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

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

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

b) Show that at the equilibrium separation

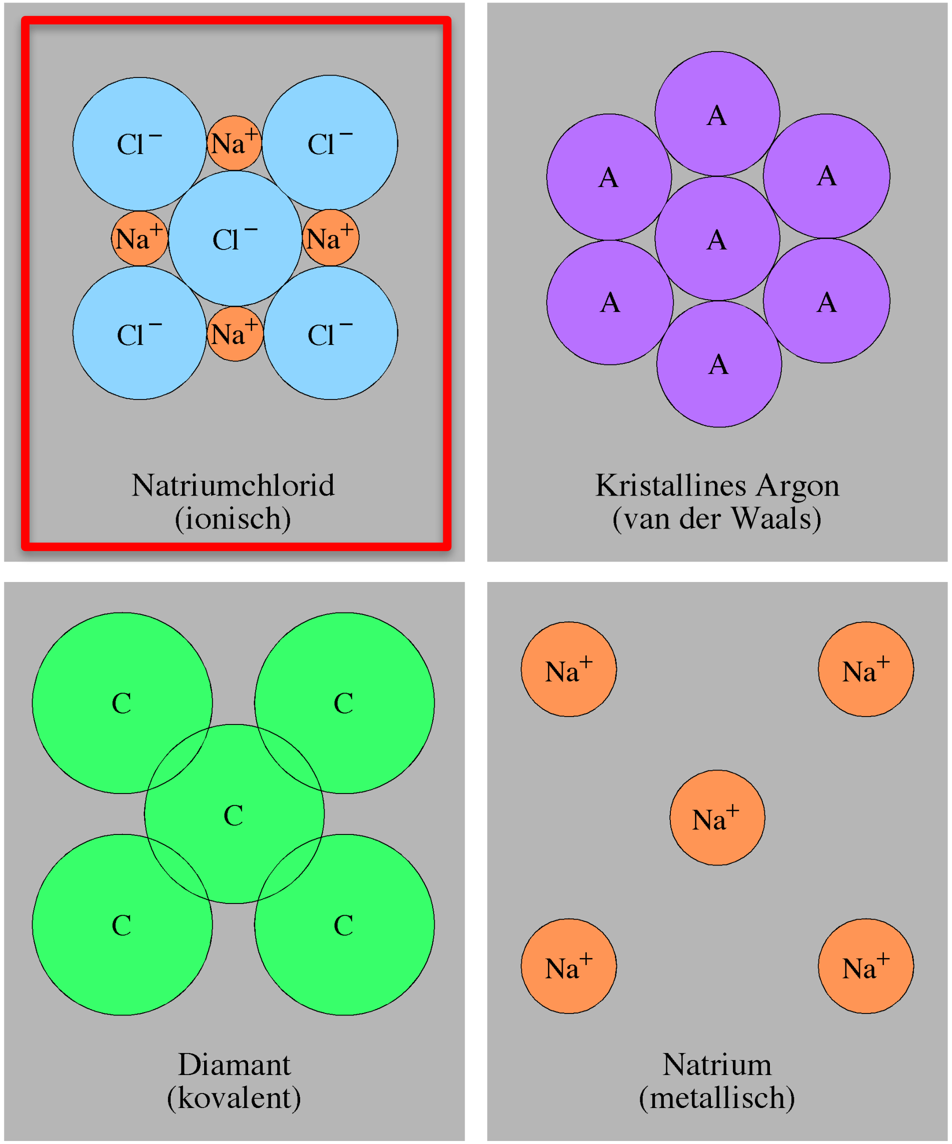
$$U(R_0) = -\frac{2Nq^2\ln 2}{4\pi\epsilon_0 R_0}\cdot\left(1-\frac{1}{n}\right).$$

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

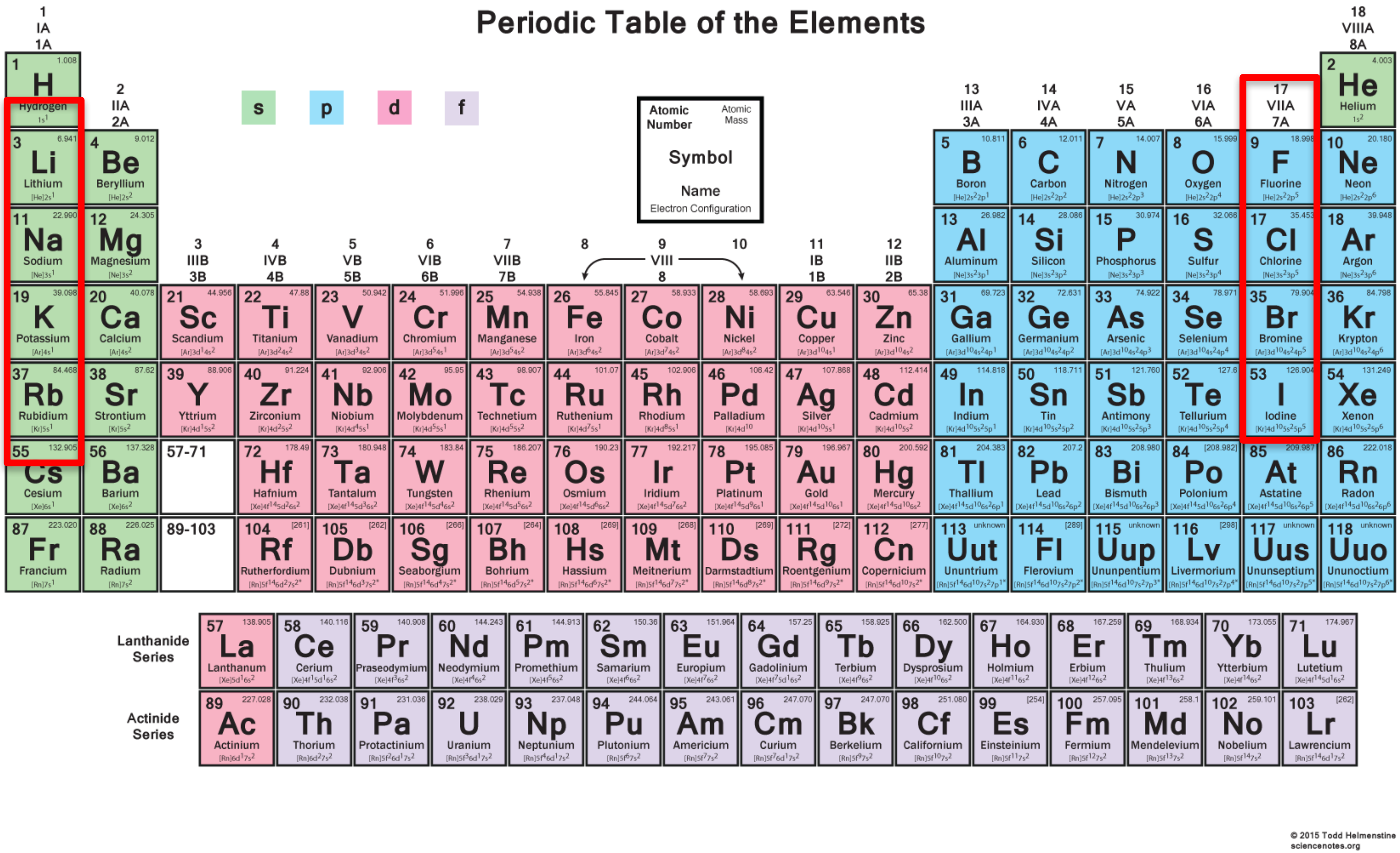
$$C = \frac{(n-1)q^2\ln 2}{4\pi\epsilon_0 R_0}.$$

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

Today’s lecture

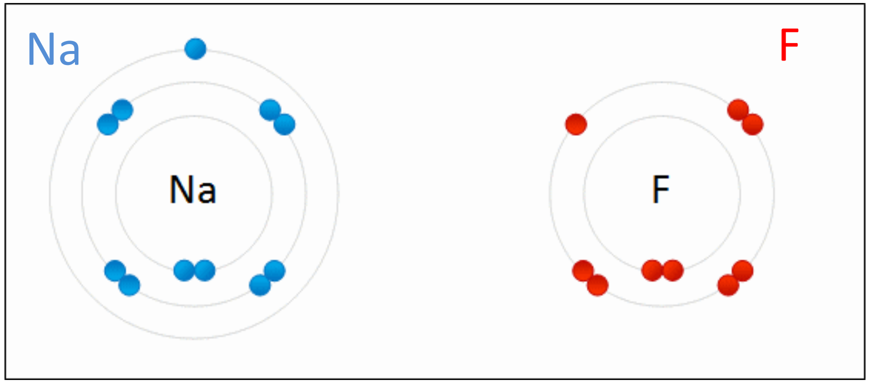


Periodic Table

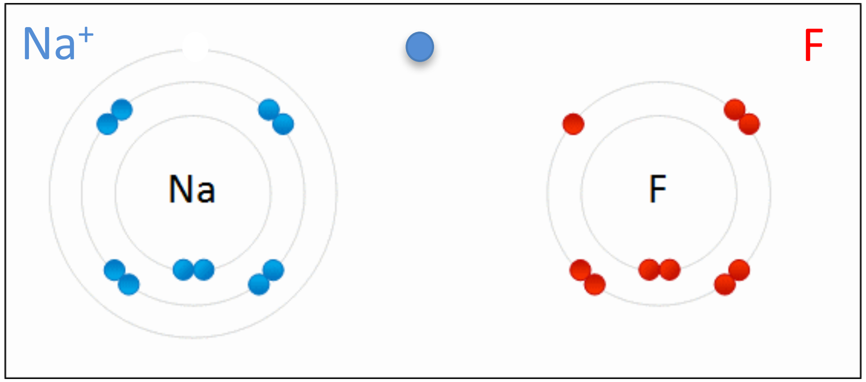


http://sciencenotes.org/periodic-table-showing-shells/

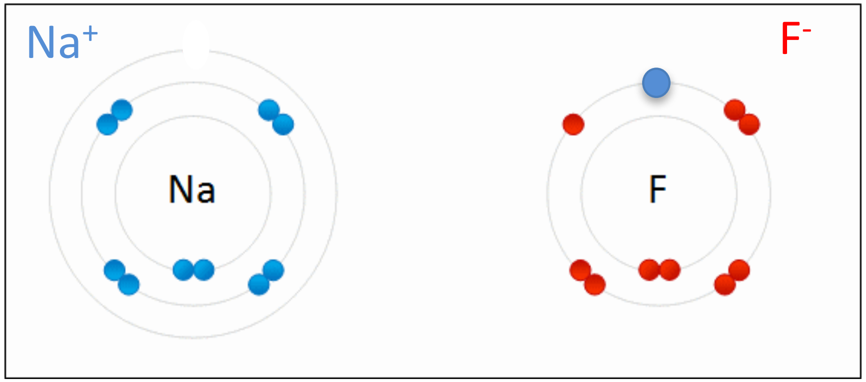
Ionic crystals



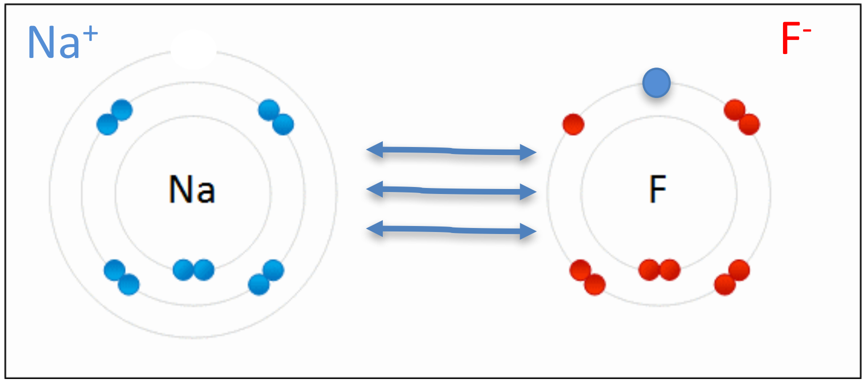
Ionization Energy = - 5.14 eV



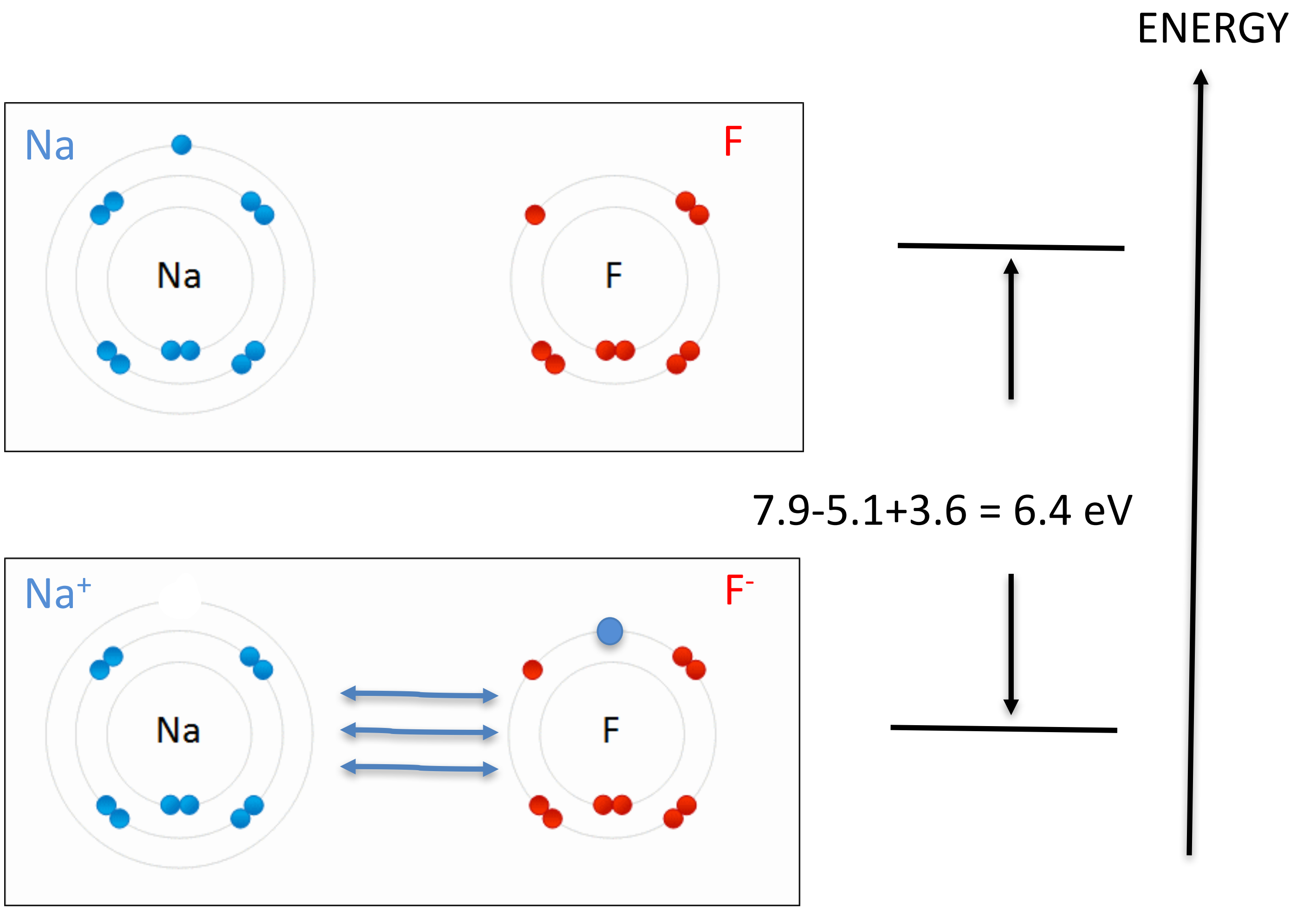
Electron affinity Energy = 3.4 eV



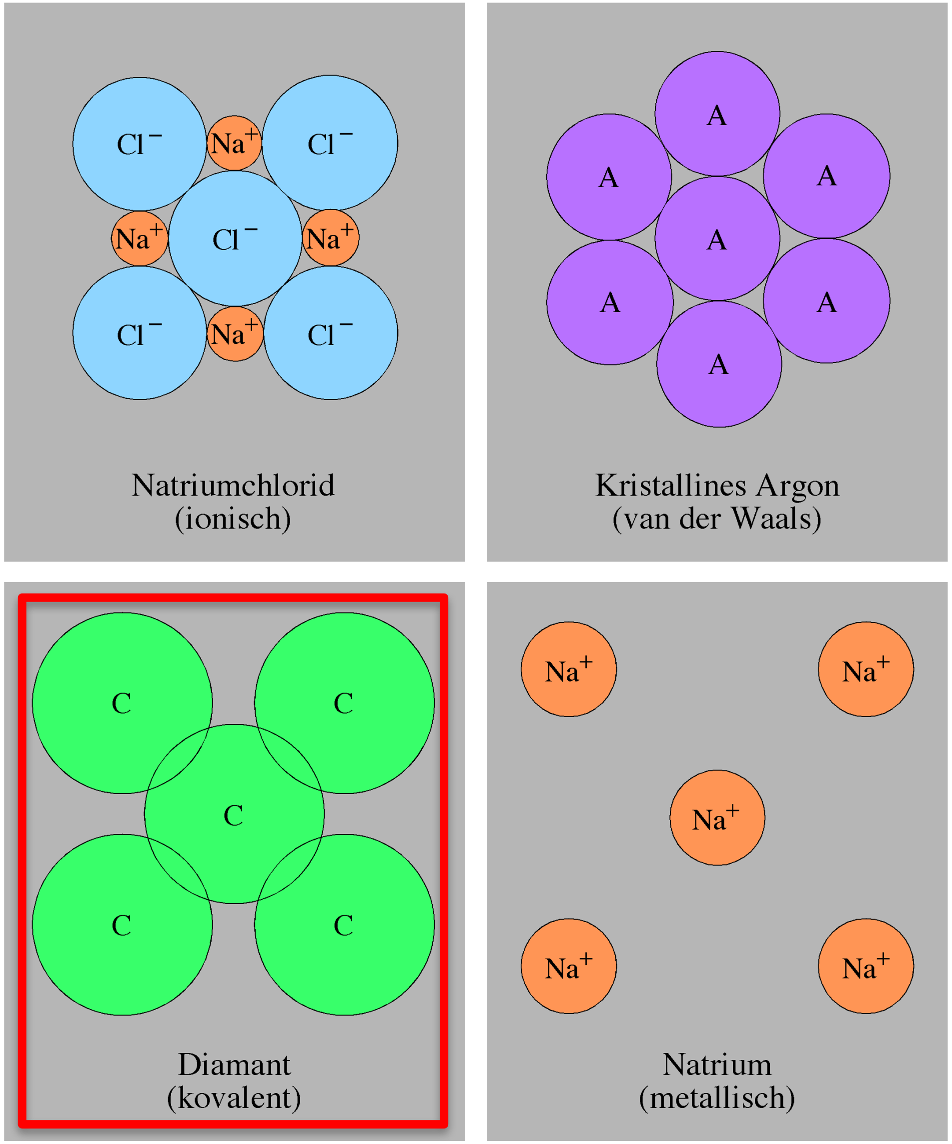
Cohesive Energy = 7.9 eV



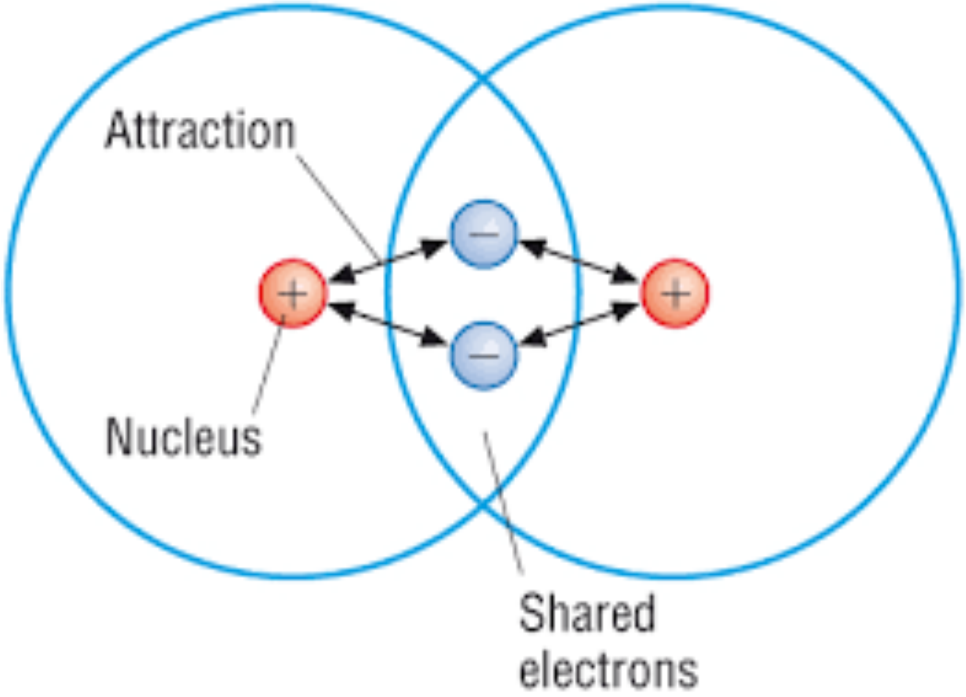
Ionic crystals



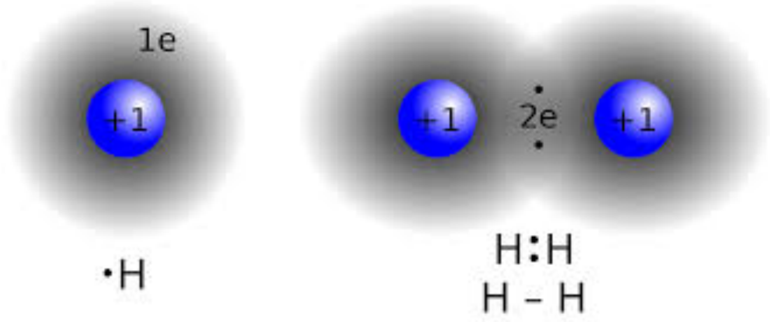
Today's lecture



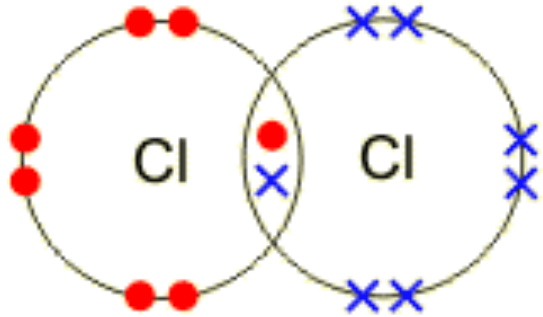
Covalent bonds



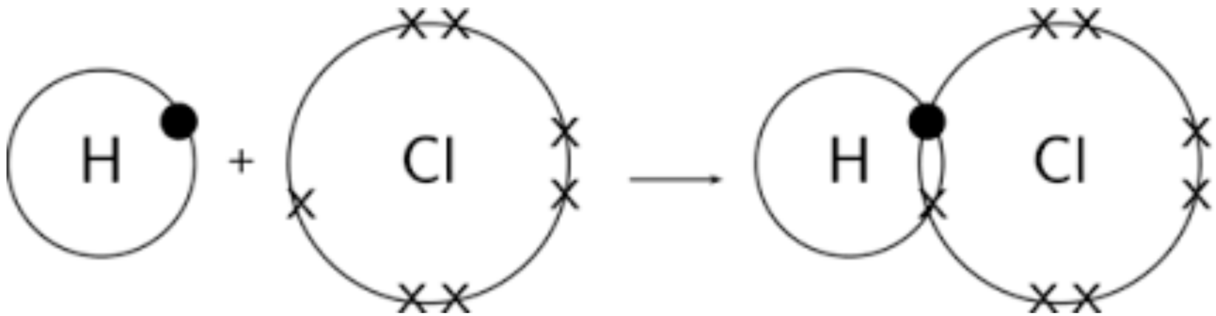
Example 1



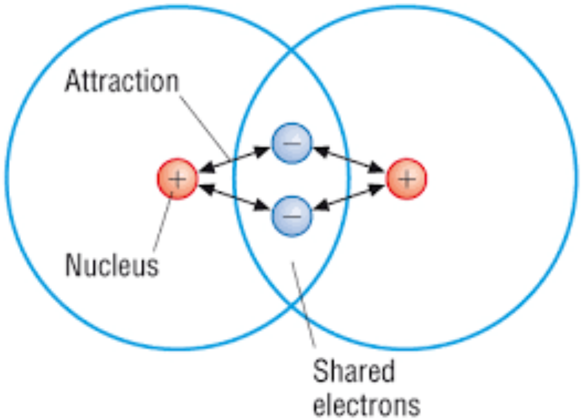
Example 2

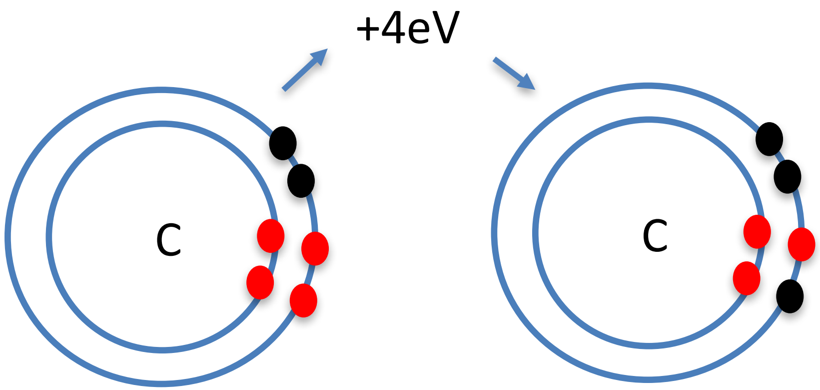


Example 3



Covalent crystals

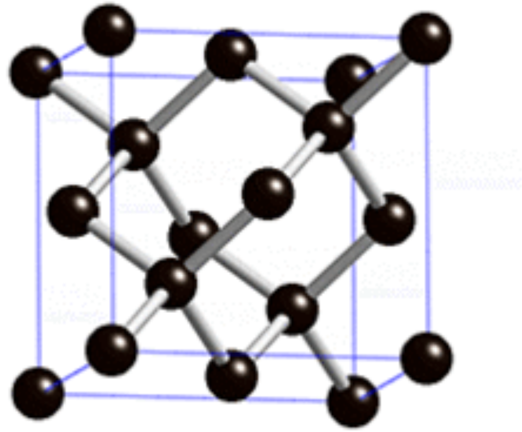




$1s^2 2s^2 2p^2$

$1s^2 2s 2p^3$

Diamond structure

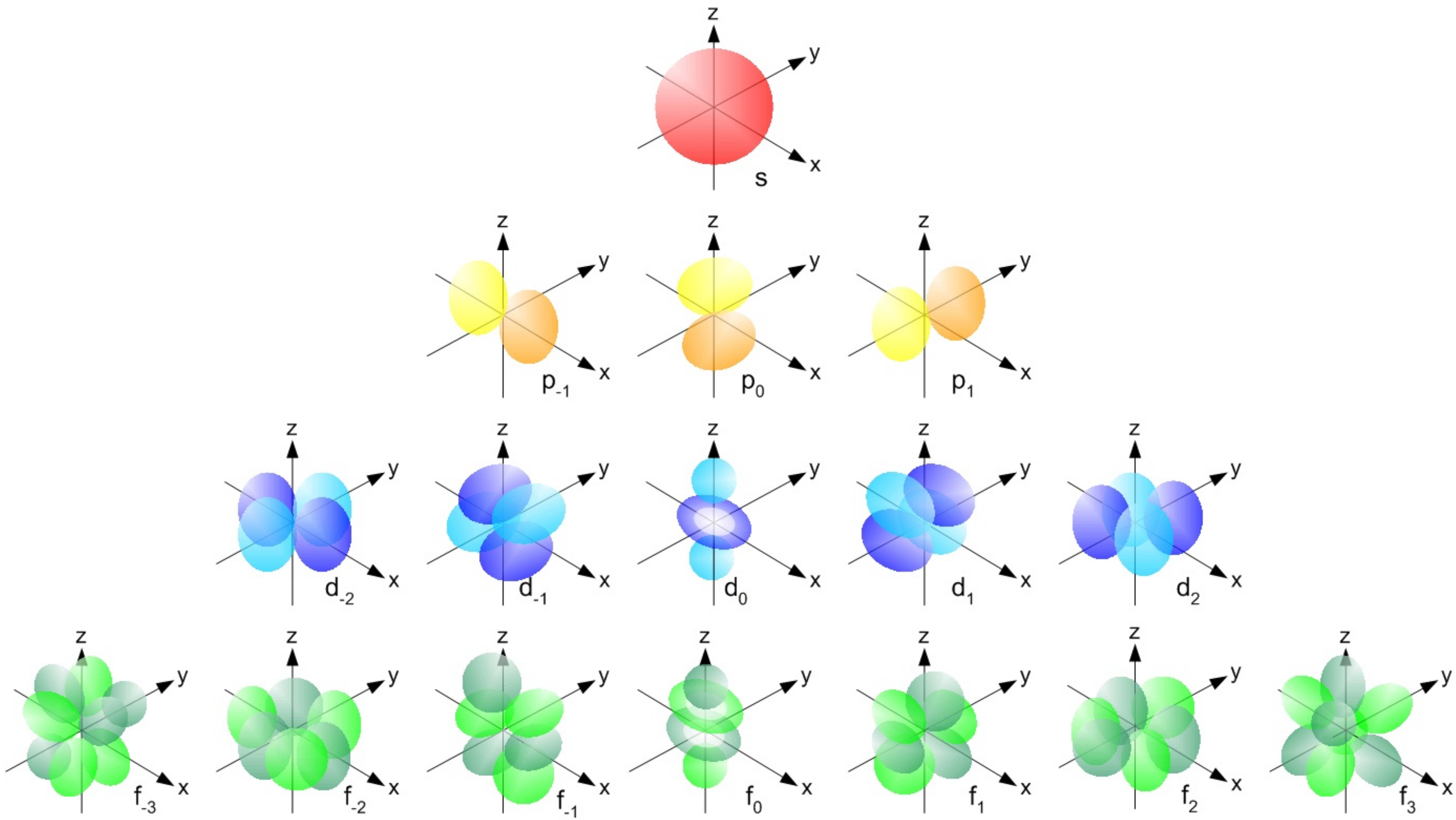


4 covalent bonds

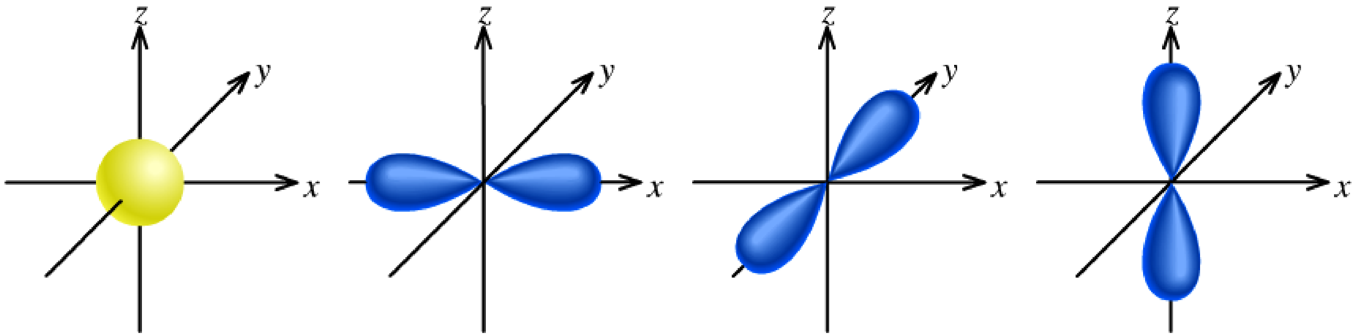
Summary

Bindungstyp	Beispiel	Bindungsenergie (eV)
Ionisch	NaCl LiF	8.23 10.92
Van-der-Waals	Ar Kr	0.080 0.116
Kovalent	Diamant Si	7.36 4.64
Metallisch	Na Fe W	1.13 4.29 8.66
Wasserstoff-Brücken	H_2O HF	0.52 0.30

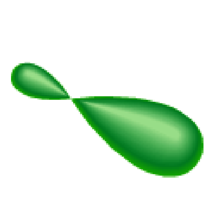
Electronic orbitals



Orbital hybridization



ψ_s ψ_{px} ψ_{py} ψ_{pz}



ψsp^3_1 ψsp^3_2 ψsp^3_3 ψsp^3_4

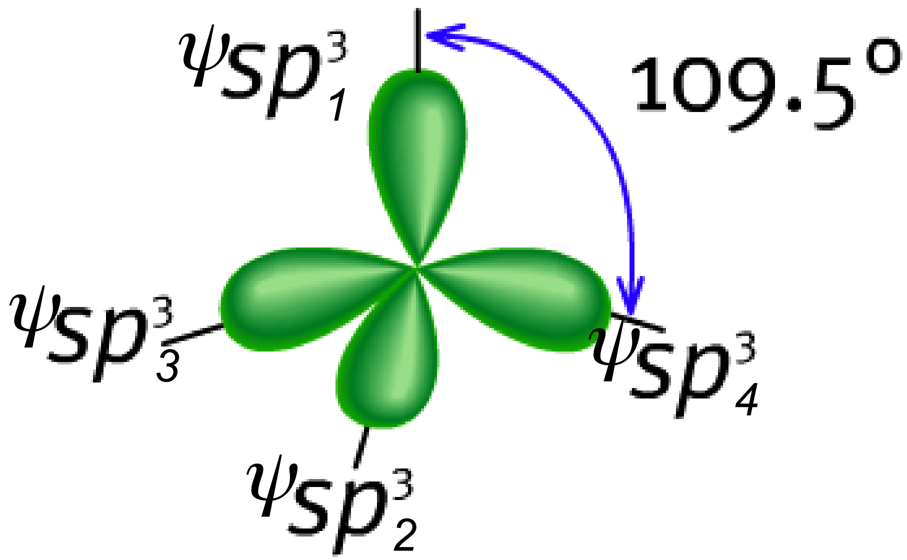
$1/2(\psi_s + \psi_{px} + \psi_{py} + \psi_{pz})$

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

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

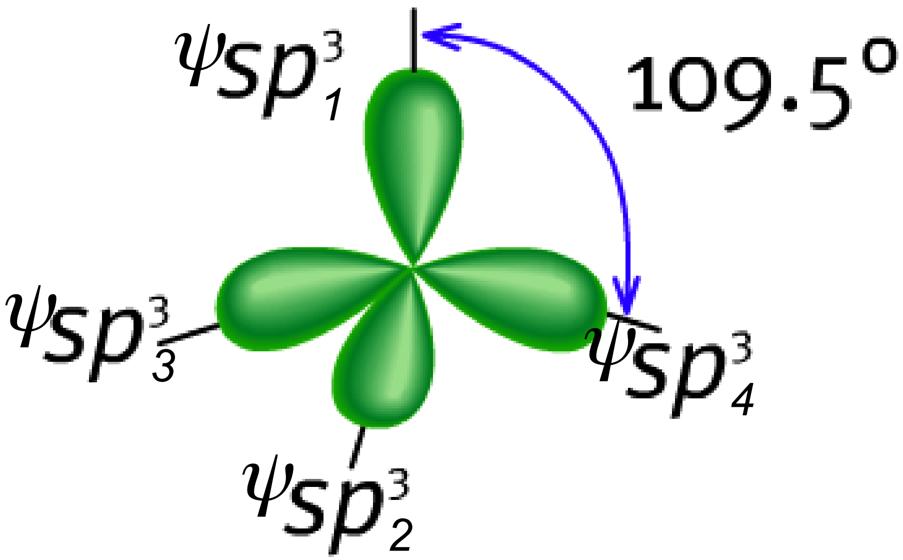
$1/2(\psi_s - \psi_{px} - \psi_{py} + \psi_{pz})$

Orbital hybridization

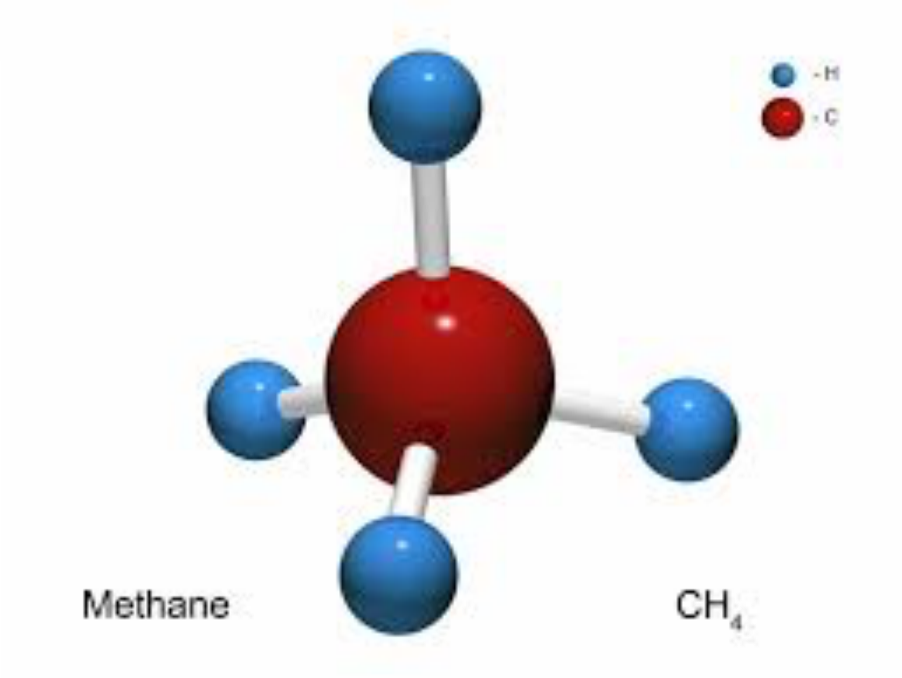


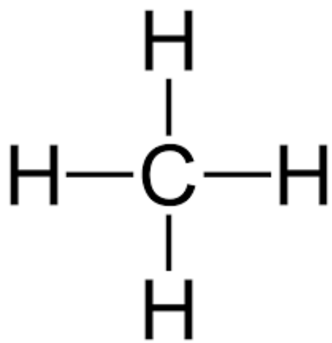
Tetraeder

Orbital molecular theory: Example CH_4 (Methane)

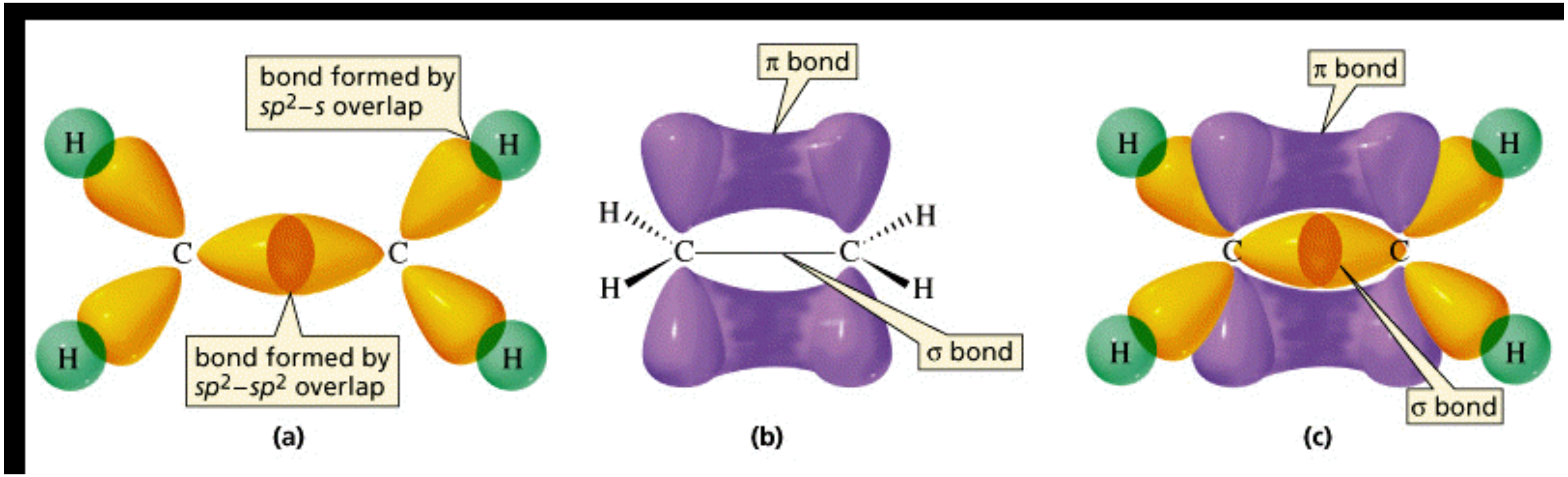


Tetraeder



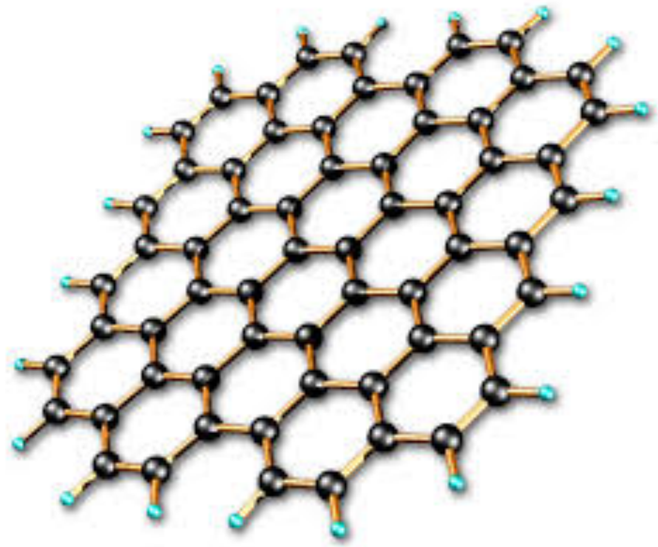


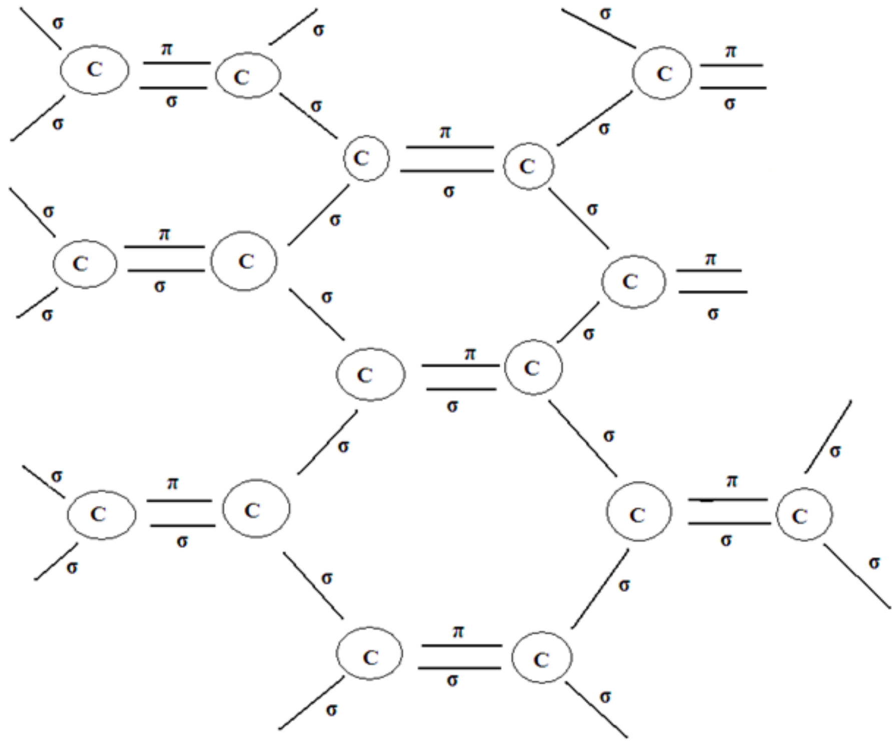
Orbital molecular theory: σ and π bonding



Graphene: σ and π bonding

Graphene





Today's lecture