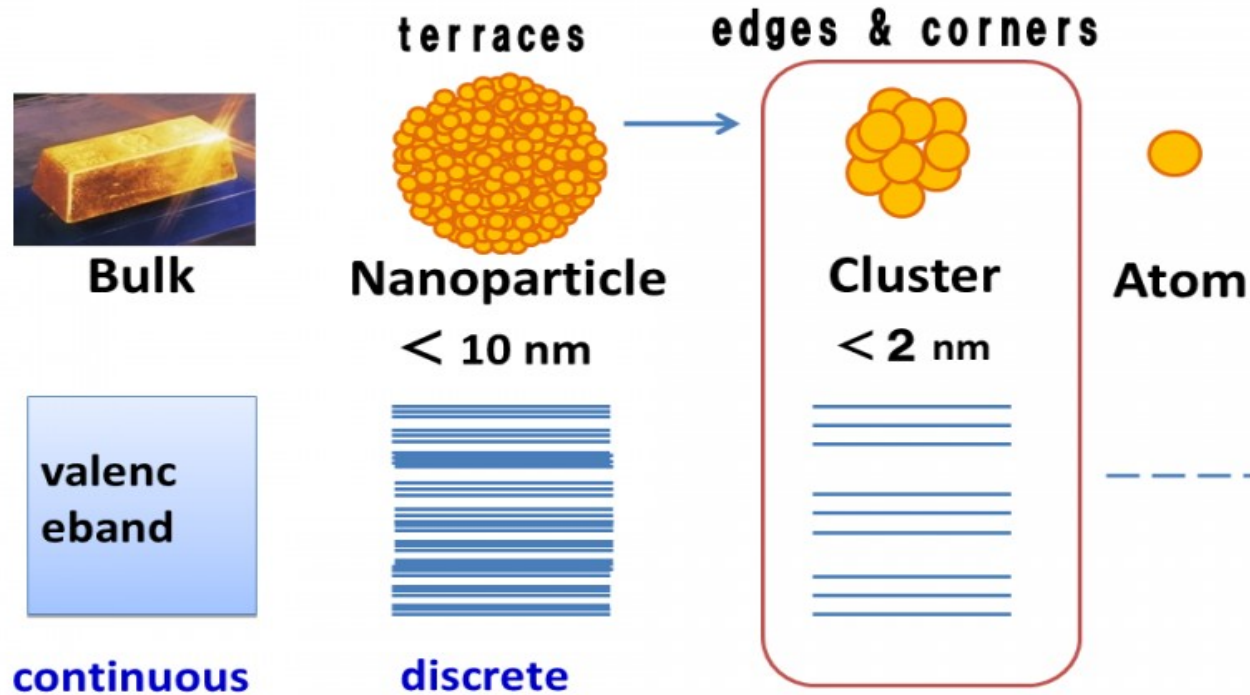
the crystal structure collapses
and this is the limit of miniaturization.

Miniaturization is possible in scalable regime



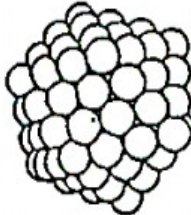
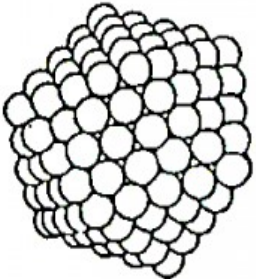
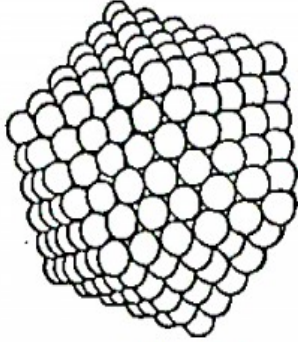
Where the surface atoms form a very
small fraction of total number of atoms

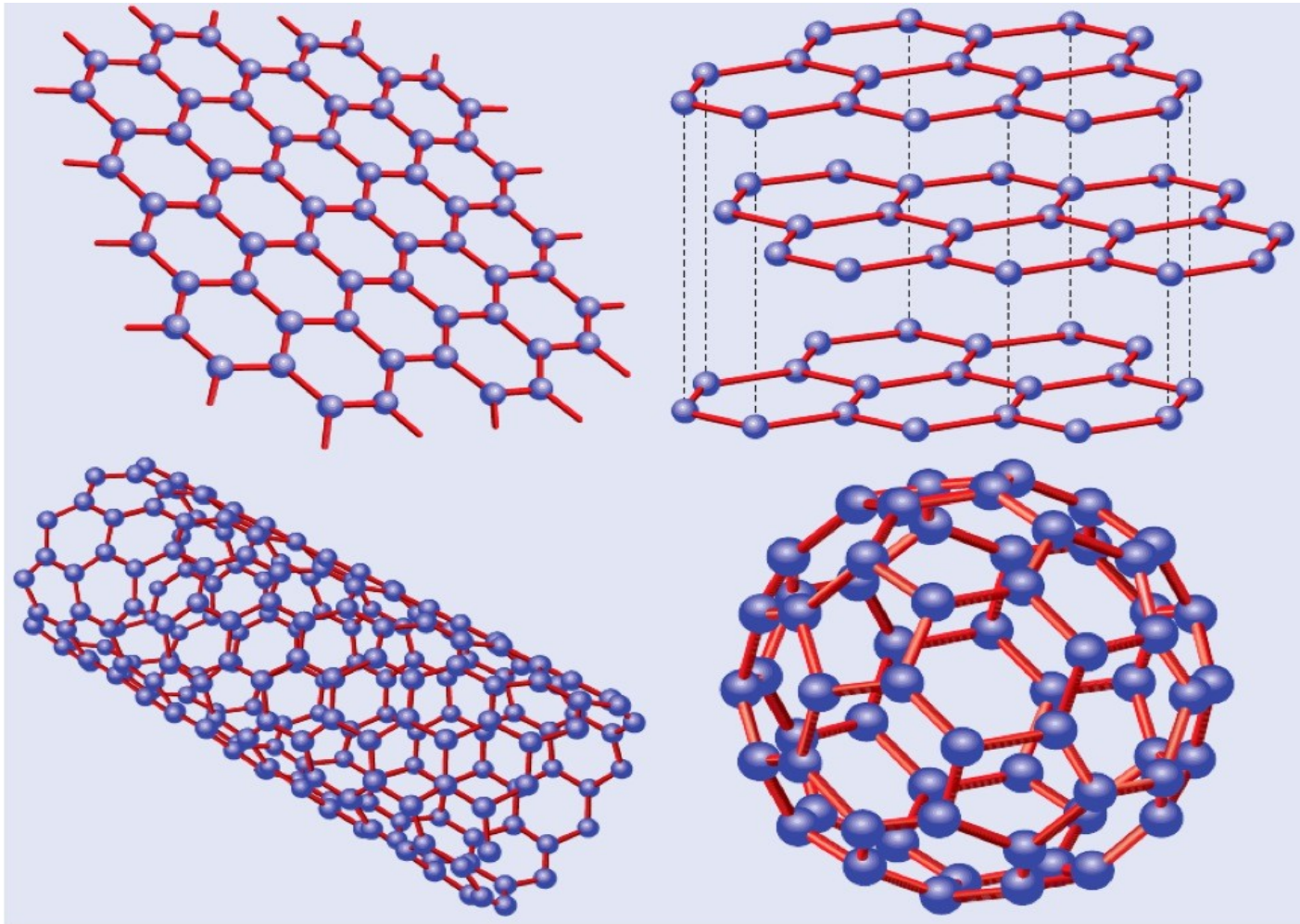
A non-scalable regime

Clusters: different from bulk!



R. Kubo, J. Phys. Soc. Jpn. 17, 975 (1962)

1.1	1.6	2.2	2.7	3.3 nm
Outer diameter				
				
13	55	147	309	561
92	76	63	52	45 surf.%
0	55	41	29	21 edge%
92	22	8	4	2 corner%

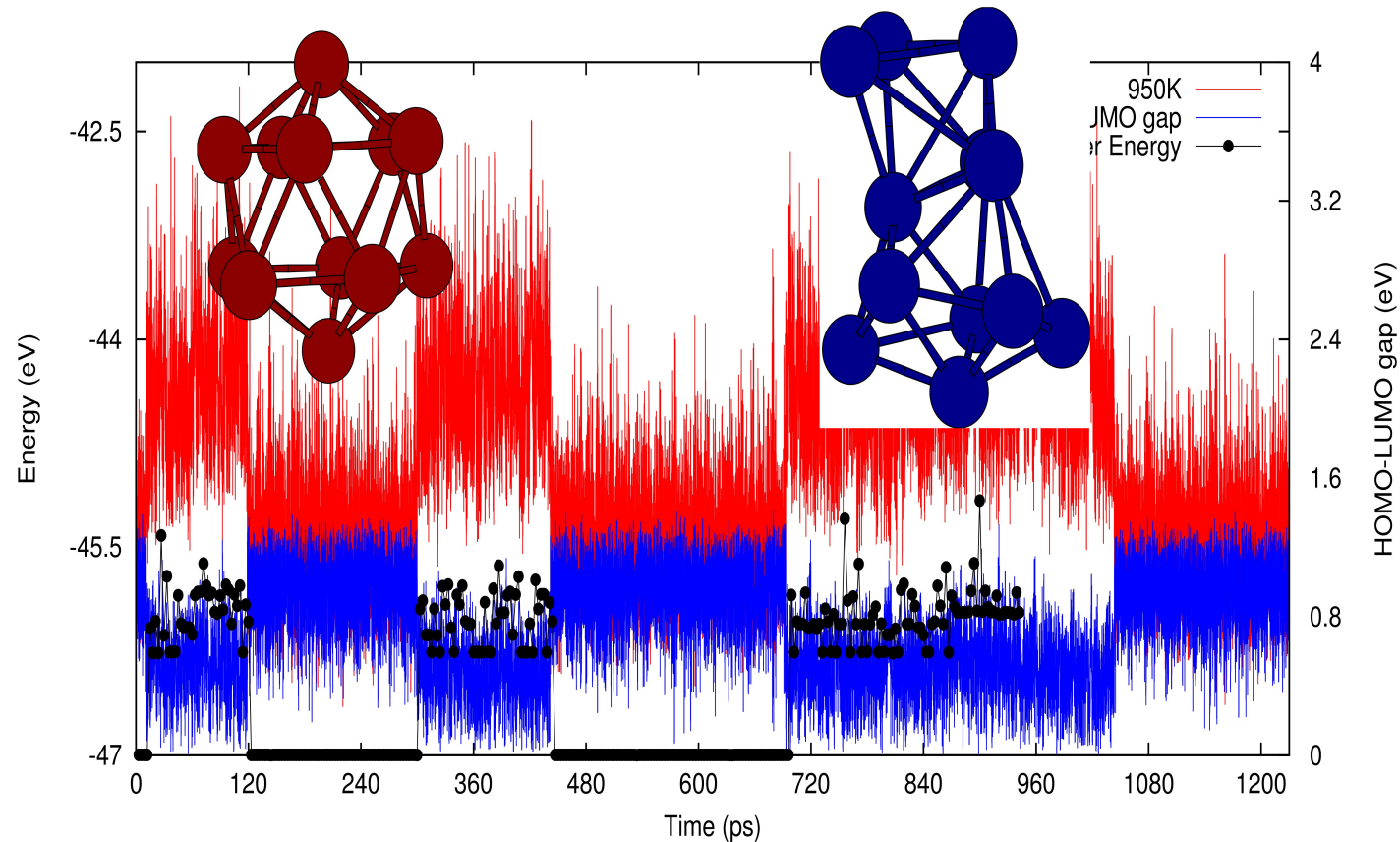


This is successful example of research field
driven by theory and computation

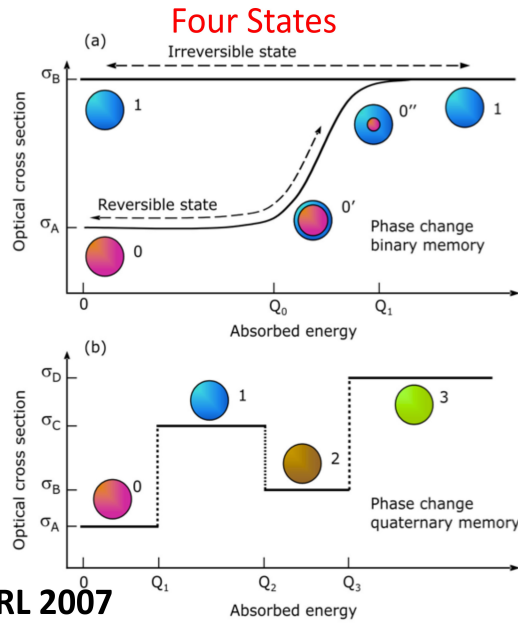
Computers as a tool

- Understanding
- Predicting
- Designing
- Control

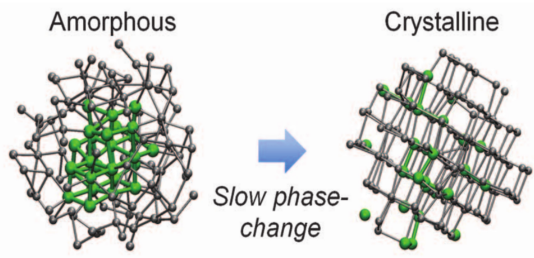
Two states: Cage and Non-Cage



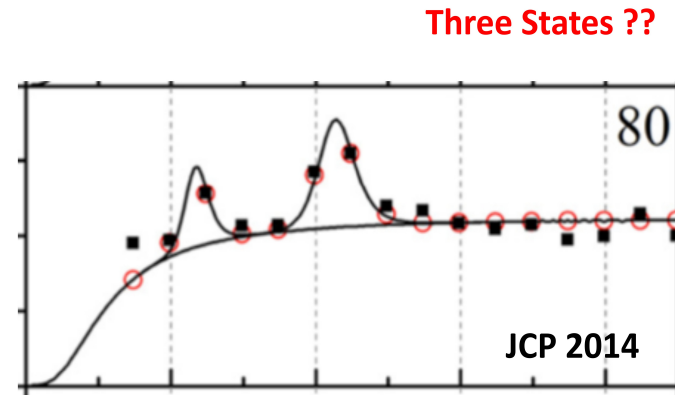
Nano Cages OR Nano Switches?



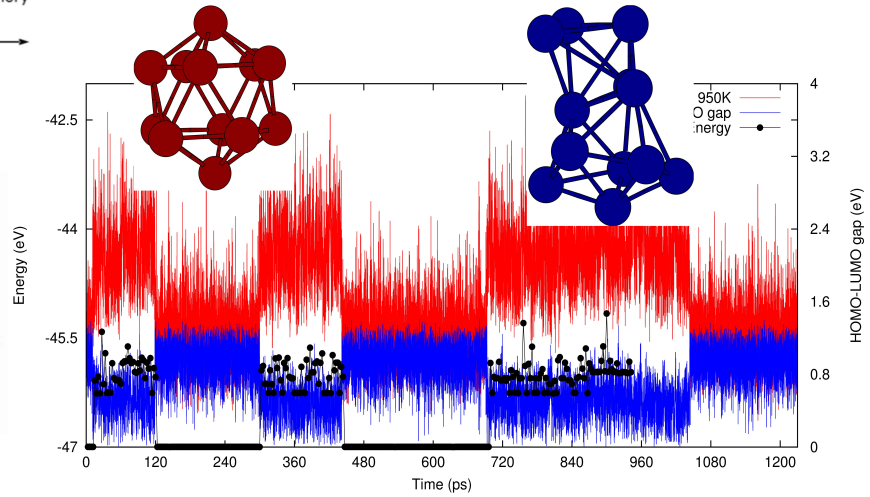
PRL 2007



Science 2012



Two states: Cage and Non-Cage



Clusters as catalyst

Inhomogeneous charge distribution
in homogeneous clusters

Thank you