

# Tasks for Next week

- (1) Read chapter 4: Phonons / Lattice Vibrations**
- (2) Solve next exercise sheets**
- (3) Summary + student presentation**

**Exercise 1** *Binding energy*

a) Show that for a potential of the form  $U(R) = -\frac{A}{R^m} + \frac{B}{R^n}$  an equilibrium can only be reached if  $n > m$ .

b) For a pure van der Waals attraction the potential is often written as

$$U(R) = 4\epsilon \left[ \left( \frac{\sigma}{R} \right)^{12} - \left( \frac{\sigma}{R} \right)^6 \right].$$

Calculate the binding energy (cohesive energy)  $E_B$  and the equilibrium distance  $R_0$ .

c) Calculate the effect of thermal expansion,  $\Delta R_0(T)/R_0$ , on a linear chain of atoms with the potential of part b. Assume that the thermal energy  $k_B T \ll E_B$  allows motion of the atoms around the equilibrium position. Think about in what boundaries the atoms can move. From this deduce the average position and compare the result with  $R_0$ .

Hint: Use the expansion  $1/(1 \pm \epsilon) \approx 1 \mp \epsilon + \epsilon^2 + \dots$  up to the second order and  $\sqrt[n]{1 + \epsilon} = 1 + \epsilon/n + \dots$  for  $\epsilon \rightarrow 0$ .

**Exercise 2** *Madelung constant*

Calculate the Madelung constant for an infinitely long, evenly spaced, linear chain of ions with alternating anions and cations of charge  $\pm e$ .

**Exercise 3** *Linear ionic crystal*

Consider a line of  $2N$  ions of alternating charge  $\pm q$  with a repulsive potential energy  $A/R^n$  between nearest neighbours.

a) Show that the expression for the potential energy can be approximated by

$$U(R) = N \left[ \frac{2A}{R^n} - \frac{2 \ln 2 q^2}{4\pi\epsilon_0 R} \right].$$

b) Show that at the equilibrium separation

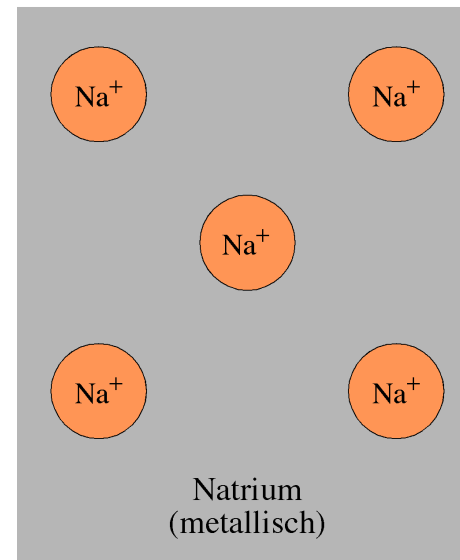
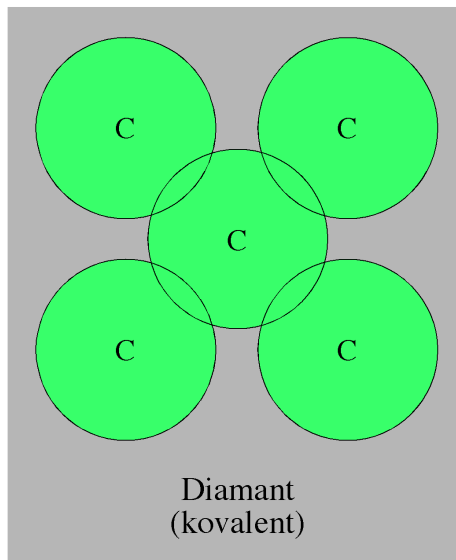
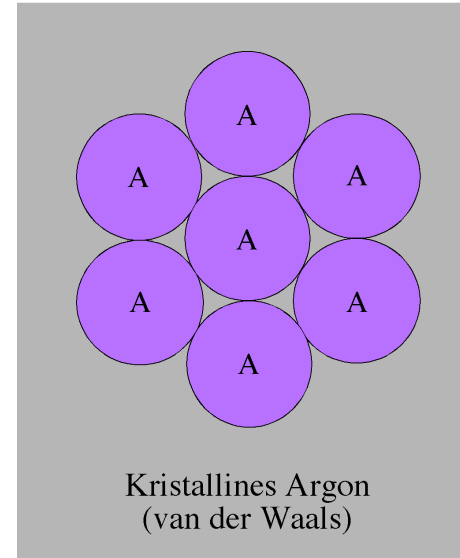
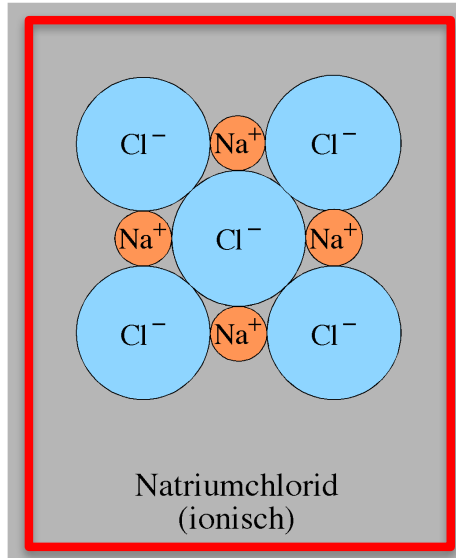
$$U(R_0) = -\frac{2Nq^2 \ln 2}{4\pi\epsilon_0 R_0} \cdot \left( 1 - \frac{1}{n} \right).$$

c) Let the crystal be compressed so that  $R_0 \rightarrow R_0(1 - \delta)$ . Show that the work done in compressing a unit length of the crystal has the leading term  $\frac{1}{2}C\delta^2$ , where

$$C = \frac{(n-1)q^2 \ln 2}{4\pi\epsilon_0 R_0}.$$

Note: Use the complete expression for  $U(R)$  instead of  $U(R_0)$ .

# Today's lecture



# Periodic Table

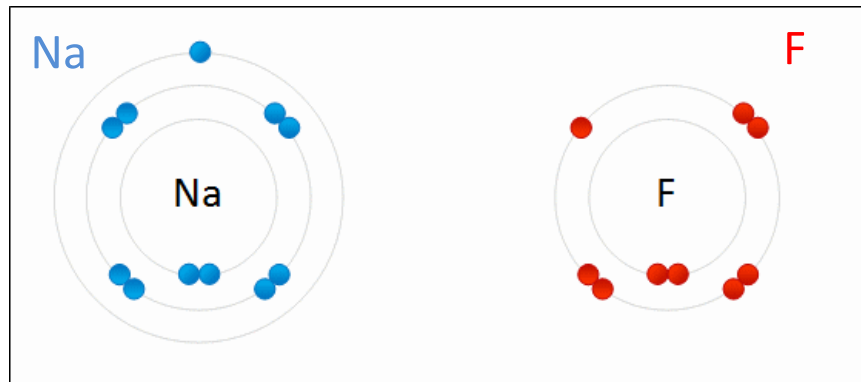
**Periodic Table of the Elements**

s   p   d   f

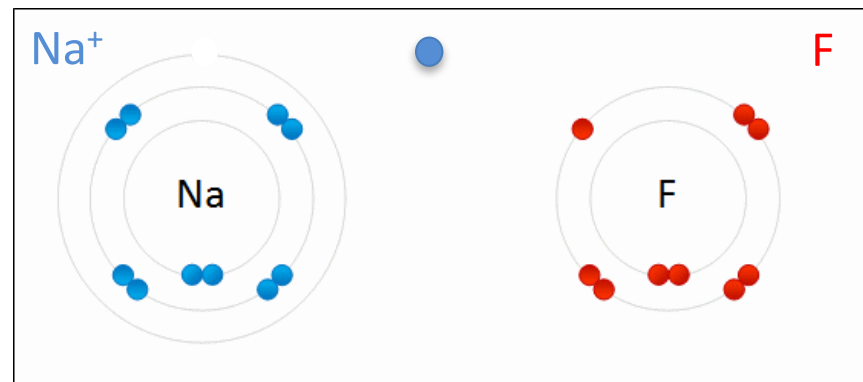
Atomic Number   Atomic Mass  
 Symbol  
 Name  
 Electron Configuration

1 IA 1A	1 H Hydrogen 1s <sup>1</sup>	2 IIA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A					
	3 Li Lithium [He]2s <sup>1</sup>	4 Be Beryllium [He]2s <sup>2</sup>																5 B Boron [He]2s <sup>2</sup> 2p <sup>1</sup>	6 C Carbon [He]2s <sup>2</sup> 2p <sup>2</sup>	7 N Nitrogen [He]2s <sup>2</sup> 2p <sup>3</sup>	8 O Oxygen [He]2s <sup>2</sup> 2p <sup>4</sup>	9 F Fluorine [He]2s <sup>2</sup> 2p <sup>5</sup>	10 Ne Neon [He]2s <sup>2</sup> 2p <sup>6</sup>
	11 Na Sodium [Ne]3s <sup>1</sup>	12 Mg Magnesium [Ne]3s <sup>2</sup>	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B						13 Al Aluminum [Ne]3s <sup>2</sup> 3p <sup>1</sup>	14 Si Silicon [Ne]3s <sup>2</sup> 3p <sup>2</sup>	15 P Phosphorus [Ne]3s <sup>2</sup> 3p <sup>3</sup>	16 S Sulfur [Ne]3s <sup>2</sup> 3p <sup>4</sup>	17 Cl Chlorine [Ne]3s <sup>2</sup> 3p <sup>5</sup>	18 Ar Argon [Ne]3s <sup>2</sup> 3p <sup>6</sup>
	19 K Potassium [Ar]4s <sup>1</sup>	20 Ca Calcium [Ar]4s <sup>2</sup>	21 Sc Scandium [Ar]3d <sup>1</sup> 4s <sup>2</sup>	22 Ti Titanium [Ar]3d <sup>2</sup> 4s <sup>2</sup>	23 V Vanadium [Ar]3d <sup>3</sup> 4s <sup>2</sup>	24 Cr Chromium [Ar]3d <sup>5</sup> 4s <sup>1</sup>	25 Mn Manganese [Ar]3d <sup>5</sup> 4s <sup>2</sup>	26 Fe Iron [Ar]3d <sup>6</sup> 4s <sup>2</sup>	27 Co Cobalt [Ar]3d <sup>7</sup> 4s <sup>2</sup>	28 Ni Nickel [Ar]3d <sup>8</sup> 4s <sup>2</sup>	29 Cu Copper [Ar]3d <sup>10</sup> 4s <sup>1</sup>	30 Zn Zinc [Ar]3d <sup>10</sup> 4s <sup>2</sup>	31 Ga Gallium [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>1</sup>	32 Ge Germanium [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup>	33 As Arsenic [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup>	34 Se Selenium [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup>	35 Br Bromine [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup>	36 Kr Krypton [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup>					
	37 Rb Rubidium [Kr]5s <sup>1</sup>	38 Sr Strontium [Kr]5s <sup>2</sup>	39 Y Yttrium [Kr]4d <sup>1</sup> 5s <sup>2</sup>	40 Zr Zirconium [Kr]4d <sup>2</sup> 5s <sup>2</sup>	41 Nb Niobium [Kr]4d <sup>4</sup> 5s <sup>1</sup>	42 Mo Molybdenum [Kr]4d <sup>5</sup> 5s <sup>1</sup>	43 Tc Technetium [Kr]4d <sup>5</sup> 5s <sup>2</sup>	44 Ru Ruthenium [Kr]4d <sup>7</sup> 5s <sup>1</sup>	45 Rh Rhodium [Kr]4d <sup>8</sup> 5s <sup>1</sup>	46 Pd Palladium [Kr]4d <sup>10</sup>	47 Ag Silver [Kr]4d <sup>10</sup> 5s <sup>1</sup>	48 Cd Cadmium [Kr]4d <sup>10</sup> 5s <sup>2</sup>	49 In Indium [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>1</sup>	50 Sn Tin [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup>	51 Sb Antimony [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup>	52 Te Tellurium [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup>	53 I Iodine [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>	54 Xe Xenon [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup>					
	55 Cs Cesium [Xe]6s <sup>1</sup>	56 Ba Barium [Xe]6s <sup>2</sup>	57-71	72 Hf Hafnium [Xe]4f <sup>14</sup> 5d <sup>2</sup> 6s <sup>2</sup>	73 Ta Tantalum [Xe]4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup>	74 W Tungsten [Xe]4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup>	75 Re Rhenium [Xe]4f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup>	76 Os Osmium [Xe]4f <sup>14</sup> 5d <sup>6</sup> 6s <sup>2</sup>	77 Ir Iridium [Xe]4f <sup>14</sup> 5d <sup>7</sup> 6s <sup>2</sup>	78 Pt Platinum [Xe]4f <sup>14</sup> 5d <sup>9</sup> 6s <sup>1</sup>	79 Au Gold [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>1</sup>	80 Hg Mercury [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup>	81 Tl Thallium [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>1</sup>	82 Pb Lead [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>2</sup>	83 Bi Bismuth [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>3</sup>	84 Po Polonium [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>4</sup>	85 At Astatine [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>5</sup>	86 Rn Radon [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>6</sup>					
	87 Fr Francium [Rn]7s <sup>1</sup>	88 Ra Radium [Rn]7s <sup>2</sup>	89-103	104 Rf Rutherfordium [Rn]5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup>	105 Db Dubnium [Rn]5f <sup>14</sup> 6d <sup>3</sup> 7s <sup>2</sup>	106 Sg Seaborgium [Rn]5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup>	107 Bh Bohrium [Rn]5f <sup>14</sup> 6d <sup>5</sup> 7s <sup>2</sup>	108 Hs Hassium [Rn]5f <sup>14</sup> 6d <sup>6</sup> 7s <sup>2</sup>	109 Mt Meitnerium [Rn]5f <sup>14</sup> 6d <sup>7</sup> 7s <sup>2</sup>	110 Ds Darmstadtium [Rn]5f <sup>14</sup> 6d <sup>8</sup> 7s <sup>2</sup>	111 Rg Roentgenium [Rn]5f <sup>14</sup> 6d <sup>9</sup> 7s <sup>2</sup>	112 Cn Copernicium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup>	113 Uut Ununtrium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>1</sup>	114 Fl Flerovium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>2</sup>	115 Uup Ununpentium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>3</sup>	116 Lv Livermorium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>4</sup>	117 Uus Ununseptium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>5</sup>	118 Uuo Ununoctium [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>6</sup>					
Lanthanide Series	57 La Lanthanum [Xe]5d <sup>1</sup> 6s <sup>2</sup>	58 Ce Cerium [Xe]4f <sup>1</sup> 5d <sup>1</sup> 6s <sup>2</sup>	59 Pr Praseodymium [Xe]4f <sup>3</sup> 6s <sup>2</sup>	60 Nd Neodymium [Xe]4f <sup>4</sup> 6s <sup>2</sup>	61 Pm Promethium [Xe]4f <sup>5</sup> 6s <sup>2</sup>	62 Sm Samarium [Xe]4f <sup>6</sup> 6s <sup>2</sup>	63 Eu Europium [Xe]4f <sup>7</sup> 6s <sup>2</sup>	64 Gd Gadolinium [Xe]4f <sup>7</sup> 5d <sup>1</sup> 6s <sup>2</sup>	65 Tb Terbium [Xe]4f <sup>9</sup> 6s <sup>2</sup>	66 Dy Dysprosium [Xe]4f <sup>10</sup> 6s <sup>2</sup>	67 Ho Holmium [Xe]4f <sup>11</sup> 6s <sup>2</sup>	68 Er Erbium [Xe]4f <sup>12</sup> 6s <sup>2</sup>	69 Tm Thulium [Xe]4f <sup>13</sup> 6s <sup>2</sup>	70 Yb Ytterbium [Xe]4f <sup>14</sup> 6s <sup>2</sup>	71 Lu Lutetium [Xe]4f <sup>14</sup> 5d <sup>1</sup> 6s <sup>2</sup>								
Actinide Series	89 Ac Actinium [Rn]6d <sup>1</sup> 7s <sup>2</sup>	90 Th Thorium [Rn]6d <sup>2</sup> 7s <sup>2</sup>	91 Pa Protactinium [Rn]5f <sup>2</sup> 6d <sup>1</sup> 7s <sup>2</sup>	92 U Uranium [Rn]5f <sup>3</sup> 6d <sup>1</sup> 7s <sup>2</sup>	93 Np Neptunium [Rn]5f <sup>4</sup> 6d <sup>1</sup> 7s <sup>2</sup>	94 Pu Plutonium [Rn]5f <sup>6</sup> 7s <sup>2</sup>	95 Am Americium [Rn]5f <sup>7</sup> 7s <sup>2</sup>	96 Cm Curium [Rn]5f <sup>7</sup> 6d <sup>1</sup> 7s <sup>2</sup>	97 Bk Berkelium [Rn]5f <sup>9</sup> 7s <sup>2</sup>	98 Cf Californium [Rn]5f <sup>10</sup> 7s <sup>2</sup>	99 Es Einsteinium [Rn]5f <sup>11</sup> 7s <sup>2</sup>	100 Fm Fermium [Rn]5f <sup>12</sup> 7s <sup>2</sup>	101 Md Mendelevium [Rn]5f <sup>13</sup> 7s <sup>2</sup>	102 No Nobelium [Rn]5f <sup>14</sup> 7s <sup>2</sup>	103 Lr Lawrencium [Rn]5f <sup>14</sup> 6d <sup>1</sup> 7s <sup>2</sup>								

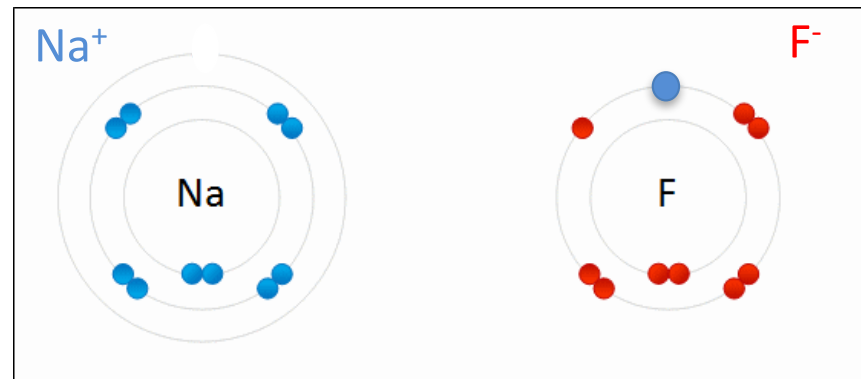
# Ionic crystals



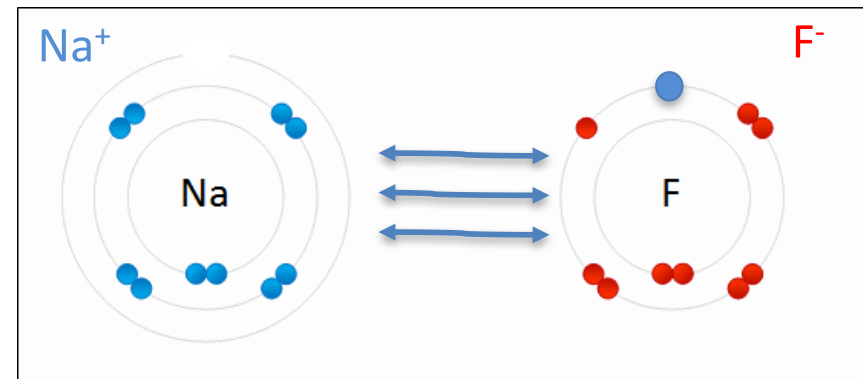
Ionization Energy = - 5.14 eV



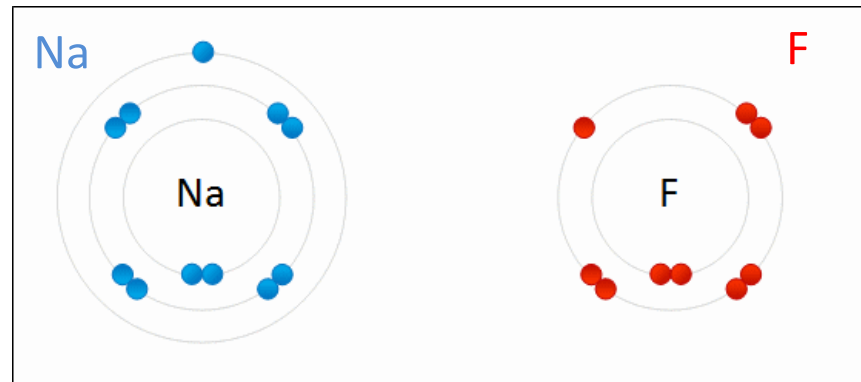
Electron affinity Energy = 3.4 eV



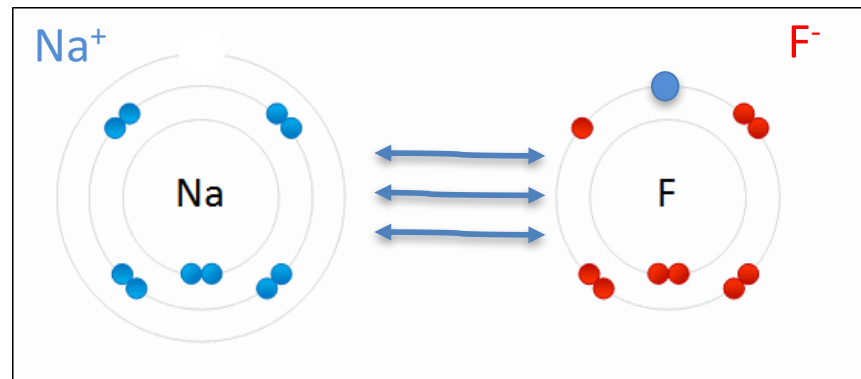
Cohesive Energy = 7.9 eV



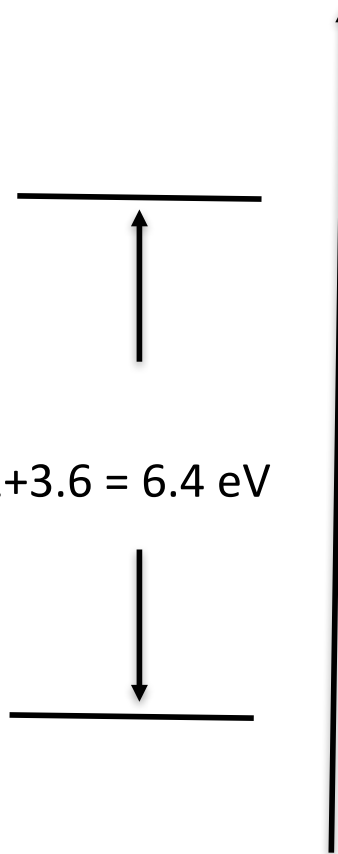
# Ionic crystals



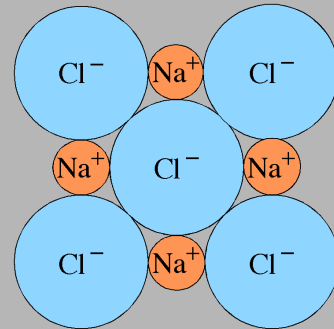
$$7.9 - 5.1 + 3.6 = 6.4 \text{ eV}$$



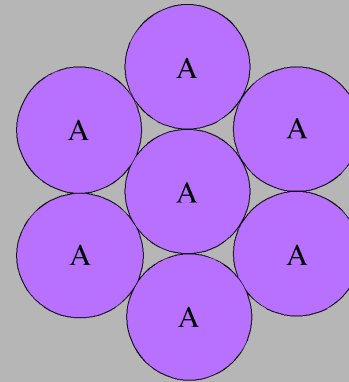
ENERGY



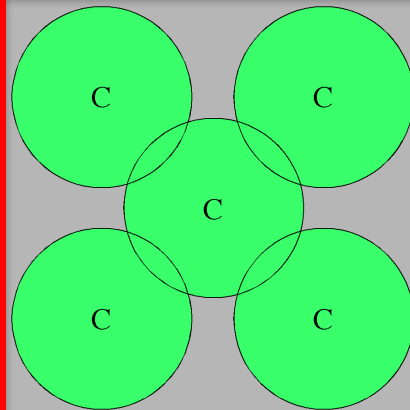
# Today's lecture



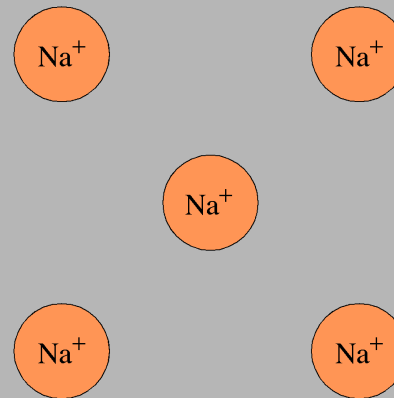
Natriumchlorid  
(ionisch)



Kristallines Argon  
(van der Waals)



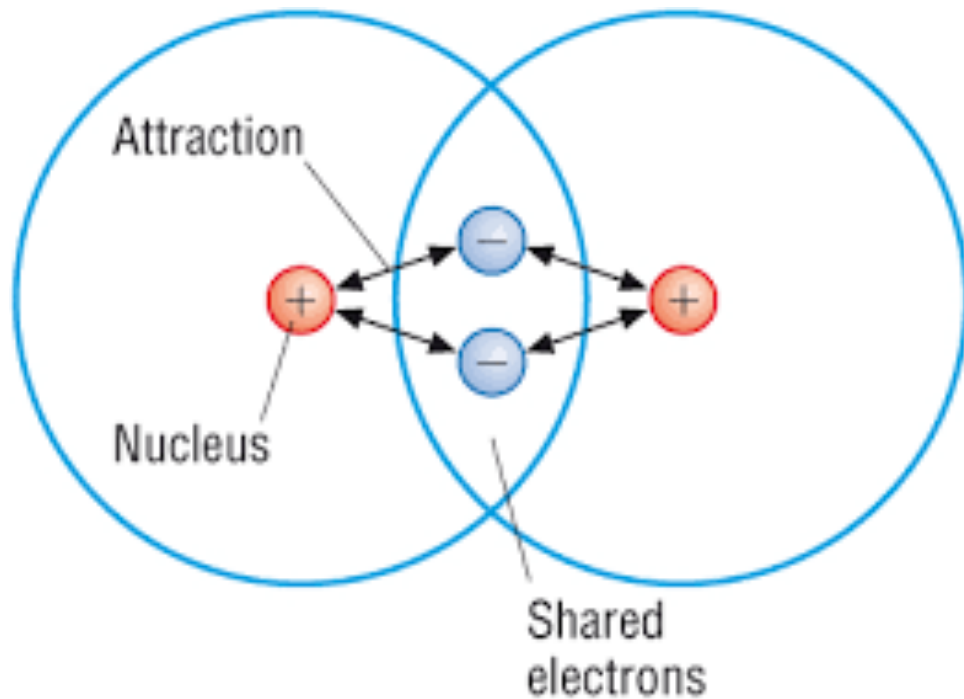
Diamant  
(kovalent)



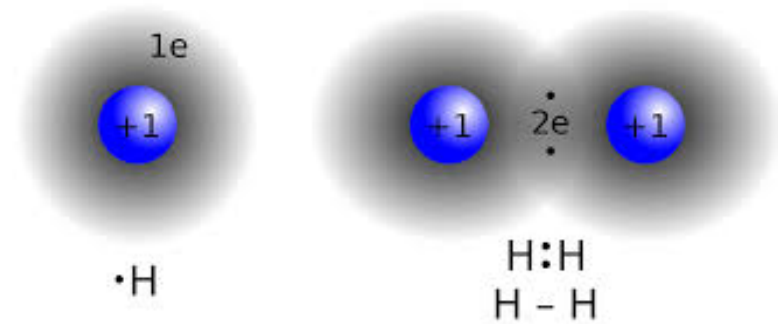
Natrium  
(metallisch)



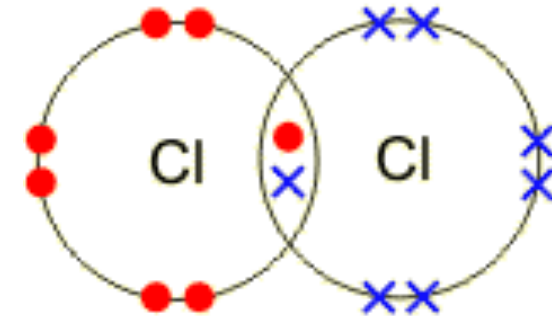
# Covalent bonds



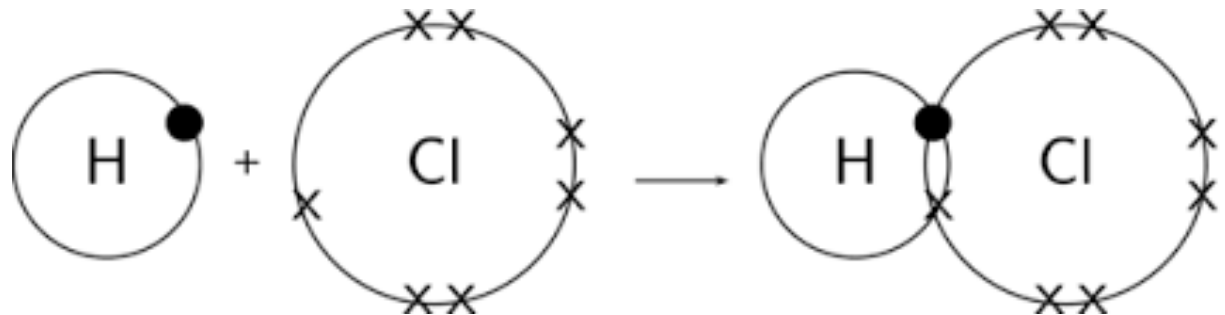
Example 1



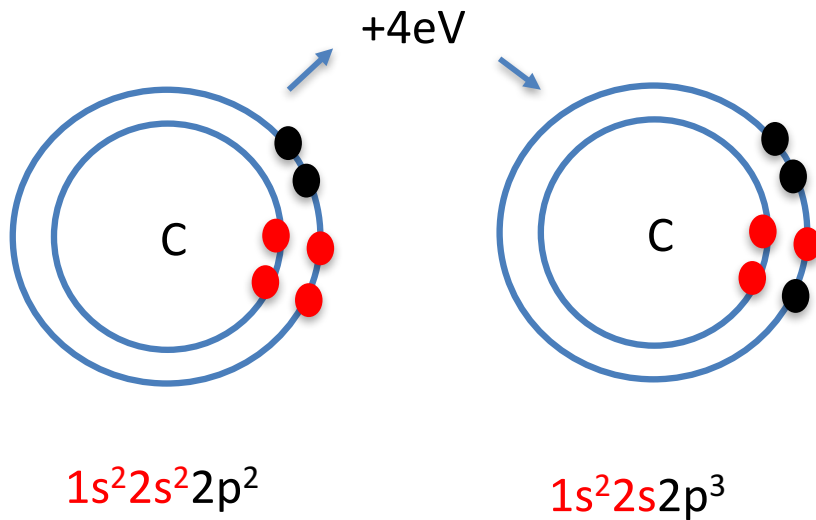
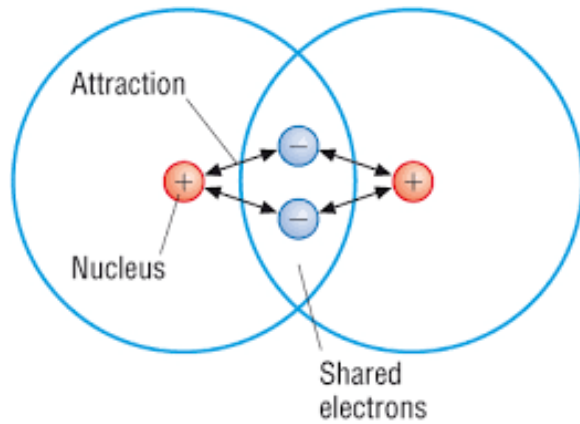
Example 2



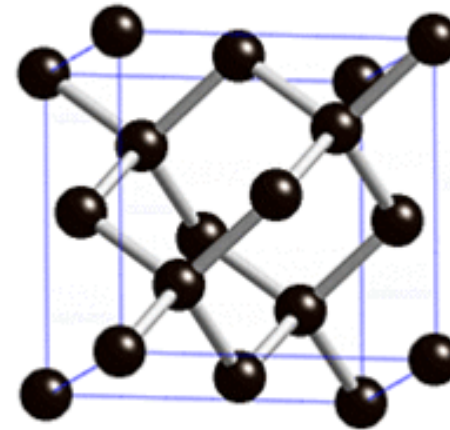
Example 3



# Covalent crystals



Diamond structure

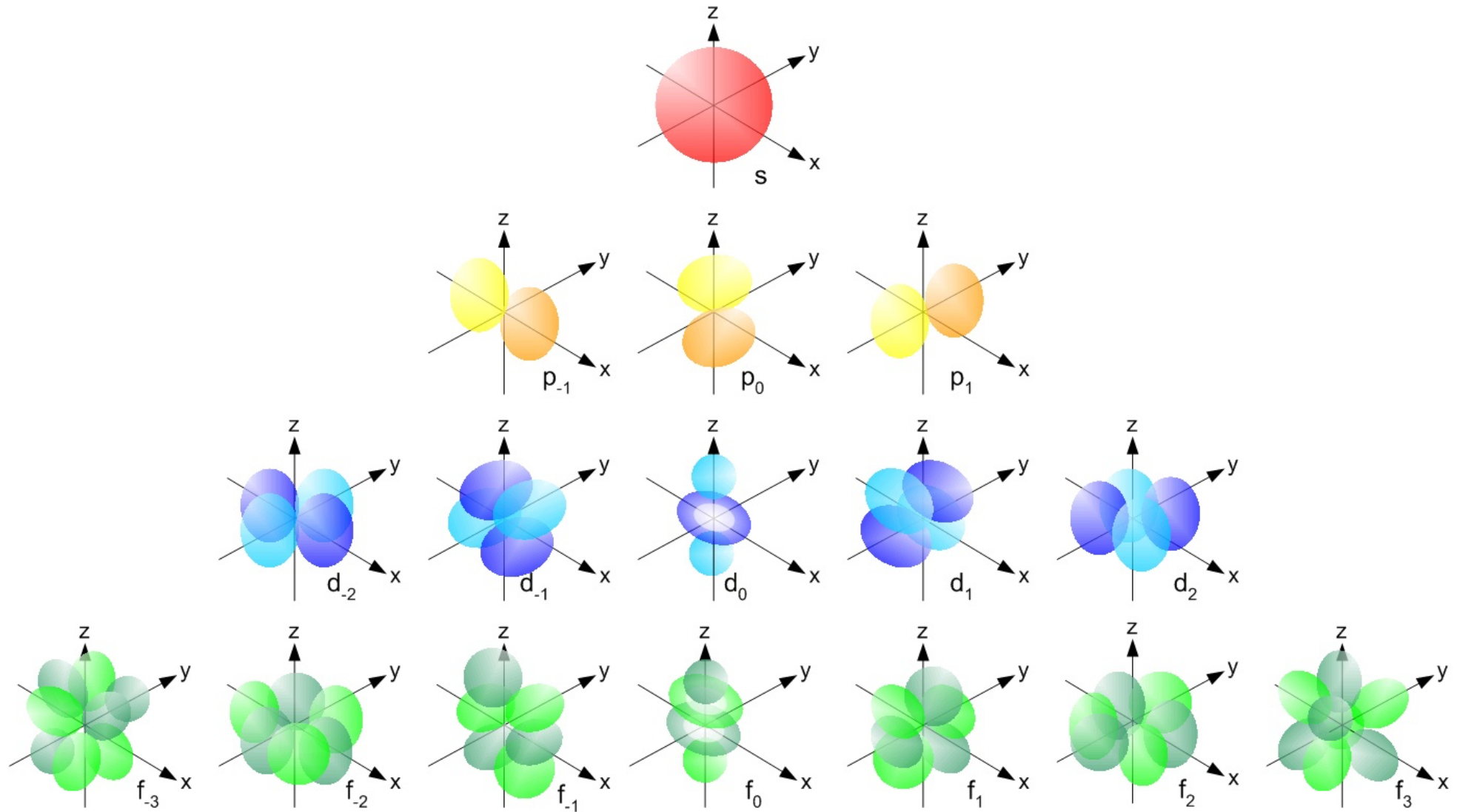


4 covalent bonds

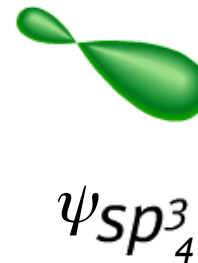
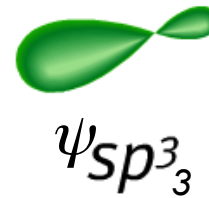
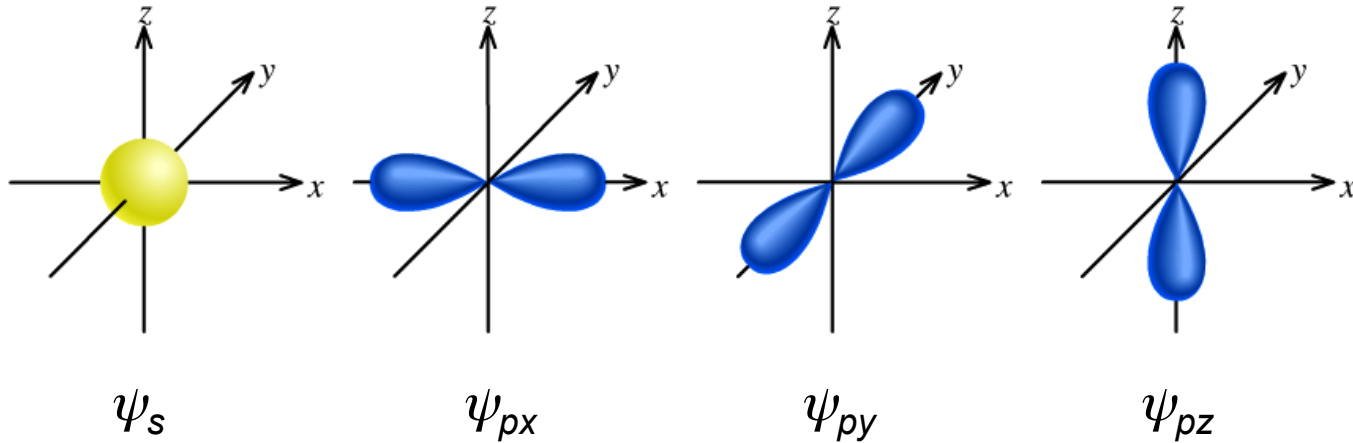
# Summary

Bindungstyp	Beispiel	Bindungsenergie (eV)
Ionisch	NaCl	8.23
	LiF	10.92
Van-der-Waals	Ar	0.080
	Kr	0.116
Kovalent	Diamant	7.36
	Si	4.64
Metallisch	Na	1.13
	Fe	4.29
	W	8.66
Wasserstoff-Brücken	H <sub>2</sub> O	0.52
	HF	0.30

# Electronic orbitals



# Orbital hybridization



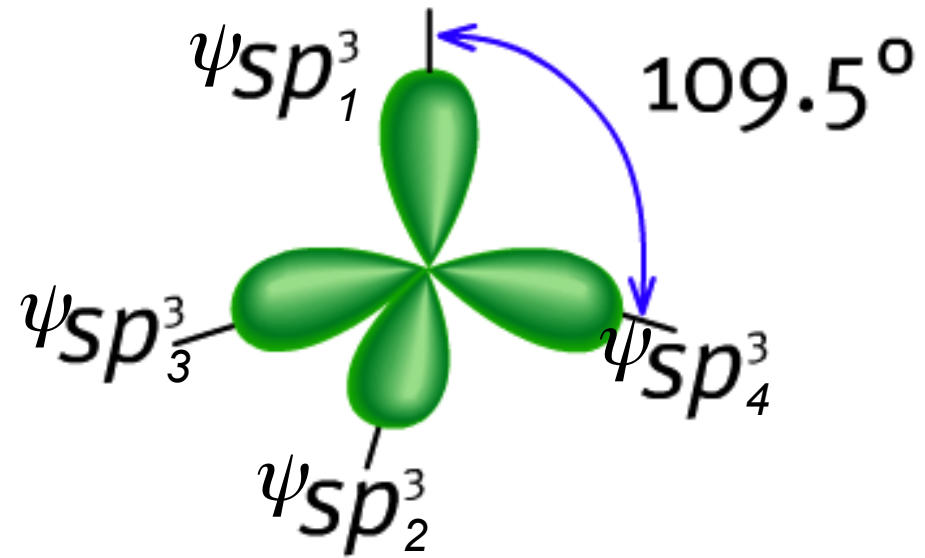
$$\frac{1}{2}(\psi_s + \psi_{px} + \psi_{py} + \psi_{pz})$$

$$\frac{1}{2}(\psi_s + \psi_{px} - \psi_{py} - \psi_{pz})$$

$$\frac{1}{2}(\psi_s - \psi_{px} + \psi_{py} - \psi_{pz})$$

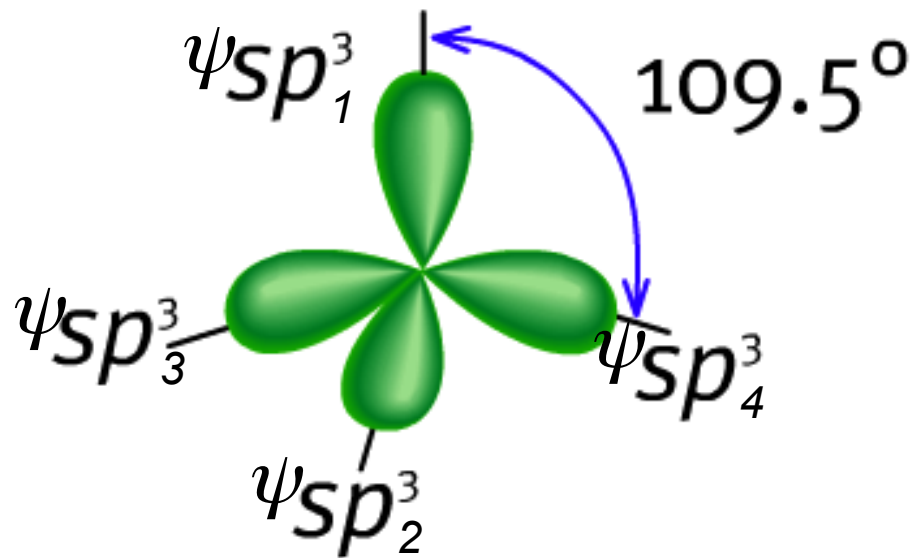
$$\frac{1}{2}(\psi_s - \psi_{px} - \psi_{py} + \psi_{pz})$$

# Orbital hybridization

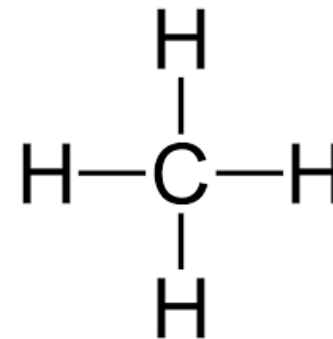
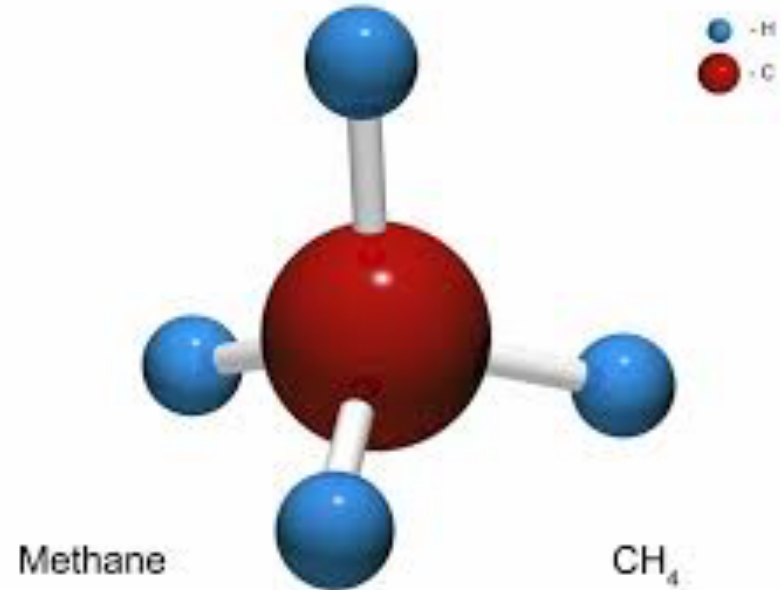


Tetraeder

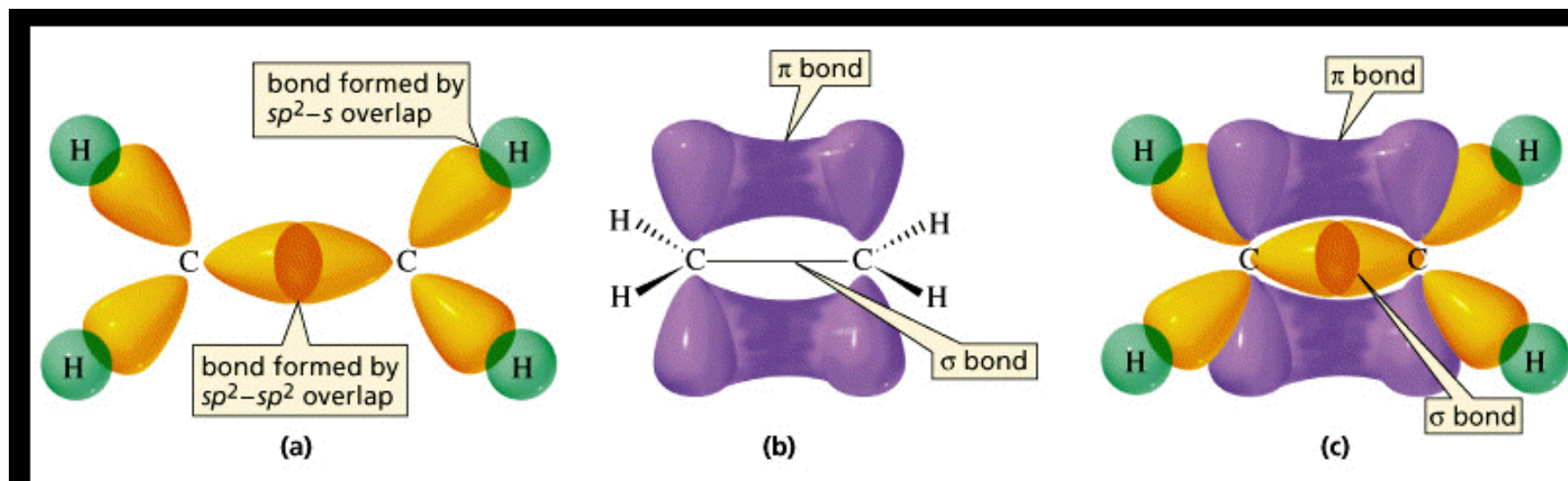
# Orbital molecular theory: Example CH<sub>4</sub> (Methane)



Tetraeder



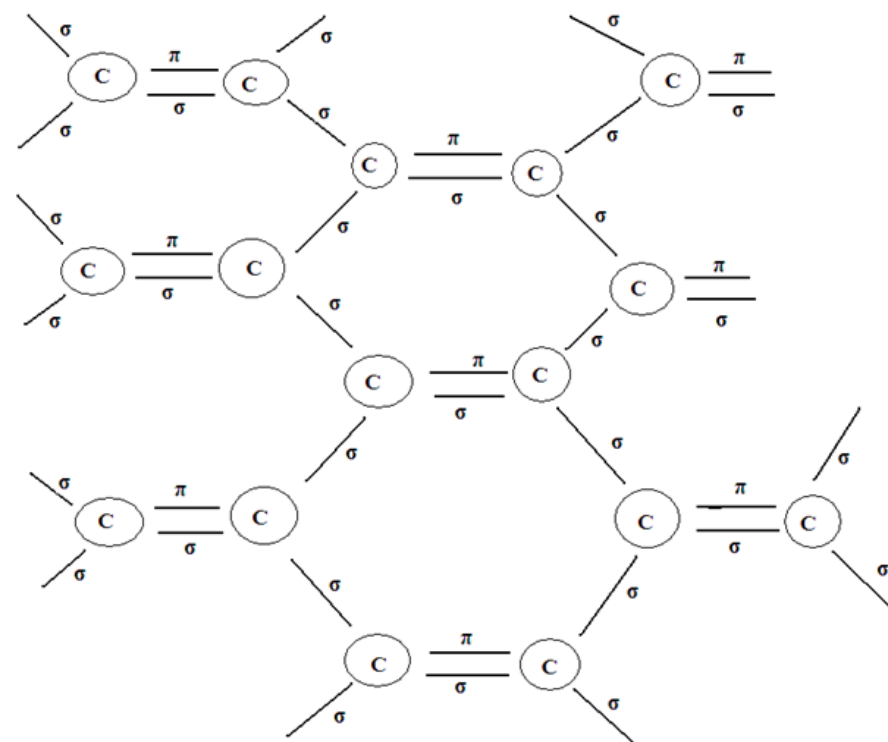
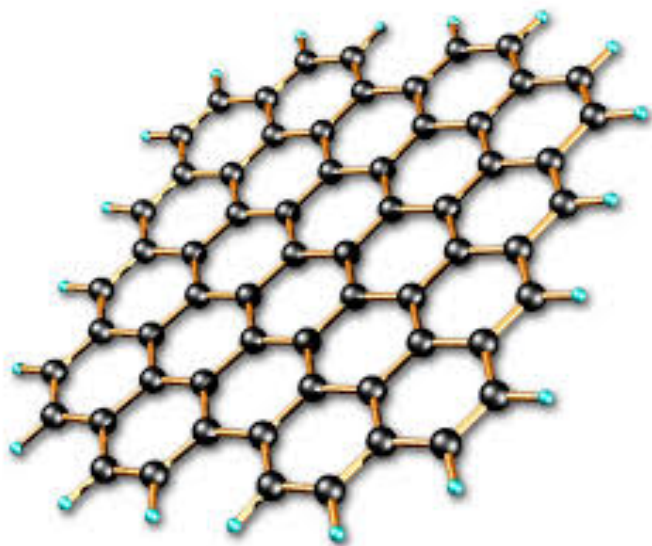
# Orbital molecular theory: $\sigma$ and $\pi$ bonding



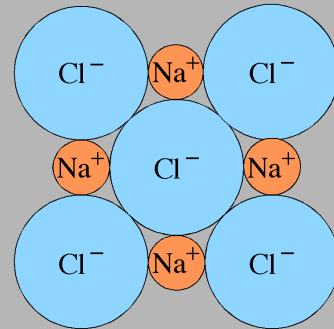


# Graphene: $\sigma$ and $\pi$ bonding

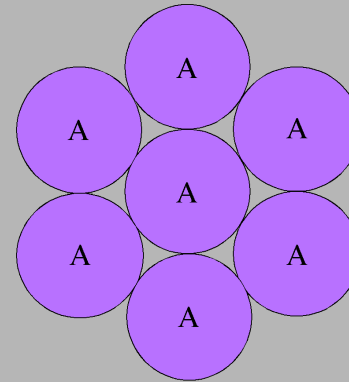
Graphene



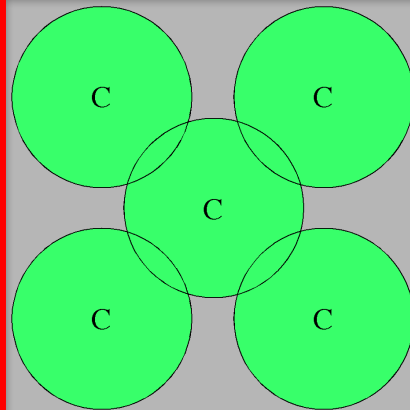
# Today's lecture



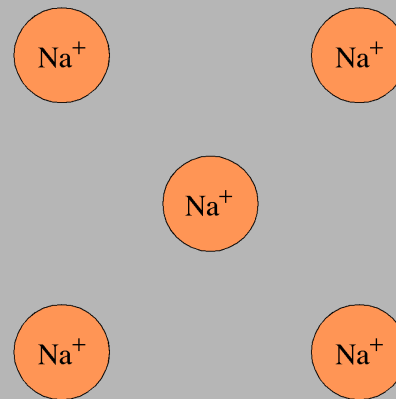
Natriumchlorid  
(ionisch)



Kristallines Argon  
(van der Waals)



Diamant  
(kovalent)



Natrium  
(metallisch)