

# **First-Principles Computational Materials Physics**

## **Part I: Fundamentals of First-principles Calculations**

台灣大學物理系 郭光宇

**Guang-Yu Guo**

**Physics Dept., National Taiwan University**

**(Fall Semester, 2017)**

# Chapter 1 Introduction to First-Principles Calculations

## 1.1 What is first-principles calculation

This course is about calculating the properties of materials (solid phase) from first-principles (*ab initio*), by directly or indirectly solving the Schrödinger equation that describes the motion of the electrons in the Coulomb potentials of the nuclei and of each other. By first-principles (*ab initio*), we meant empirical parameter-free calculations; that is, calculations in which the only input is the atomic numbers of the atoms and the macroscopic constraints (pressure, temperature, etc).

# Periodic Table of the Elements

Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
	IA 1A	IIA 2A											IIIA 3A	IVA 4A	VA 5A	VIA 6A	VIIA 7A	VIIIA 8A
1	1 H Hydrogen 1 1s <sup>1</sup>																	2 He Helium 2 1s <sup>2</sup>
2	3 Li Lithium 2.1 [He]2s <sup>1</sup>	4 Be Beryllium 2.2 [He]2s <sup>2</sup>											5 B Boron 2.3 [He]2s <sup>2</sup> 2p <sup>1</sup>	6 C Carbon 2.4 [He]2s <sup>2</sup> 2p <sup>2</sup>	7 N Nitrogen 2.5 [He]2s <sup>2</sup> 2p <sup>3</sup>	8 O Oxygen 2.6 [He]2s <sup>2</sup> 2p <sup>4</sup>	9 F Fluorine 2.7 [He]2s <sup>2</sup> 2p <sup>5</sup>	10 Ne Neon 2.8 [He]2s <sup>2</sup> 2p <sup>6</sup>
3	11 Na Sodium 2.8.1 [Ne]3s <sup>1</sup>	12 Mg Magnesium 2.8.2 [Ne]3s <sup>2</sup>											13 Al Aluminum 2.8.3 [Ne]3s <sup>2</sup> 3p <sup>1</sup>	14 Si Silicon 2.8.4 [Ne]3s <sup>2</sup> 3p <sup>2</sup>	15 P Phosphorus 2.8.5 [Ne]3s <sup>2</sup> 3p <sup>3</sup>	16 S Sulfur 2.8.6 [Ne]3s <sup>2</sup> 3p <sup>4</sup>	17 Cl Chlorine 2.8.7 [Ne]3s <sup>2</sup> 3p <sup>5</sup>	18 Ar Argon 2.8.8 [Ne]3s <sup>2</sup> 3p <sup>6</sup>
4	19 K Potassium 2.8.8.1 [Ar]4s <sup>1</sup>	20 Ca Calcium 2.8.9.2 [Ar]4s <sup>2</sup>	21 Sc Scandium 2.8.9.2 [Ar]3d <sup>1</sup> 4s <sup>2</sup>	22 Ti Titanium 2.8.10.2 [Ar]3d <sup>2</sup> 4s <sup>2</sup>	23 V Vanadium 2.8.11.2 [Ar]3d <sup>3</sup> 4s <sup>2</sup>	24 Cr Chromium 2.8.11.2 [Ar]3d <sup>5</sup> 4s <sup>1</sup>	25 Mn Manganese 2.8.13.2 [Ar]3d <sup>5</sup> 4s <sup>2</sup>	26 Fe Iron 2.8.14.2 [Ar]3d <sup>6</sup> 4s <sup>2</sup>	27 Co Cobalt 2.8.15.2 [Ar]3d <sup>7</sup> 4s <sup>2</sup>	28 Ni Nickel 2.8.16.2 [Ar]3d <sup>8</sup> 4s <sup>2</sup>	29 Cu Copper 2.8.18.1 [Ar]3d <sup>10</sup> 4s <sup>1</sup>	30 Zn Zinc 2.8.18.2 [Ar]3d <sup>10</sup> 4s <sup>2</sup>	31 Ga Gallium 2.8.18.3 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>1</sup>	32 Ge Germanium 2.8.18.4 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup>	33 As Arsenic 2.8.18.5 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup>	34 Se Selenium 2.8.18.6 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup>	35 Br Bromine 2.8.18.7 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup>	36 Kr Krypton 2.8.18.8 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup>
5	37 Rb Rubidium 2.8.18.8.1 [Kr]5s <sup>1</sup>	38 Sr Strontium 2.8.18.9.2 [Kr]5s <sup>2</sup>	39 Y Yttrium 2.8.18.9.2 [Kr]4d <sup>1</sup> 5s <sup>2</sup>	40 Zr Zirconium 2.8.18.10.2 [Kr]4d <sup>2</sup> 5s <sup>2</sup>	41 Nb Niobium 2.8.18.11.2 [Kr]4d <sup>4</sup> 5s <sup>1</sup>	42 Mo Molybdenum 2.8.18.13.2 [Kr]4d <sup>5</sup> 5s <sup>1</sup>	43 Tc Technetium 2.8.18.14.2 [Kr]4d <sup>5</sup> 5s <sup>2</sup>	44 Ru Ruthenium 2.8.18.15.2 [Kr]4d <sup>7</sup> 5s <sup>1</sup>	45 Rh Rhodium 2.8.18.16.2 [Kr]4d <sup>8</sup> 5s <sup>1</sup>	46 Pd Palladium 2.8.18.18 [Kr]4d <sup>10</sup>	47 Ag Silver 2.8.18.18.1 [Kr]4d <sup>10</sup> 5s <sup>1</sup>	48 Cd Cadmium 2.8.18.18.2 [Kr]4d <sup>10</sup> 5s <sup>2</sup>	49 In Indium 2.8.18.18.3 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>1</sup>	50 Sn Tin 2.8.18.18.4 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup>	51 Sb Antimony 2.8.18.18.5 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup>	52 Te Tellurium 2.8.18.18.6 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup>	53 I Iodine 2.8.18.18.7 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>	54 Xe Xenon 2.8.18.18.8 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup>
6	55 Cs Cesium 2.8.18.18.8.1 [Xe]6s <sup>1</sup>	56 Ba Barium 2.8.18.18.8.2 [Xe]6s <sup>2</sup>	57-71 Lanthanide Series	72 Hf Hafnium 2.8.18.32.10.2 [Xe]4f <sup>14</sup> 5d <sup>2</sup> 6s <sup>2</sup>	73 Ta Tantalum 2.8.18.32.11.2 [Xe]4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup>	74 W Tungsten 2.8.18.32.12.2 [Xe]4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup>	75 Re Rhenium 2.8.18.32.13.2 [Xe]4f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup>	76 Os Osmium 2.8.18.32.14.2 [Xe]4f <sup>14</sup> 5d <sup>6</sup> 6s <sup>2</sup>	77 Ir Iridium 2.8.18.32.15.2 [Xe]4f <sup>14</sup> 5d <sup>7</sup> 6s <sup>2</sup>	78 Pt Platinum 2.8.18.32.17.1 [Xe]4f <sup>14</sup> 5d <sup>9</sup> 6s <sup>1</sup>	79 Au Gold 2.8.18.32.18.1 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>1</sup>	80 Hg Mercury 2.8.18.32.18.2 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup>	81 Tl Thallium 2.8.18.32.18.3 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>1</sup>	82 Pb Lead 2.8.18.32.18.4 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>2</sup>	83 Bi Bismuth 2.8.18.32.18.5 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>3</sup>	84 Po Polonium 2.8.18.32.18.6 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>4</sup>	85 At Astatine 2.8.18.32.18.7 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>5</sup>	86 Rn Radon 2.8.18.32.18.8 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>6</sup>
7	87 Fr Francium 2.8.18.32.18.8.1 [Rn]7s <sup>1</sup>	88 Ra Radium 2.8.18.32.18.8.2 [Rn]7s <sup>2</sup>	89-103 Actinide Series	104 Rf Rutherfordium 2.8.18.32.32.10.2 [Rn]5f <sup>14</sup> 6d <sup>2</sup> 7s <sup>2</sup>	105 Db Dubnium 2.8.18.32.32.11.2 [Rn]5f <sup>14</sup> 6d <sup>3</sup> 7s <sup>2</sup>	106 Sg Seaborgium 2.8.18.32.32.12.2 [Rn]5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup>	107 Bh Bohrium 2.8.18.32.32.13.2 [Rn]5f <sup>14</sup> 6d <sup>5</sup> 7s <sup>2</sup>	108 Hs Hassium 2.8.18.32.32.14.2 [Rn]5f <sup>14</sup> 6d <sup>6</sup> 7s <sup>2</sup>	109 Mt Meitnerium 2.8.18.32.32.15.2 [Rn]5f <sup>14</sup> 6d <sup>7</sup> 7s <sup>2</sup>	110 Ds Darmstadtium 2.8.18.32.32.16.2 [Rn]5f <sup>14</sup> 6d <sup>8</sup> 7s <sup>2</sup>	111 Rg Roentgenium 2.8.18.32.32.17.2 [Rn]5f <sup>14</sup> 6d <sup>9</sup> 7s <sup>2</sup>	112 Cn Copernicium 2.8.18.32.32.18.2 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup>	113 Uut Ununtrium 2.8.18.32.32.18.3 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>1</sup>	114 Fl Flerovium 2.8.18.32.32.18.4 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>2</sup>	115 Uup Ununpentium 2.8.18.32.32.18.5 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>3</sup>	116 Lv Livermorium 2.8.18.32.32.18.6 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>4</sup>	117 Uus Ununseptium 2.8.18.32.32.18.7 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>5</sup>	118 Uuo Ununoctium 2.8.18.32.32.18.8 [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>6</sup>

Lanthanide Series

Actinide Series

57 La Lanthanum 2.8.18.9.2 [Xe]5d <sup>1</sup> 6s <sup>2</sup>	58 Ce Cerium 2.8.18.9.2 [Xe]4f <sup>1</sup> 5d <sup>1</sup> 6s <sup>2</sup>	59 Pr Praseodymium 2.8.18.9.2 [Xe]4f <sup>3</sup> 6s <sup>2</sup>	60 Nd Neodymium 2.8.18.9.2 [Xe]4f <sup>4</sup> 6s <sup>2</sup>	61 Pm Promethium 2.8.18.9.2 [Xe]4f <sup>5</sup> 6s <sup>2</sup>	62 Sm Samarium 2.8.18.9.2 [Xe]4f <sup>6</sup> 6s <sup>2</sup>	63 Eu Europium 2.8.18.9.2 [Xe]4f <sup>7</sup> 6s <sup>2</sup>	64 Gd Gadolinium 2.8.18.9.2 [Xe]4f <sup>7</sup> 5d <sup>1</sup> 6s <sup>2</sup>	65 Tb Terbium 2.8.18.9.2 [Xe]4f <sup>9</sup> 6s <sup>2</sup>	66 Dy Dysprosium 2.8.18.9.2 [Xe]4f <sup>10</sup> 6s <sup>2</sup>	67 Ho Holmium 2.8.18.9.2 [Xe]4f <sup>11</sup> 6s <sup>2</sup>	68 Er Erbium 2.8.18.9.2 [Xe]4f <sup>12</sup> 6s <sup>2</sup>	69 Tm Thulium 2.8.18.9.2 [Xe]4f <sup>13</sup> 6s <sup>2</sup>	70 Yb Ytterbium 2.8.18.9.2 [Xe]4f <sup>14</sup> 6s <sup>2</sup>	71 Lu Lutetium 2.8.18.9.2 [Xe]4f <sup>14</sup> 5d <sup>1</sup> 6s <sup>2</sup>
89 Ac Actinium 2.8.18.9.2 [Rn]6d <sup>1</sup> 7s <sup>2</sup>	90 Th Thorium 2.8.18.9.2 [Rn]6d <sup>2</sup> 7s <sup>2</sup>	91 Pa Protactinium 2.8.18.9.2 [Rn]5f <sup>2</sup> 6d <sup>1</sup> 7s <sup>2</sup>	92 U Uranium 2.8.18.9.2 [Rn]5f <sup>3</sup> 6d <sup>1</sup> 7s <sup>2</sup>	93 Np Neptunium 2.8.18.9.2 [Rn]5f <sup>4</sup> 6d <sup>1</sup> 7s <sup>2</sup>	94 Pu Plutonium 2.8.18.9.2 [Rn]5f <sup>6</sup> 7s <sup>2</sup>	95 Am Americium 2.8.18.9.2 [Rn]5f <sup>7</sup> 7s <sup>2</sup>	96 Cm Curium 2.8.18.9.2 [Rn]5f <sup>7</sup> 6d <sup>1</sup> 7s <sup>2</sup>	97 Bk Berkelium 2.8.18.9.2 [Rn]5f <sup>9</sup> 7s <sup>2</sup>	98 Cf Californium 2.8.18.9.2 [Rn]5f <sup>10</sup> 7s <sup>2</sup>	99 Es Einsteinium 2.8.18.9.2 [Rn]5f <sup>11</sup> 7s <sup>2</sup>	100 Fm Fermium 2.8.18.9.2 [Rn]5f <sup>12</sup> 7s <sup>2</sup>	101 Md Mendelevium 2.8.18.9.2 [Rn]5f <sup>13</sup> 7s <sup>2</sup>	102 No Nobelium 2.8.18.9.2 [Rn]5f <sup>14</sup> 7s <sup>2</sup>	103 Lr Lawrencium 2.8.18.9.2 [Rn]5f <sup>14</sup> 6d <sup>1</sup> 7s <sup>2</sup>

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

[from Internet]



**Table 3 Crystal structures of the elements**

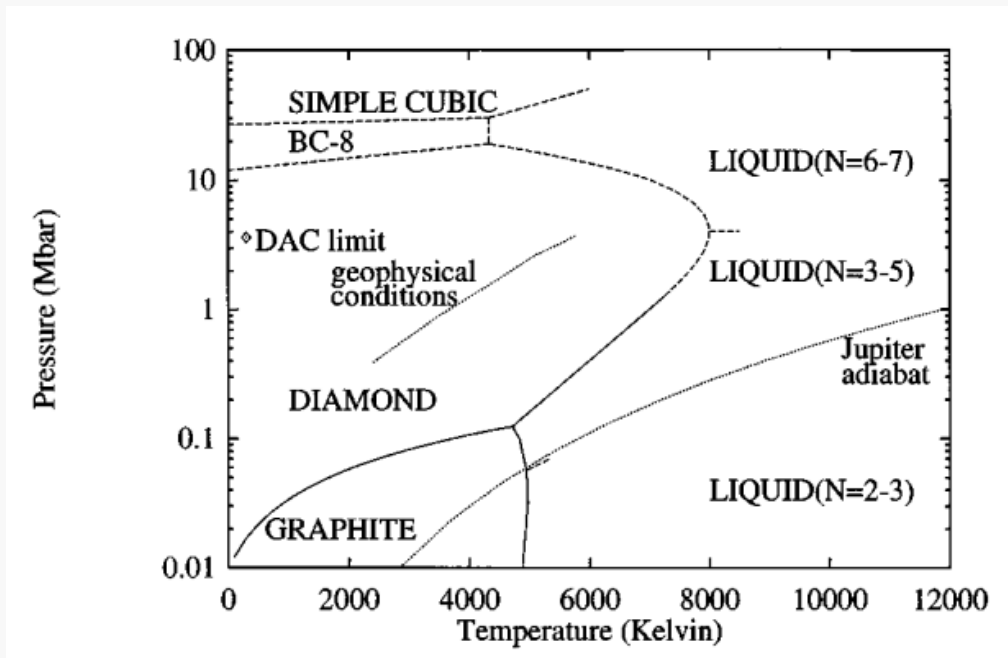
The data given are at room temperature for the most common form, or at the stated temperature in deg K. For further descriptions of the elements see Wyckoff, Vol. 1, Chap. 2. Structures labeled complex are described there.

Table 3 Crystal structures of the elements																		He <sup>4</sup> 2K											
H <sup>1</sup> 4K																				hcp									
3.75																				3.57									
6.12																				5.83									
Li 78K		Be																B		C		N 20K		O		F		Ne 4K	
bcc		hcp																rhomb.		diamond		cubic		complex		fcc			
3.491		2.27																		3.567		5.66		(O <sub>2</sub> )		4.46			
		3.59																				(N <sub>2</sub> )							
Na 5K		Mg																Al		Si		P		S		Cl		Ar 4K	
bcc		hcp																fcc		diamond		complex		complex		complex		fcc	
4.225		3.21																4.05		5.430						(Cl <sub>2</sub> )		5.31	
		5.21																											
																		Crystal structure											
																		a lattice parameter, in Å											
																		c lattice parameter, in Å											
K 5K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr 4K												
bcc	fcc	hcp	hcp	bcc	bcc	cubic	bcc	hcp	fcc	fcc	hcp	complex	diamond	rhomb.	hex.	complex	fcc												
5.225	5.58	3.31	2.95	3.03	2.88	complex	2.87	2.51	3.52	3.61	2.66	complex	5.658		chains	(Br <sub>2</sub> )	5.64												
		5.27	4.68				4.07				4.95																		
Rb 5K	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn (α)	Sb	Te	I	Xe 4K												
bcc	fcc	hcp	hcp	bcc	bcc	hcp	hcp	fcc	fcc	fcc	hcp	tetr.	diamond	rhomb.	hex.	complex	fcc												
5.585	6.08	3.65	3.23	3.30	3.15	2.74	2.71	3.80	3.89	4.09	2.98	3.25	6.49		chains	(I <sub>2</sub> )	6.13												
		5.73	5.15			4.40	4.28				5.62	4.95																	
Cs 5K	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn												
bcc	bcc	hex.	hcp	bcc	bcc	hcp	hcp	fcc	fcc	fcc	rhomb.	hcp	fcc	rhomb.	sc	—	—												
6.045	5.02	3.77	3.19	3.30	3.16	2.76	2.74	3.84	3.92	4.08		3.46	4.95		3.34														
		ABAC	5.05			4.46	4.32					5.52																	
Fr	Ra	Ac																											
—	—	fcc	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu													
		5.31	fcc	hex.	hex.	—	complex	bcc	hcp	hcp	hcp	hcp	hcp	hcp	fcc	hcp													
			5.16	3.67	3.66			4.58	3.63	3.60	3.59	3.58	3.56	3.54	5.48	3.50													
				ABAC				5.78	5.70	5.65	5.62	5.59	5.56	5.55		5.55													
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr													
			fcc	tetr.	complex	complex	complex	hex.	—	—	—	—	—	—	—	—													
			5.08	3.92				3.64																					
				3.24				ABAC																					

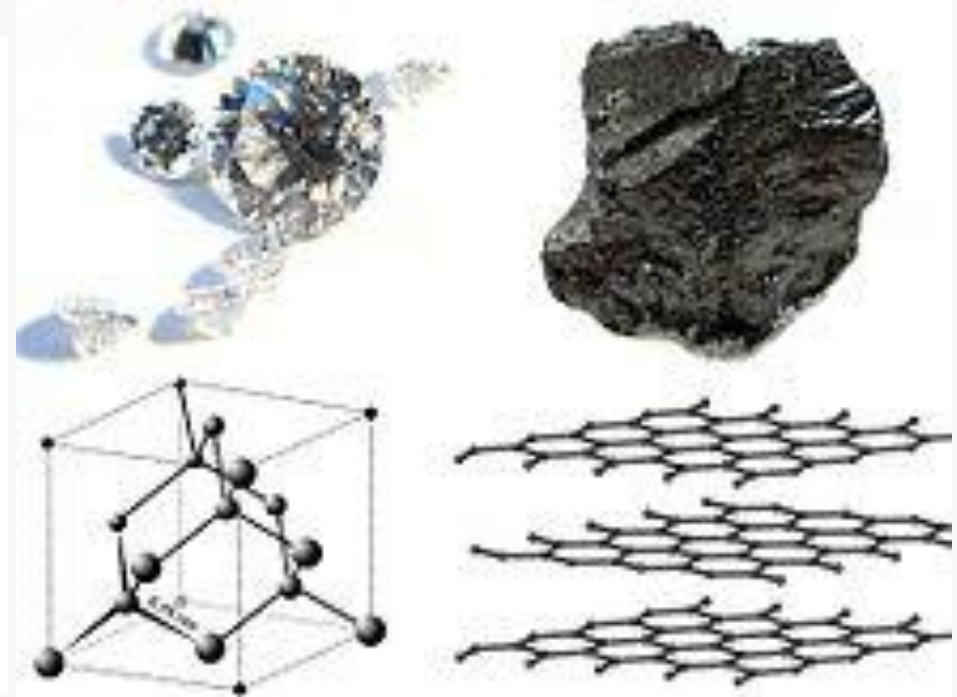
in Kittel's book]

[from Kittel's book]

## Phase diagram of carbon



## Carbon allotropes: diamond and graphite

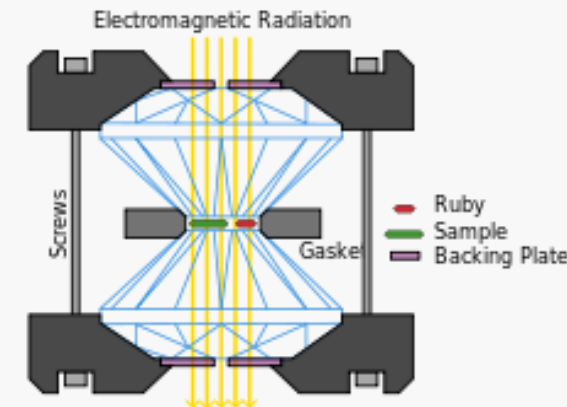
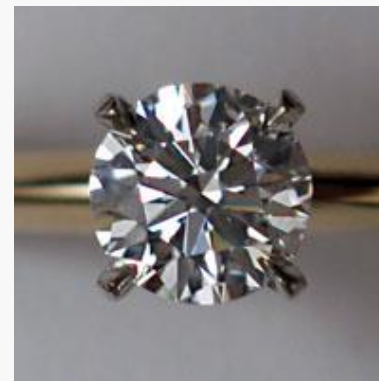


Diamond

Diamond anvil cell

[from Martin's book, p. 28]

[from Internet]





**Table 3 Isothermal bulk moduli and compressibilities at room temperature**

After K. Gschneidner, Jr., Solid state physics **16**, 275–426 (1964); several data are from F. Birch, in *Handbook of physical constants*, Geological Society of America Memoir **97**, 107–173 (1966). Original references should be consulted when values are needed for research purposes. Values in parentheses are estimates. Letters in parentheses refer to the crystal form. Letters in brackets refer to the temperature:

[a] = 77 K; [b] = 273 K; [c] = 1 K; [d] = 4 K; [e] = 81 K.

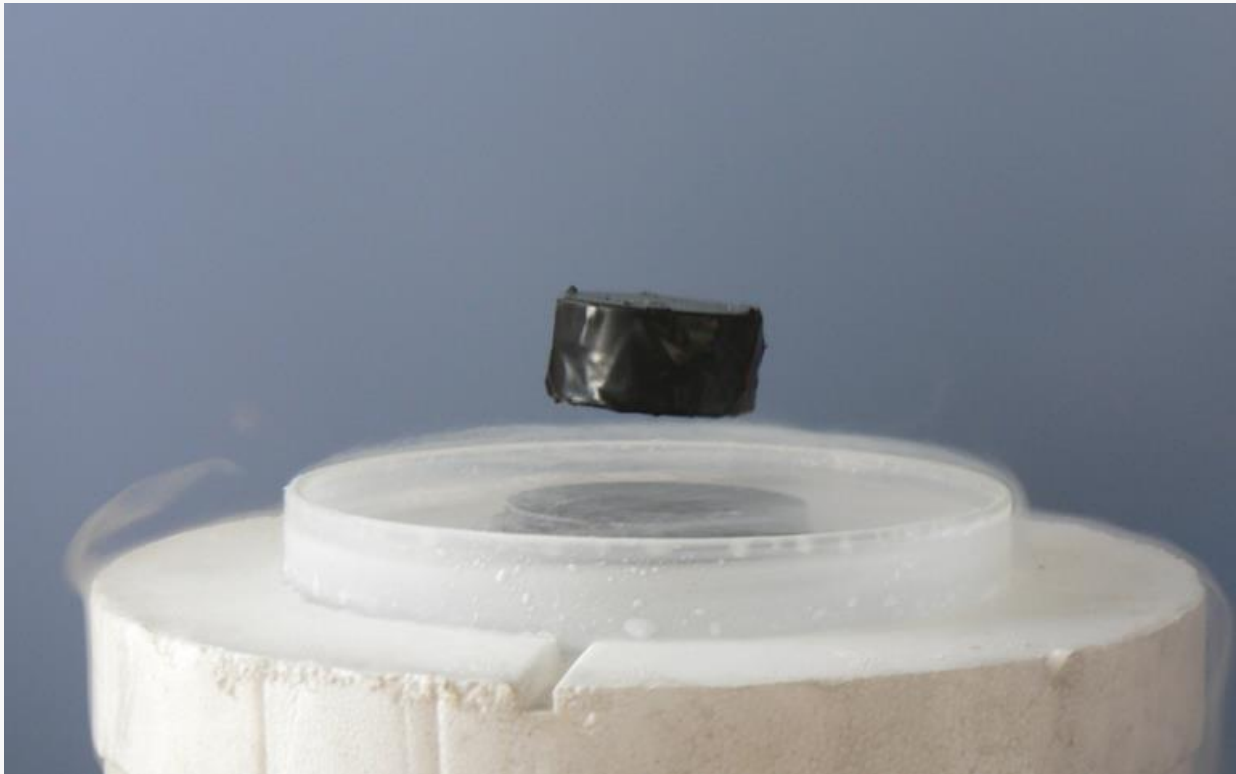
Bulk modulus in units  $10^{12}$  dyn/cm<sup>2</sup> or  $10^{11}$  N/m<sup>2</sup>  
Compressibility in units  $10^{-12}$  cm<sup>2</sup>/dyn or  $10^{-11}$  m<sup>2</sup>/N

Table 3 Isothermal bulk moduli and compressibilities at room temperature																		He [d]					
H [d]																		0.00					
0.002																		1168					
500																							
Li	Be																B	C [d]	N [e]	O	F	Ne [d]	
0.116	1.003																1.78	4.43	0.012			0.010	
8.62	0.997																0.562	0.226	80			100	
Na	Mg																Al	Si	P (b)	S (r)	Cl	Ar [a]	
0.068	0.354																0.722	0.988	0.304	0.178		0.013	
14.7	2.82																1.385	1.012	3.29	5.62		79	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga [b]	Ge	As	Se	Br	Kr [a]						
0.032	0.152	0.435	1.051	1.619	1.901	0.596	1.683	1.914	1.86	1.37	0.598	0.569	0.772	0.394	0.091		0.018						
31.	6.58	2.30	0.951	0.618	0.526	1.68	0.594	0.522	0.538	0.73	1.67	1.76	1.29	2.54	11.0		56						
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn (g)	Sb	Te	I	Xe						
0.031	0.116	0.366	0.833	1.702	2.725	(2.97)	3.208	2.704	1.808	1.007	0.467	0.411	1.11	0.383	0.230								
32.	8.62	2.73	1.20	0.587	0.366	(0.34)	0.311	0.369	0.553	0.993	2.14	2.43	0.901	2.61	4.35								
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg [c]	Tl	Pb	Bi	Po	At	Rn						
0.020	0.103	0.243	1.09	2.00	3.232	3.72	(4.18)	3.55	2.783	1.732	0.382	0.359	0.430	0.315	(0.26)								
50.	9.97	4.12	0.92	0.50	0.309	0.269	(0.24)	0.282	0.359	0.577	2.60	2.79	2.33	3.17	(3.8)								
Fr	Ra	Ac																					
(0.020)	(0.132)	(0.25)	Ce (γ)	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu							
(50.)	(7.6)	(4.)	0.239	0.306	0.327	(0.35)	0.294	0.147	0.383	0.399	0.384	0.397	0.411	0.397	0.133	0.411							
			4.18	3.27	3.06	(2.85)	3.40	6.80	2.61	2.51	2.60	2.52	2.43	2.52	7.52	2.43							
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr							
			0.543	(0.76)	0.987	(0.68)	0.54																
			1.84	(1.3)	1.01	(1.5)	1.9																

om Kittel's book]

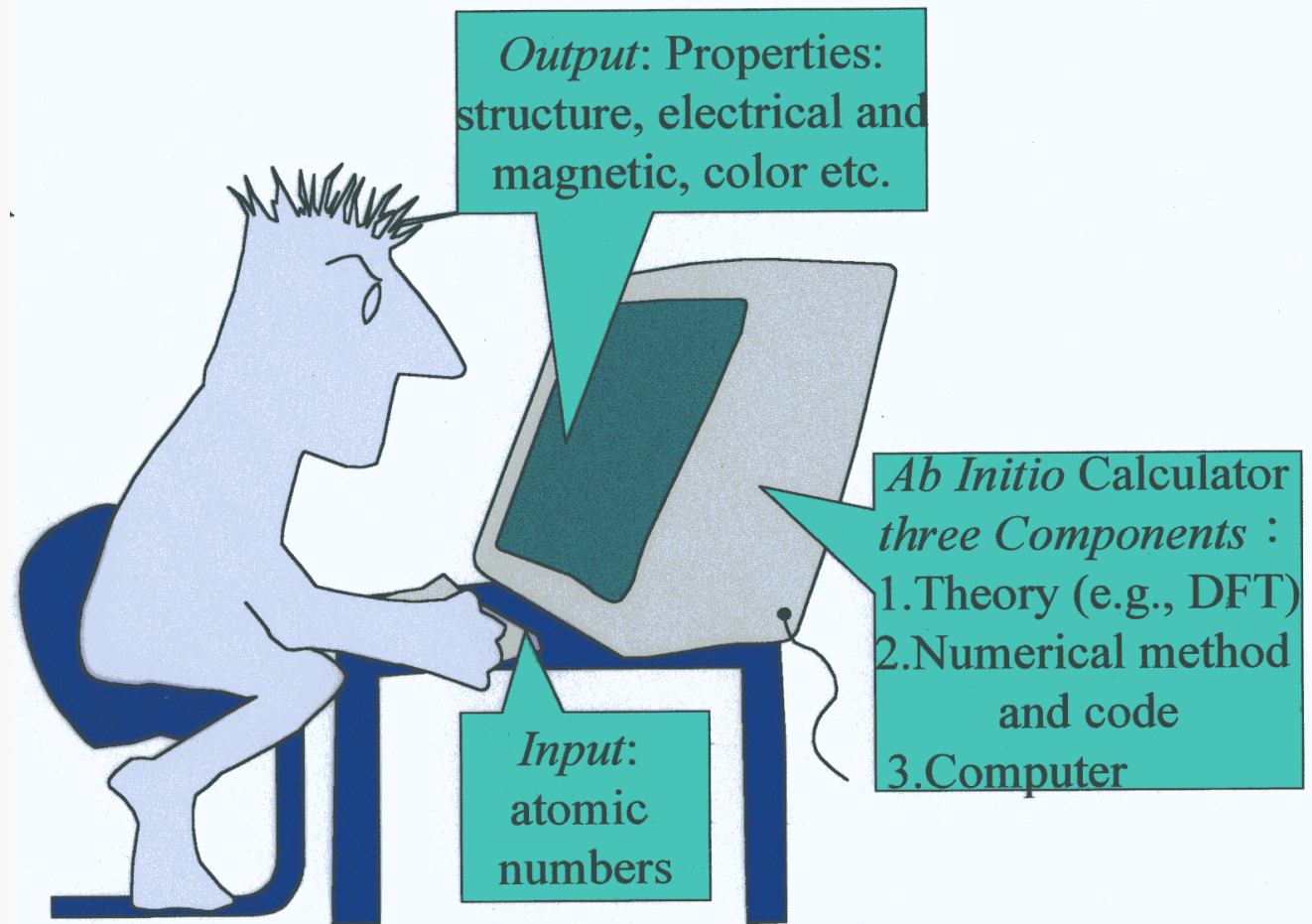
[from Kittel's book]

A metal becomes superconducting below  $T_c$  and floats in a magnetic field.



[from Internet]

## Cartoon of first-principles (*ab initio*) calculations



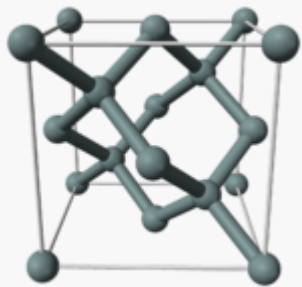
The calculation is really a “computer experiment”, as we can make intricate changes in the “experimental conditions” and measure our “observables” in arbitrarily minute details. It can make materials-specific predictions and also provide first-principles parameters for otherwise empirical models.



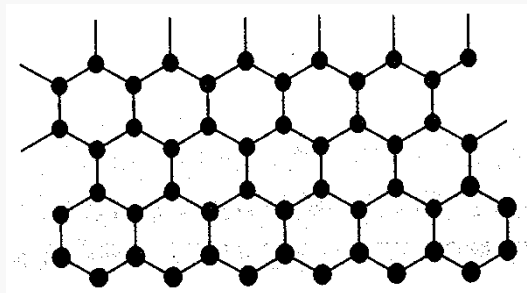
## 1.2 Significances of first-principles calculation

Today, due to fast computers, efficient algorithms, advanced quantum theory, first-principles calculations have become essential to understand the intricate phenomena in condensed matter systems, to search for and/or design for new materials with desired properties.

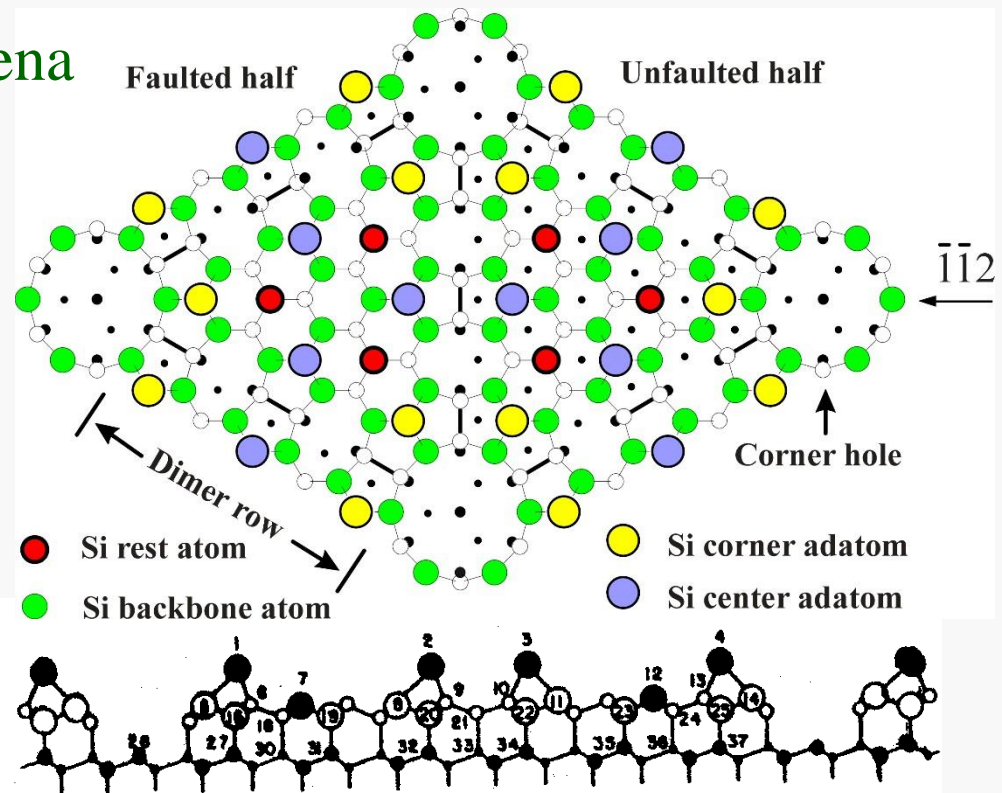
### Understanding of complex phenomena



Si (111) surface



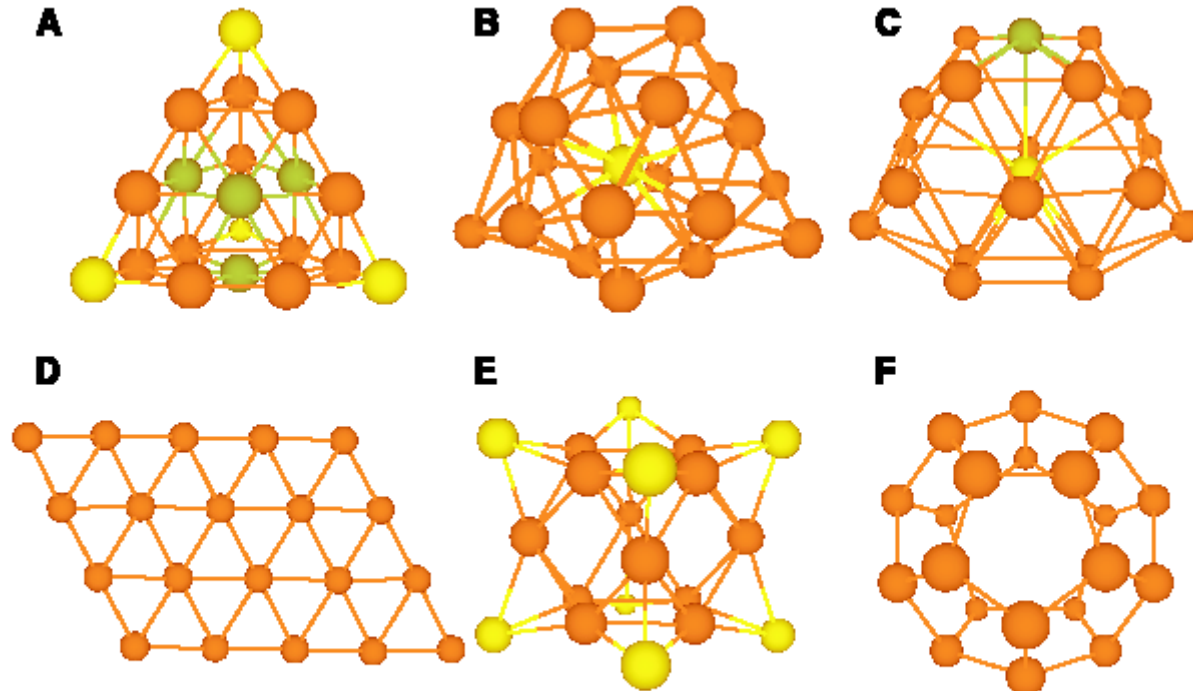
Si (111) surface reconstruction



[PRL 68 (1992) 1355]

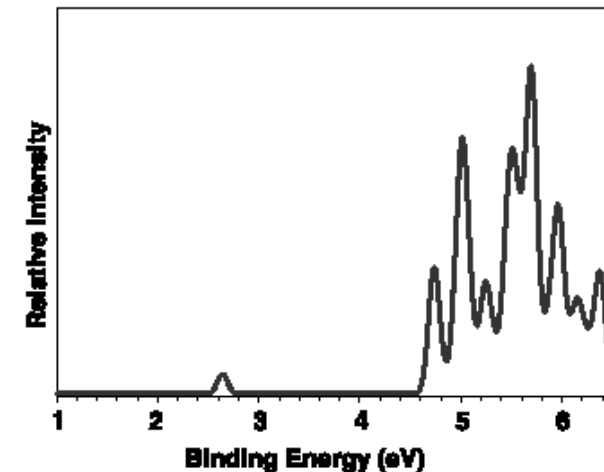
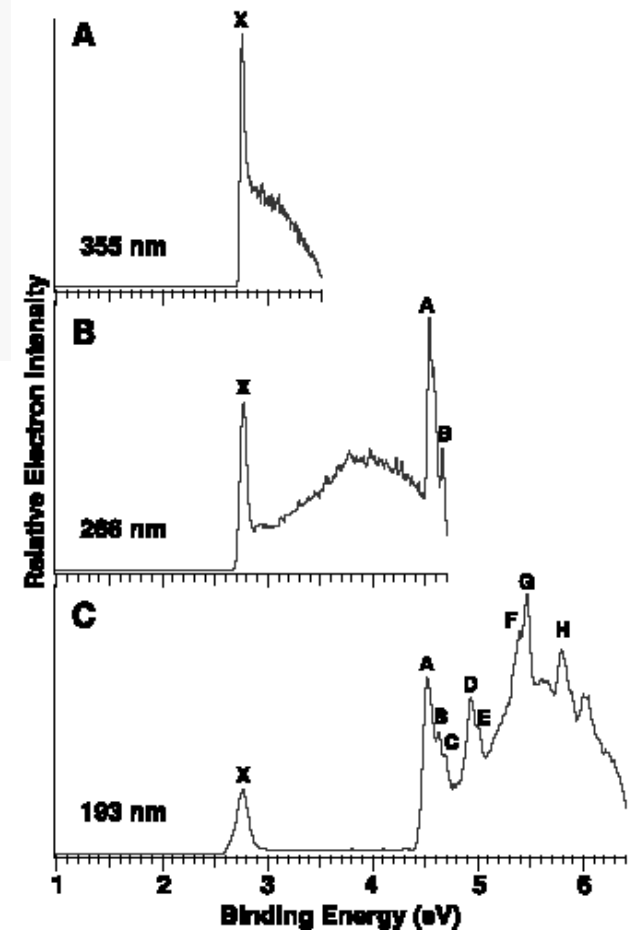
# Materials characterization

Another example, the structure of  $\text{Au}_{20}^-$  *determined jointly* by photoelectron spectroscopy and *ab initio* calculations



**Fig. 3.** Selected optimized  $\text{Au}_{20}$  structures. (A) Tetrahedral structure ( $T_d$ ). (B) Amorphous structure ( $C_1$ ). (C) Capped decahedron ( $C_{2v}$ ). (D) Planar structure ( $C_{2h}$ ). (E) Octahedral structure ( $O_h$ ). (F) Dodecahedral structure ( $I_h$ ).

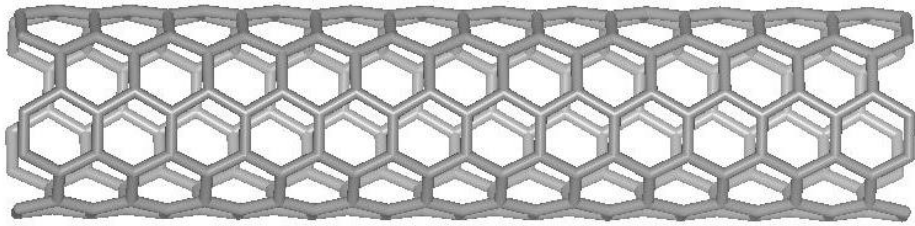
[Science 299, 864 (2003) 1355]



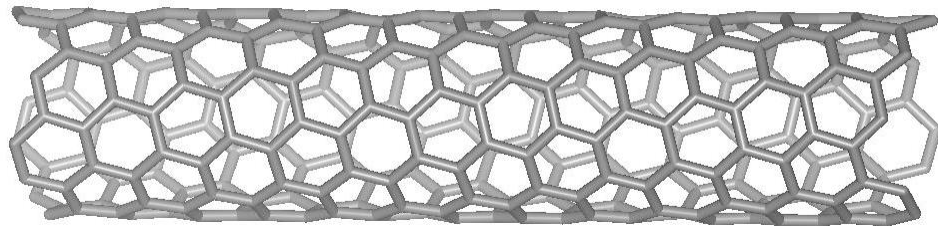
## Materials prediction/design

### Carbon nanotubes

(Iijima, 1991)

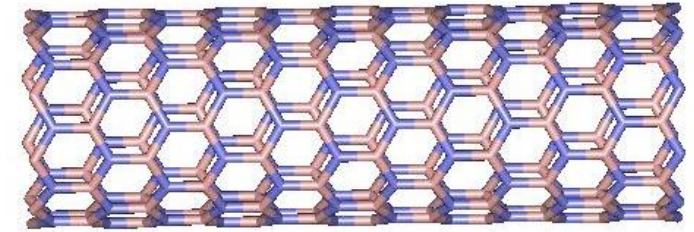


armchair (5,5) nanotube

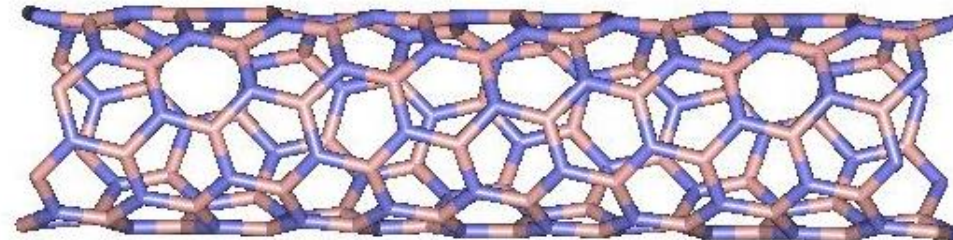


chiral (7,3) nanotube

### BN nanotubes



zigzag (10,0) nanotube



chiral (6,2) nanotube

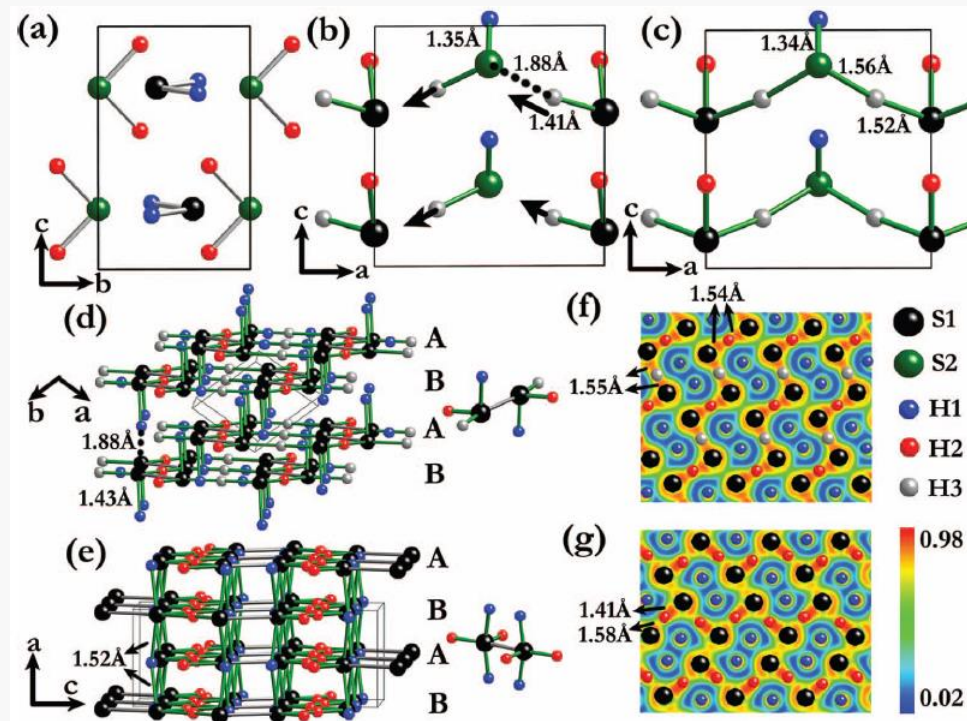
[predicted and subsequently synthesized by  
Berkeley groups in the mid-90's]

[Rubio et al., PRB 1994;  
Chopra, et al., Science, 1994]

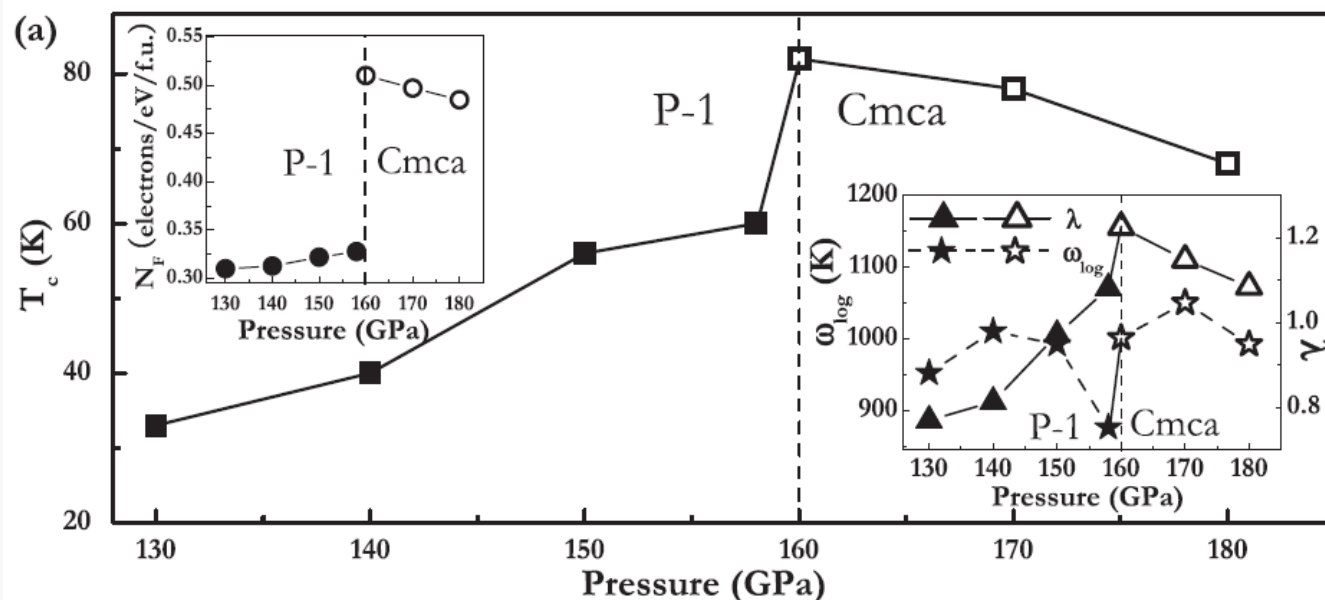


# New materials prediction

Prediction of metallization and superconductivity of dense hydrogen sulfide (2014)



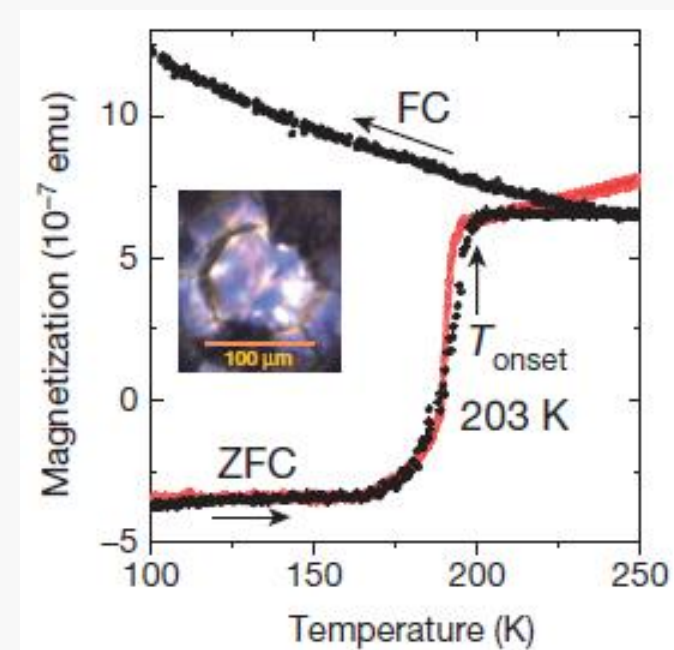
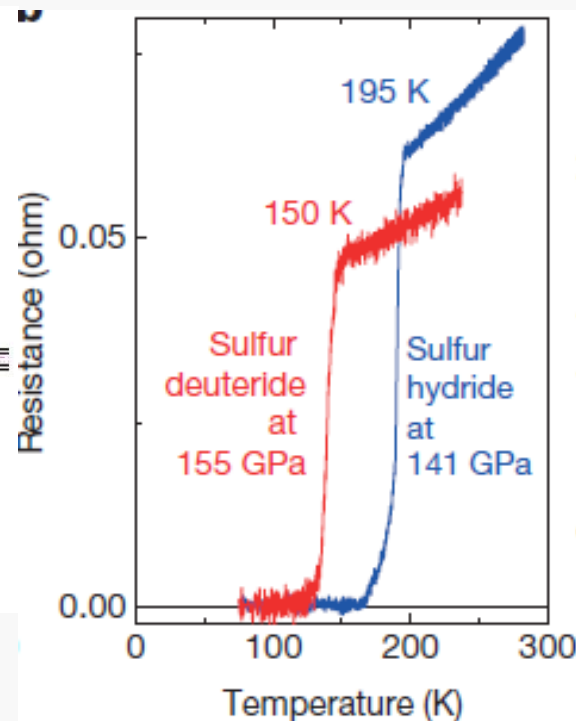
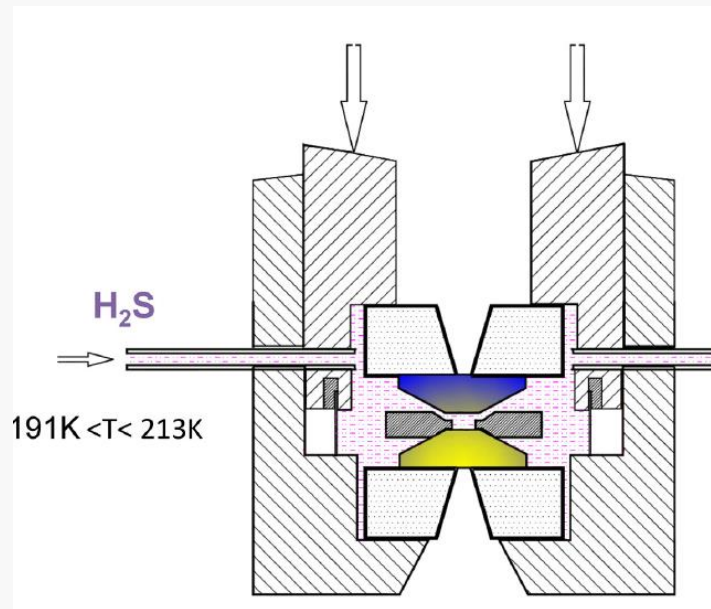
[Li, Hao, Liu, Li, Ma,  
JCP 140 (2014) 174712]



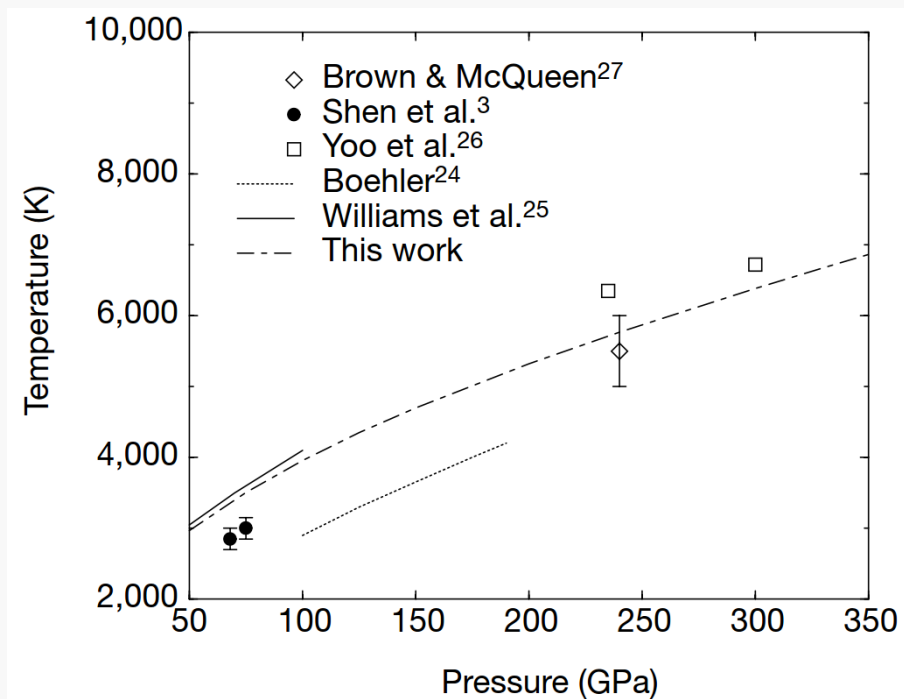
# Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov<sup>1\*</sup>, M. I. Erements<sup>1\*</sup>, I. A. Troyan<sup>1</sup>, V. Ksenofontov<sup>2</sup> & S. I. Shylin<sup>2</sup>

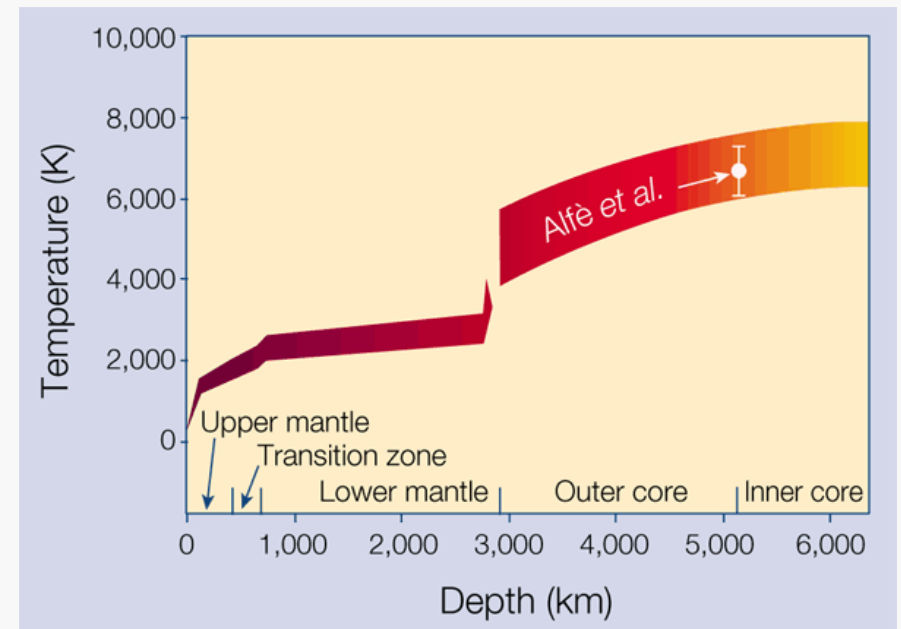
[Nature 525 (2015) 73]



Through “computer experiments”, theoreticians can now investigate some important **systems where human being cannot conduct experiments yet**, such as the physical and chemical processes happening in the interior of our planet.



[*Ab initio* melting curve of iron compared with experiments.]



[Nature 401 (1999) 462]

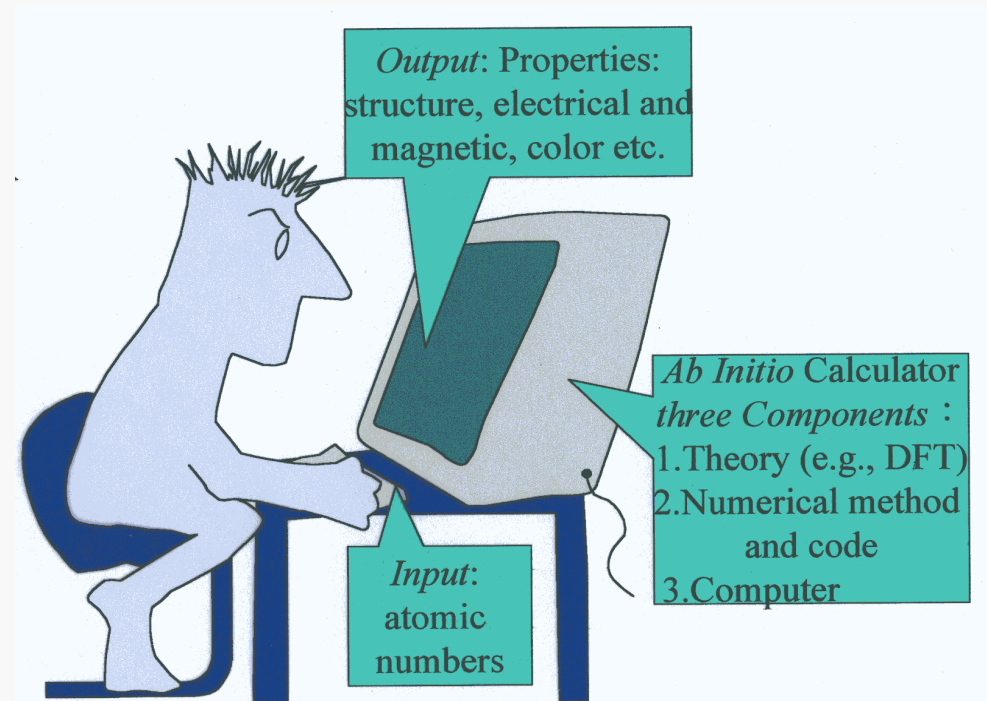


## 1.3 Outline of this course

This lecture consists of two parts.

**Part one** is on the fundamentals of first-principles materials calculations. This part will cover basic concepts of crystals, theories of electrons in periodic potentials, fundamentals of density functional theory and computational (numerical) techniques.

**Part two** is about determination of materials properties. This part consists of several units made up of lectures and hands-on exercises, given by senior researchers in field. Each unit focus on one major physical property of materials or one topic of current interest in materials physics.



# Course Materials

## 1. Main Information Source:

The course will be largely based on lecture notes and hand-outs.

## 2. Principal Reference Book

[1] *Electronic Structure: Basic Theory and Practical Methods*  
by Richard M. Martin (Cambridge U. P., 2004).

## 3. Other References:

[2] *Introduction to Solid State Physics*  
by Charles Kittel (John Wiley & Sons).

[3] *Solid State Physics* by Neil W. Ashcroft and N. David Mermin.

[4] *Planewaves, Pseudopotentials and the LAPW Method*  
by David J. Singh and Lars Nordstrom (2nd edition) (Springer, 2006)

[5] *Theory of Itinerant Electron Magnetism*, J. Kübler (Oxford, 2000).