Kvantová chemie

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Ivan Rishko
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- Počítání vlastností sloučenin

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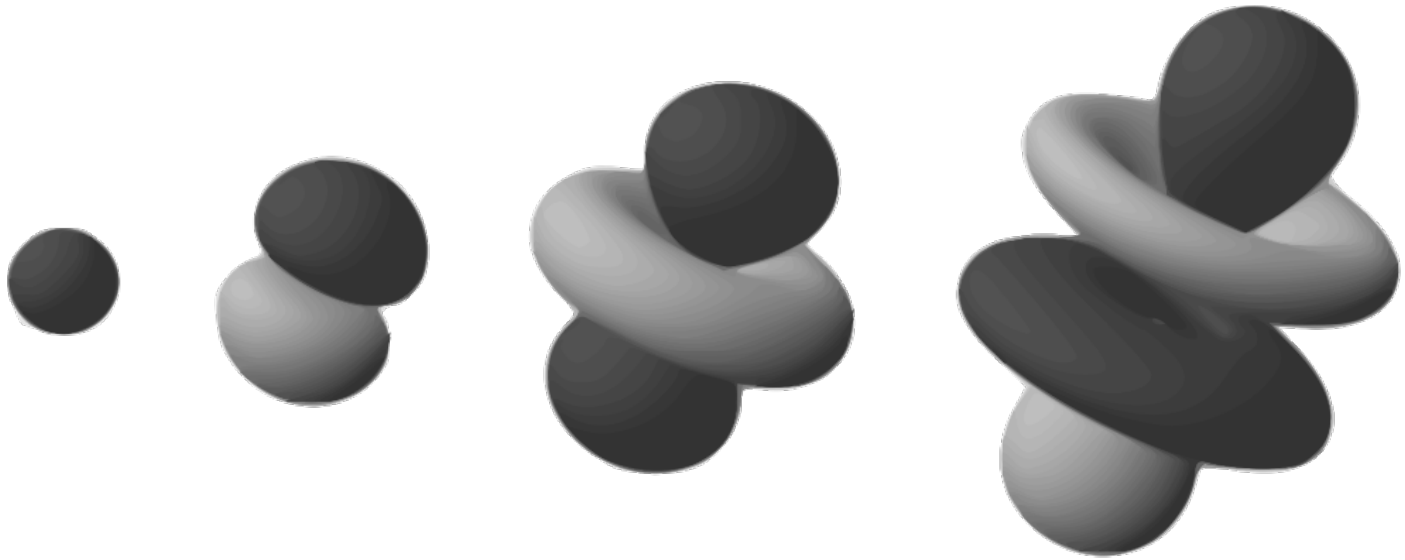
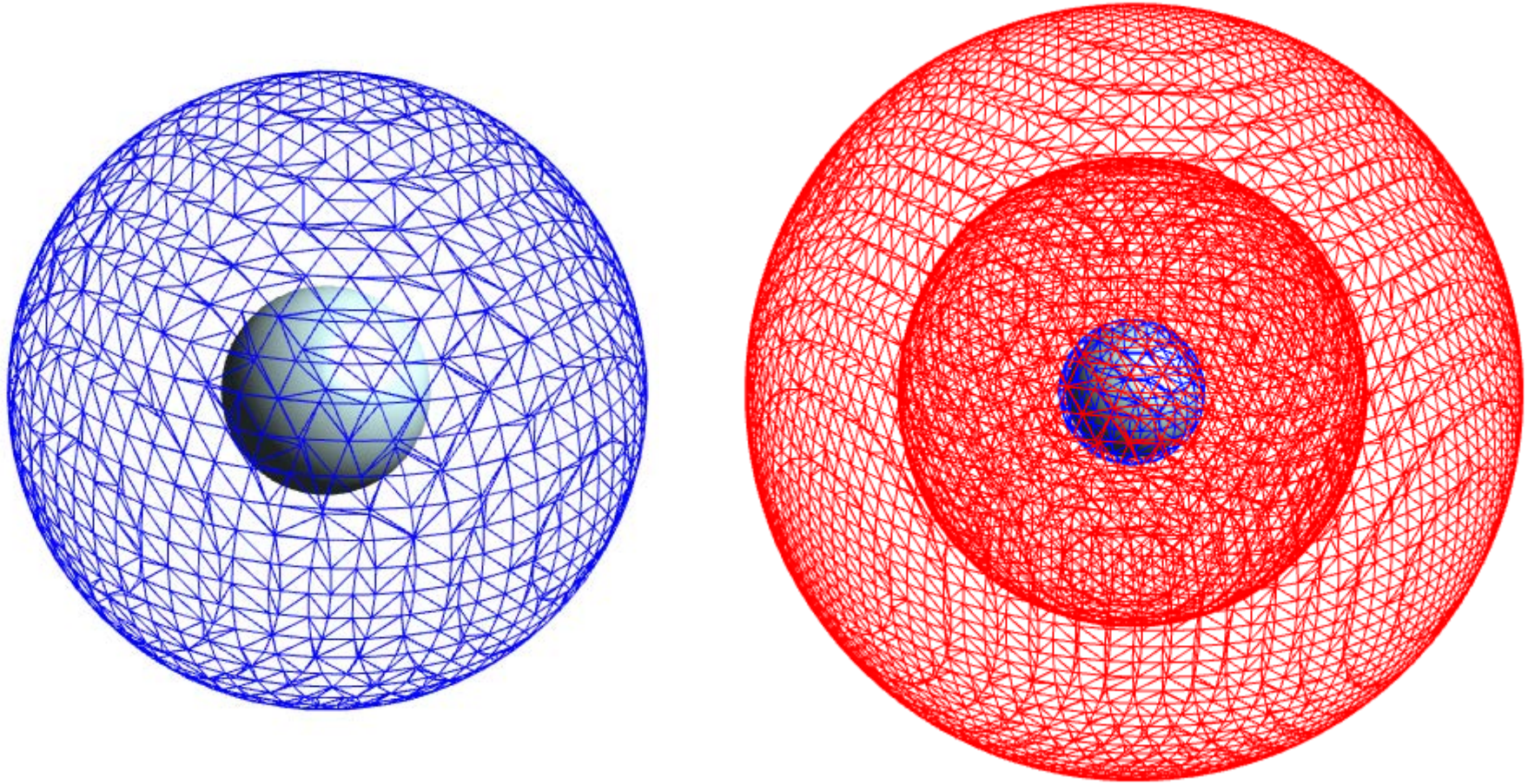
- Báze *aug-cc-pVDZ*
- Programy: Avogadro, Psi4

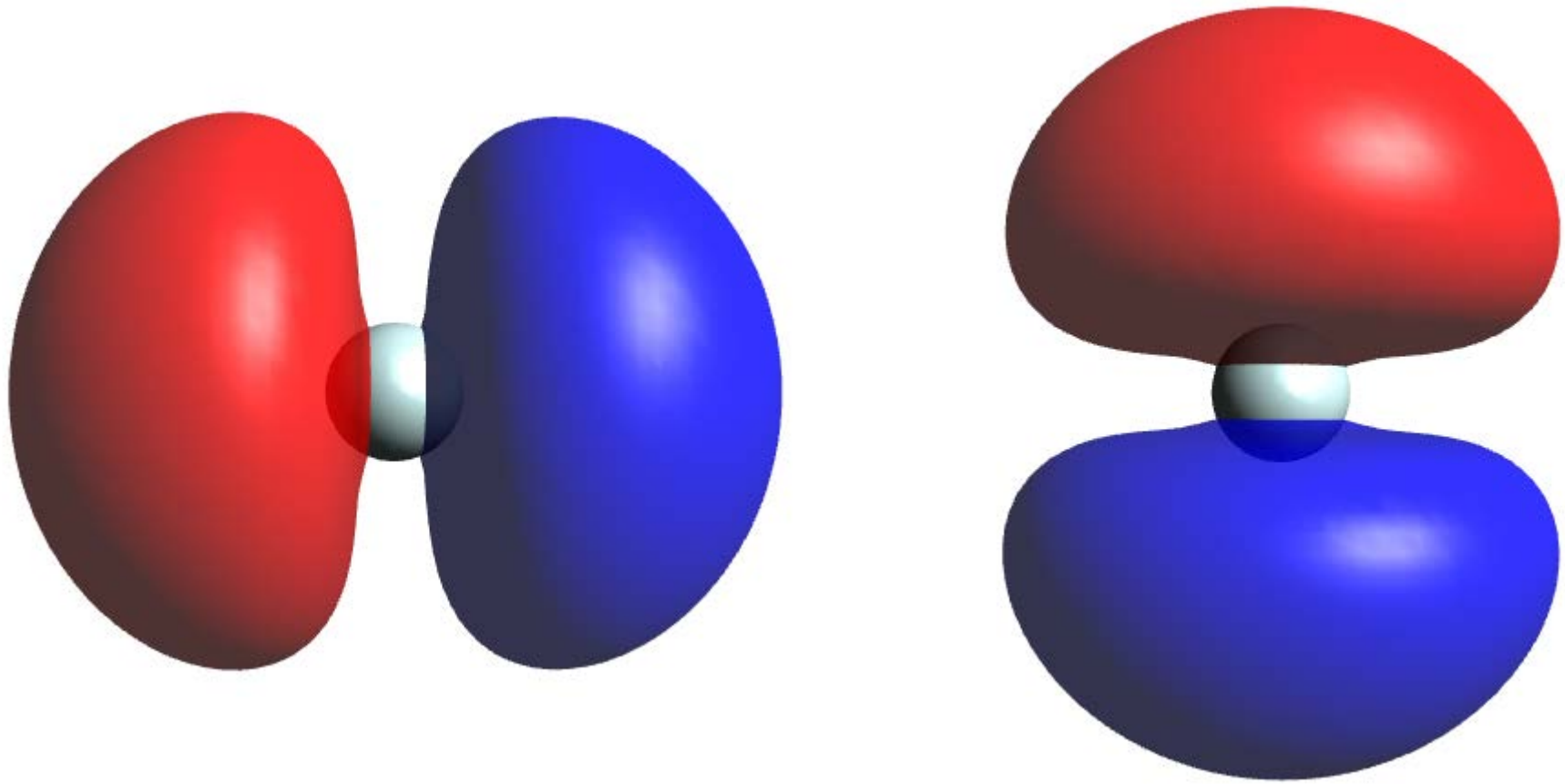
$$\hat{H}\Psi = E\Psi$$

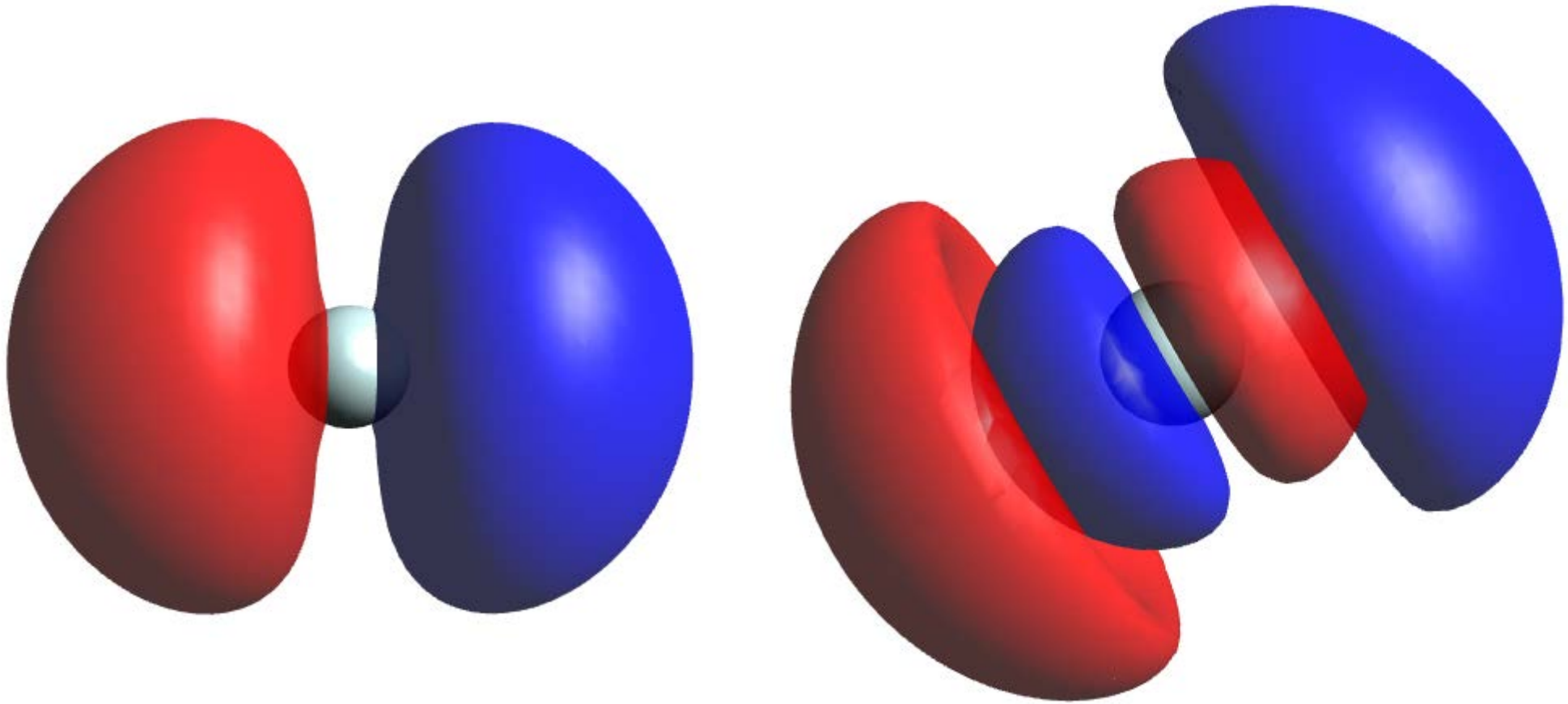
Výstavbový model

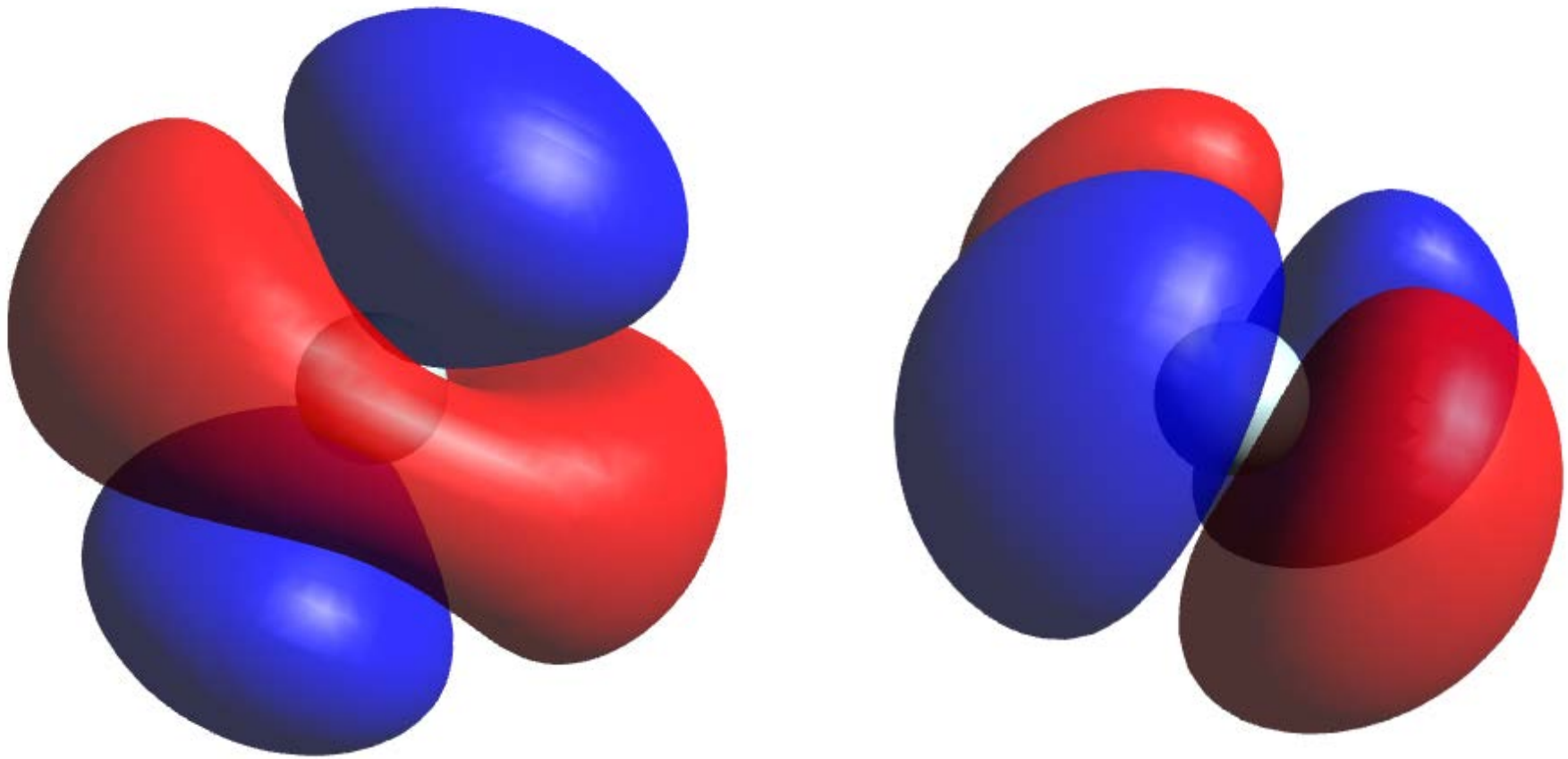


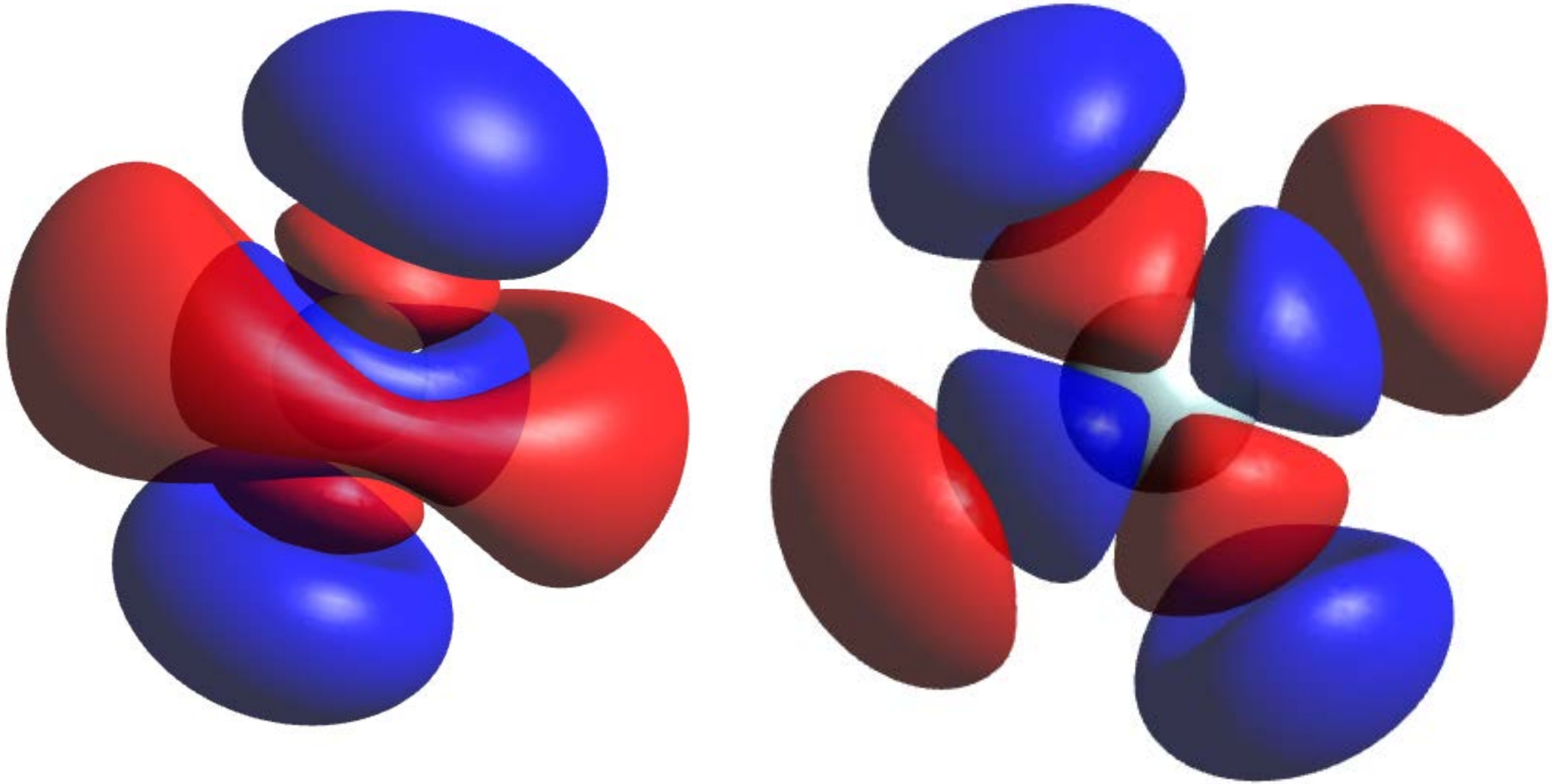
$$\rho = |\Psi(x)|^2$$

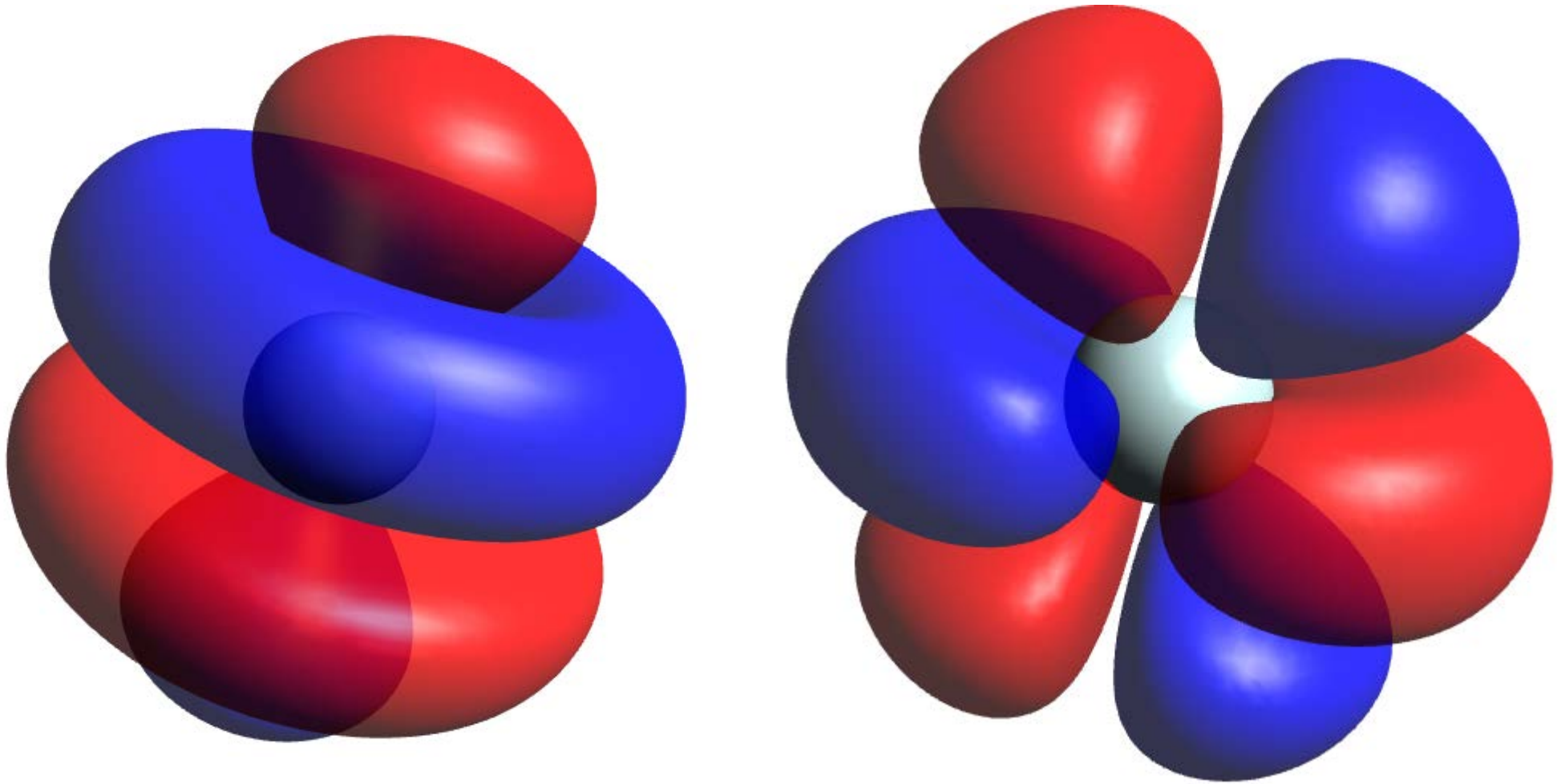


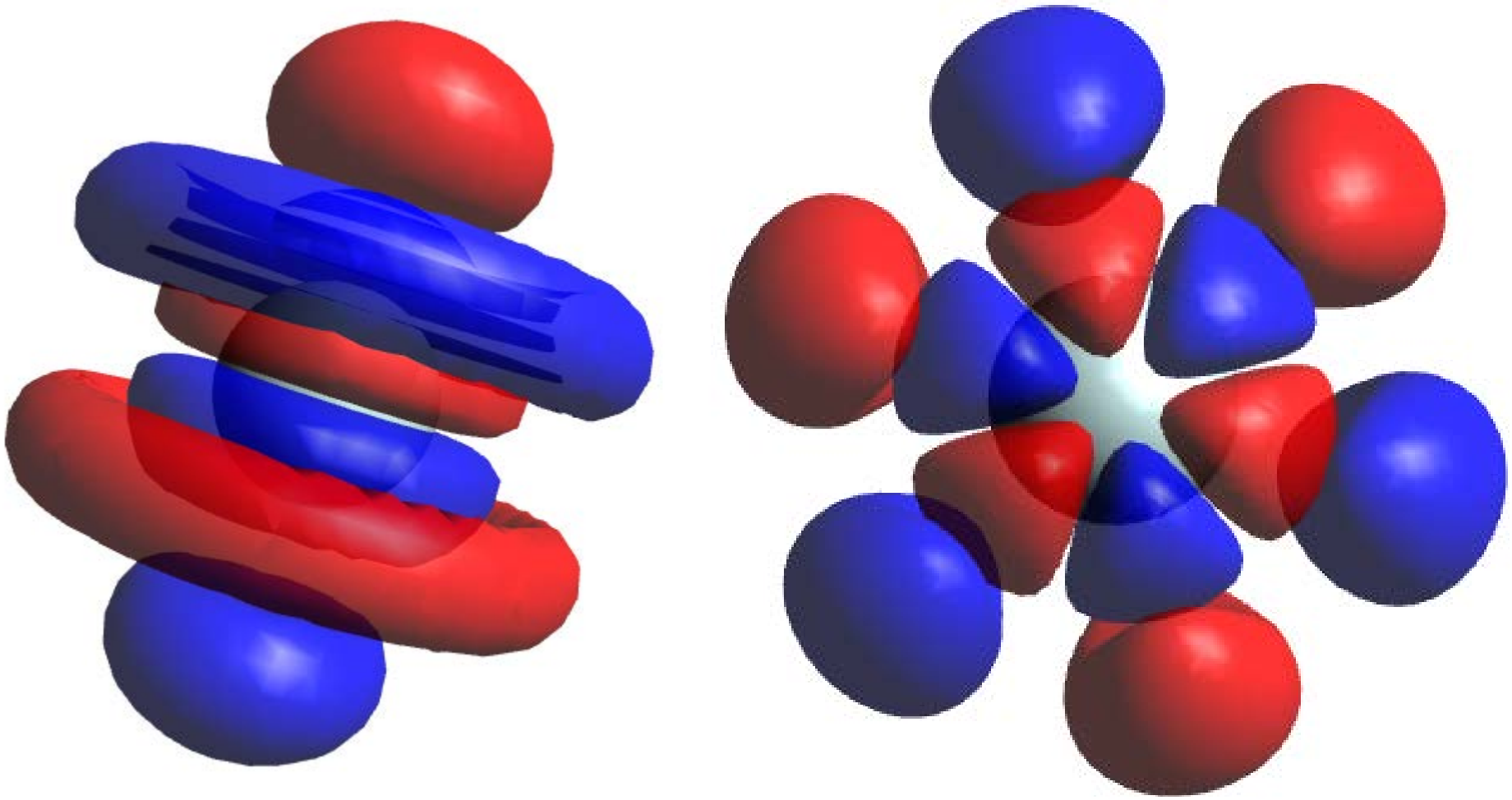




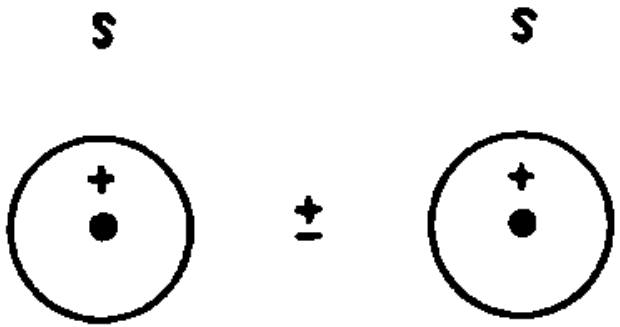


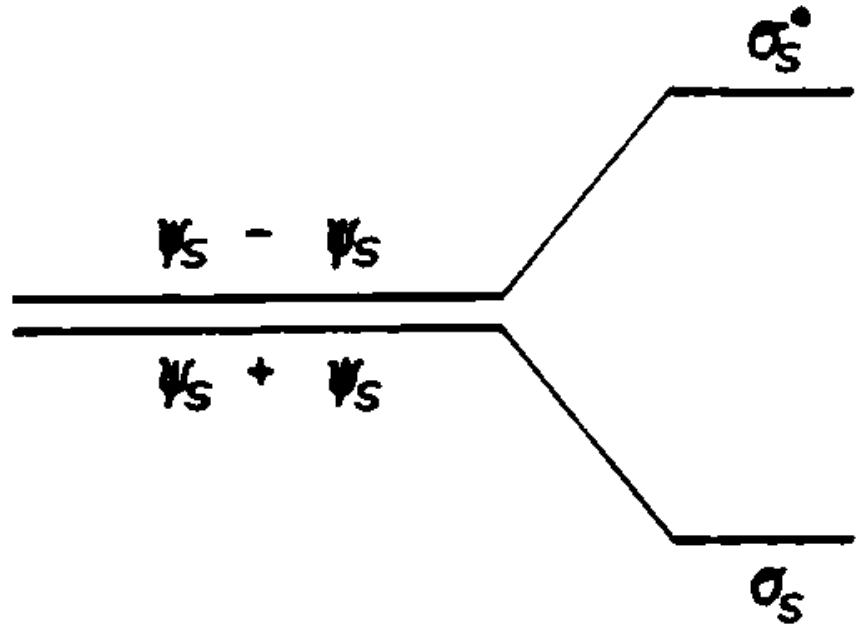


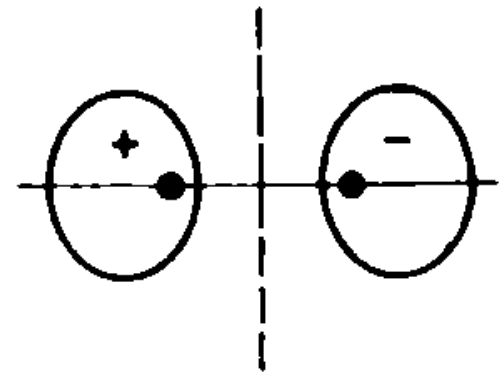


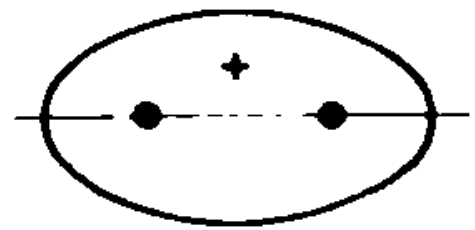


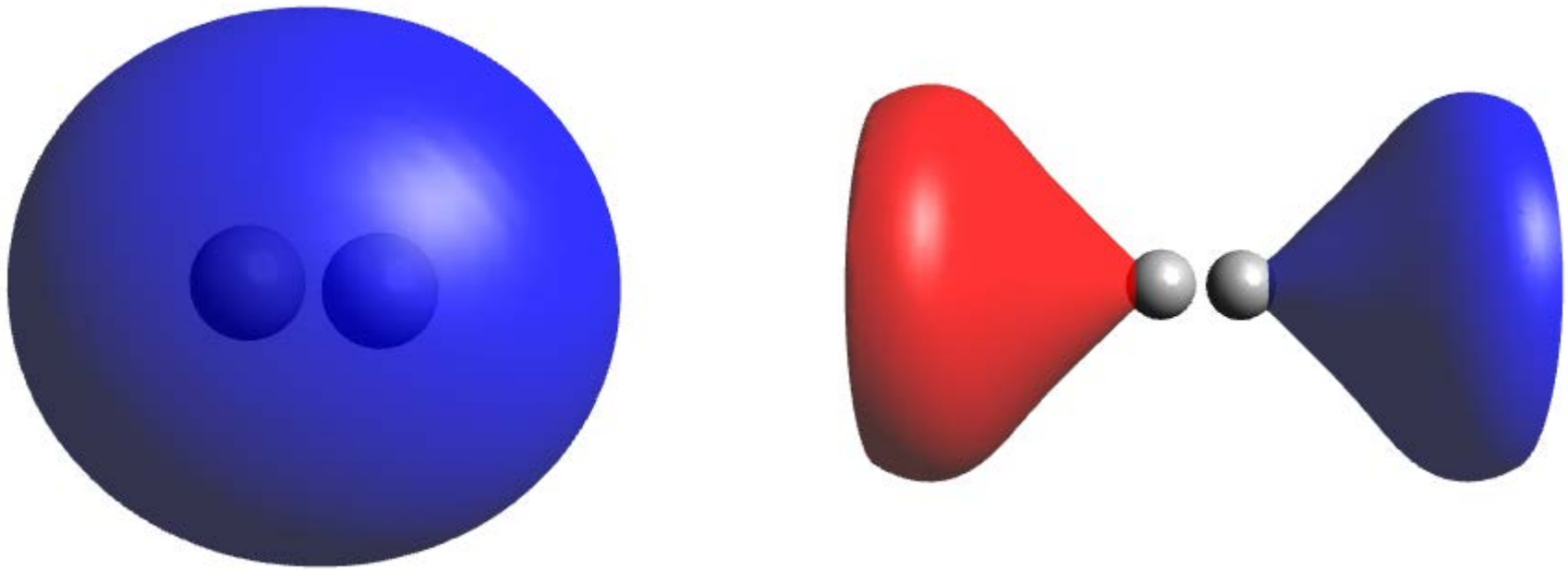
Molekulové vazby

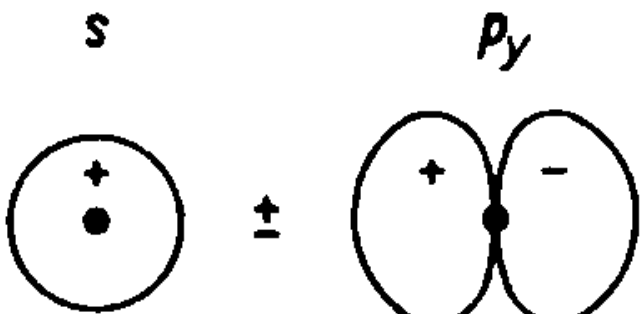


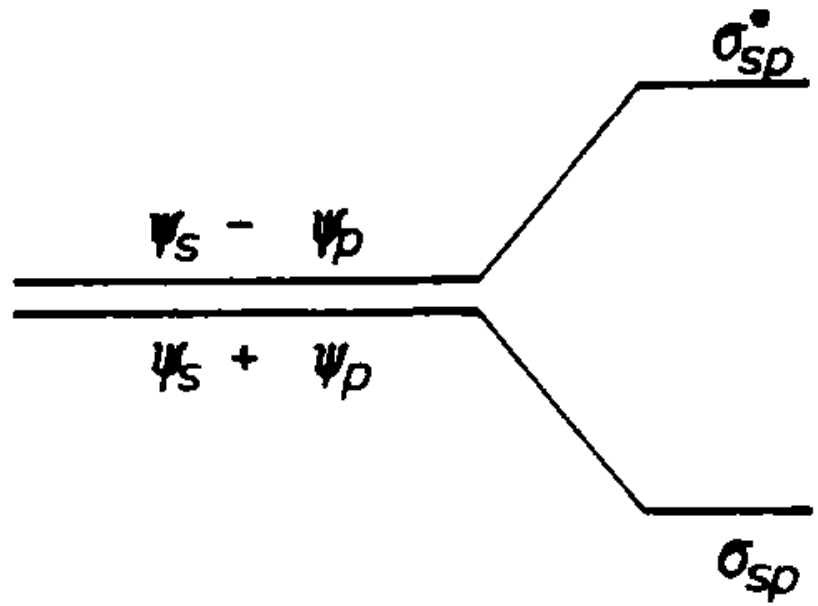


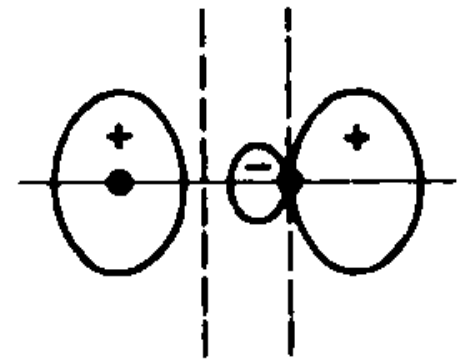


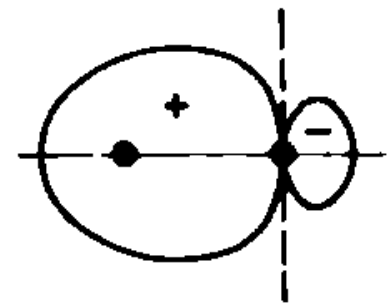


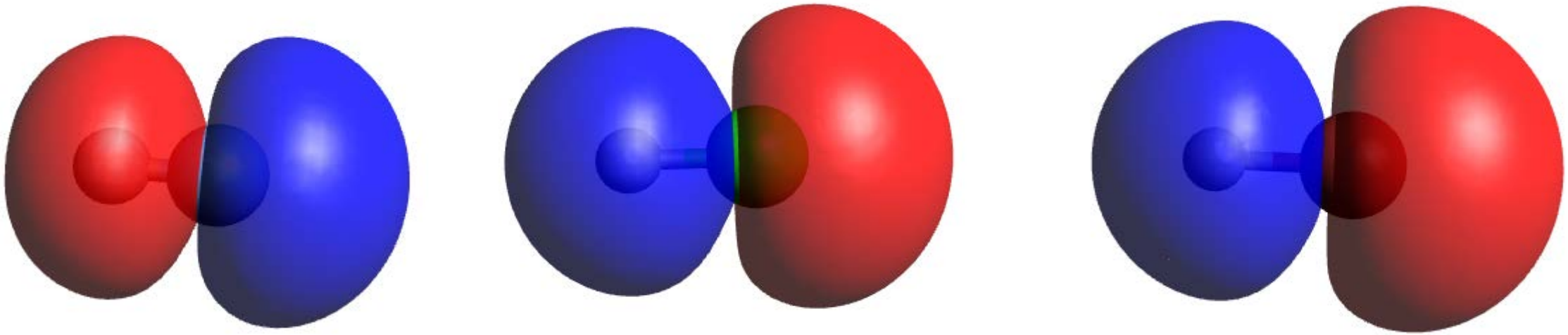


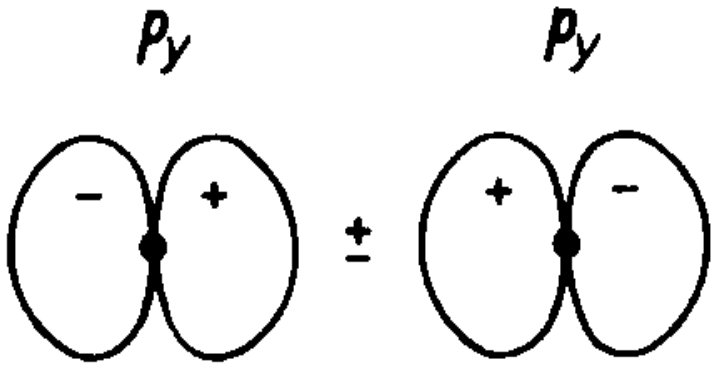

s
p_y
+
±
+
−

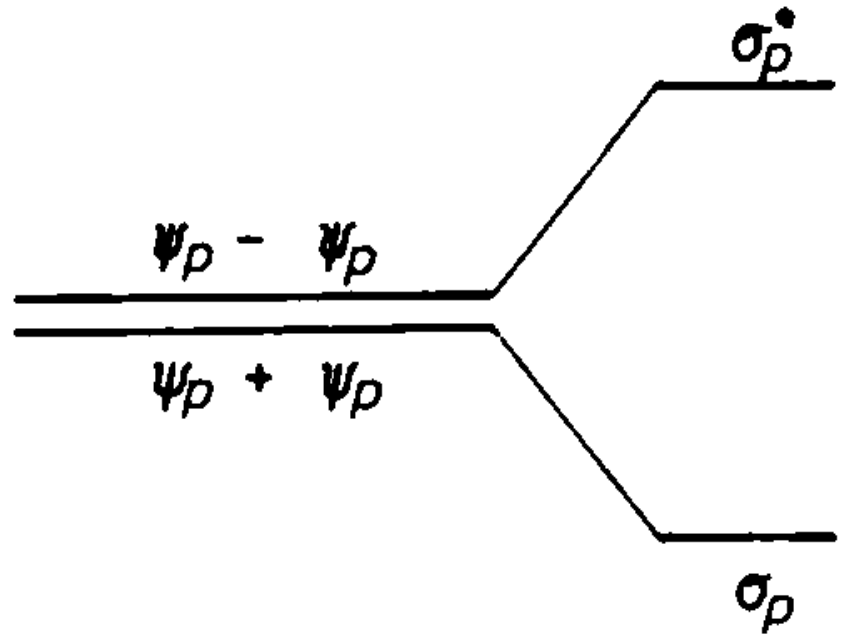

σ^*_{sp}
$\psi_s - \psi_p$
$\psi_s + \psi_p$
σ_{sp}

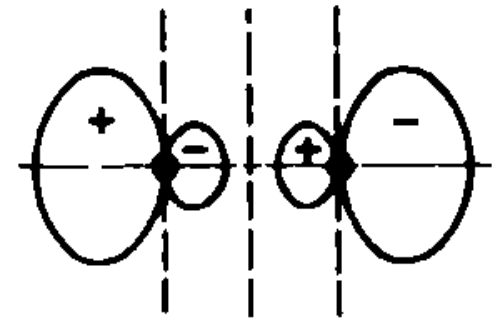

+
−
+

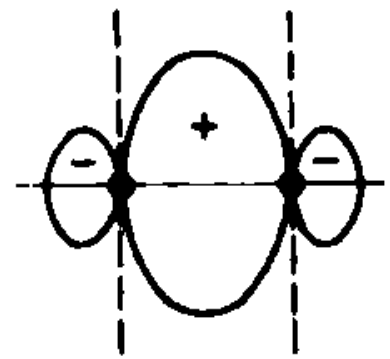

+
−

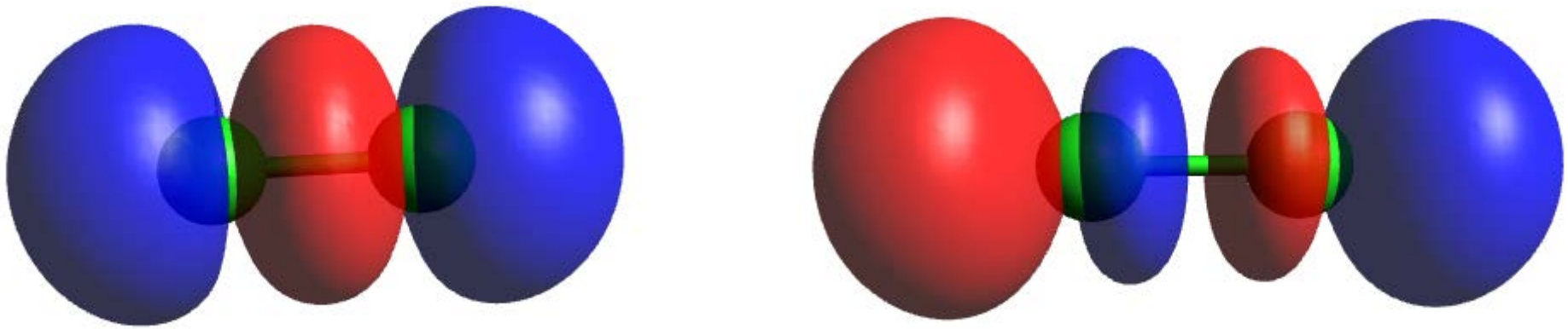


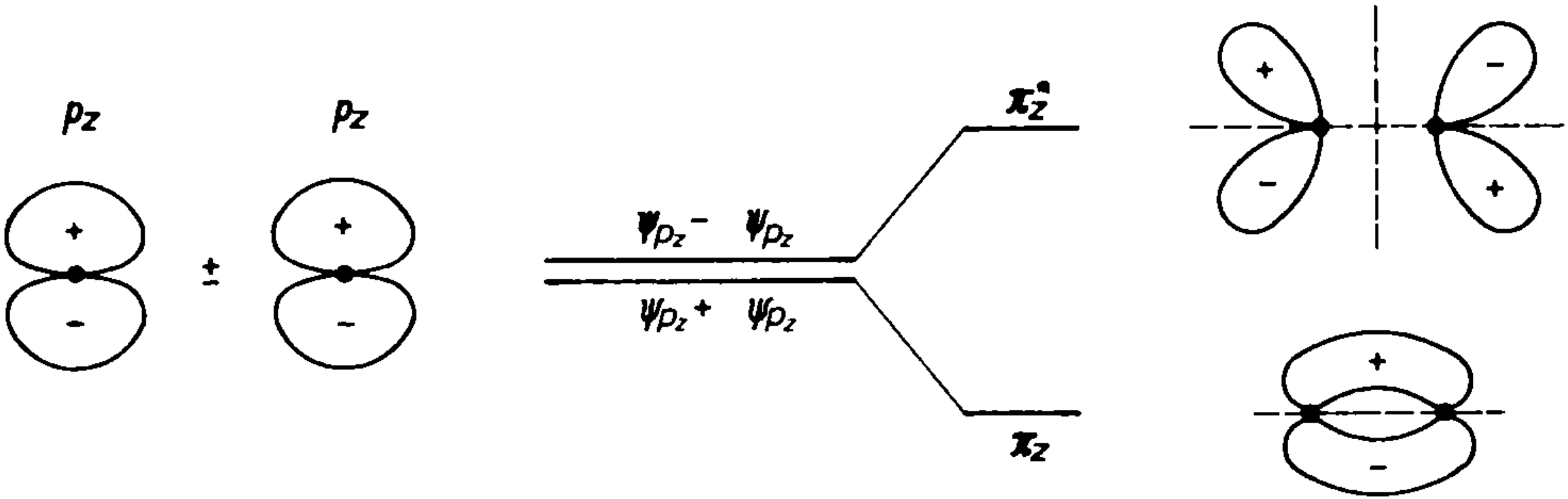

p_y
p_y
−
+
±
+
−

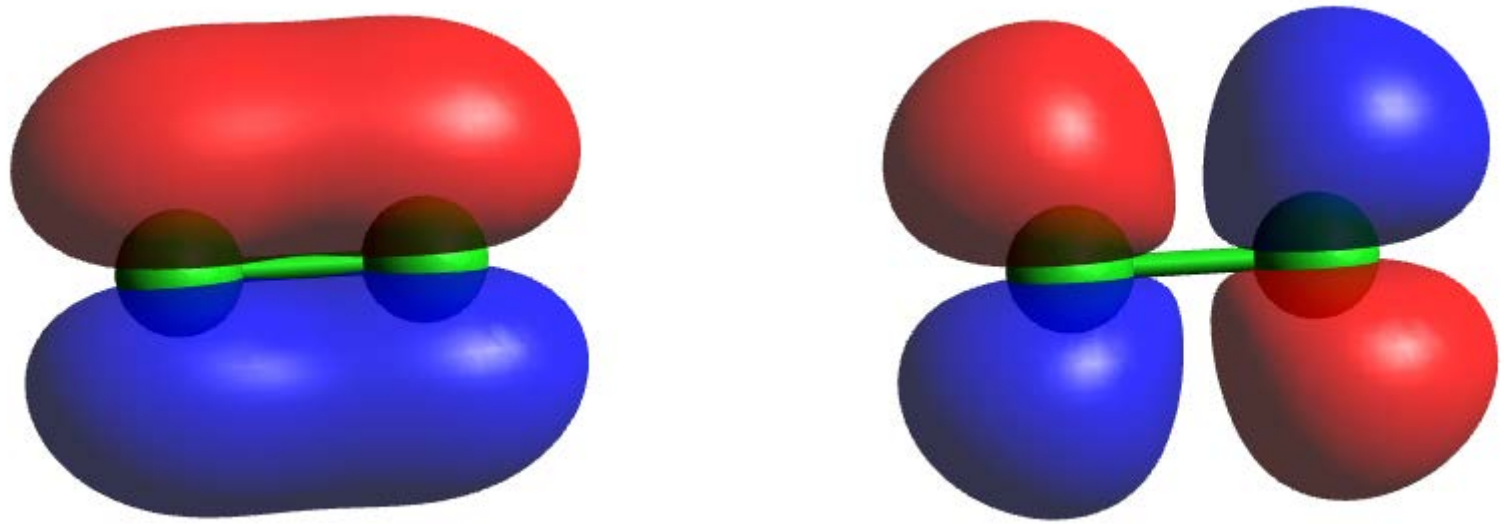

σ_p^*
$\psi_p - \psi_p$
$\psi_p + \psi_p$
σ_p

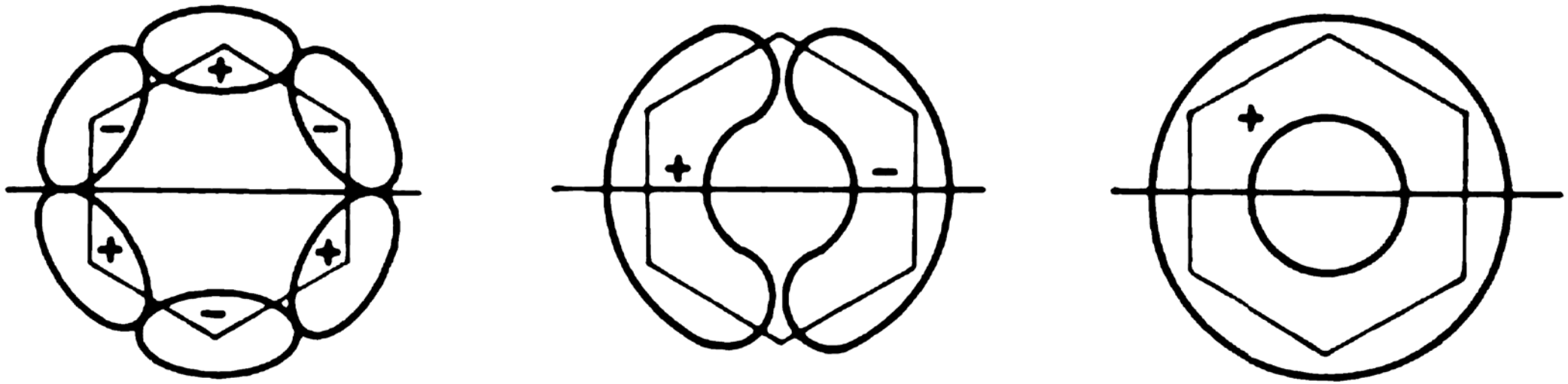

+
−
+
−

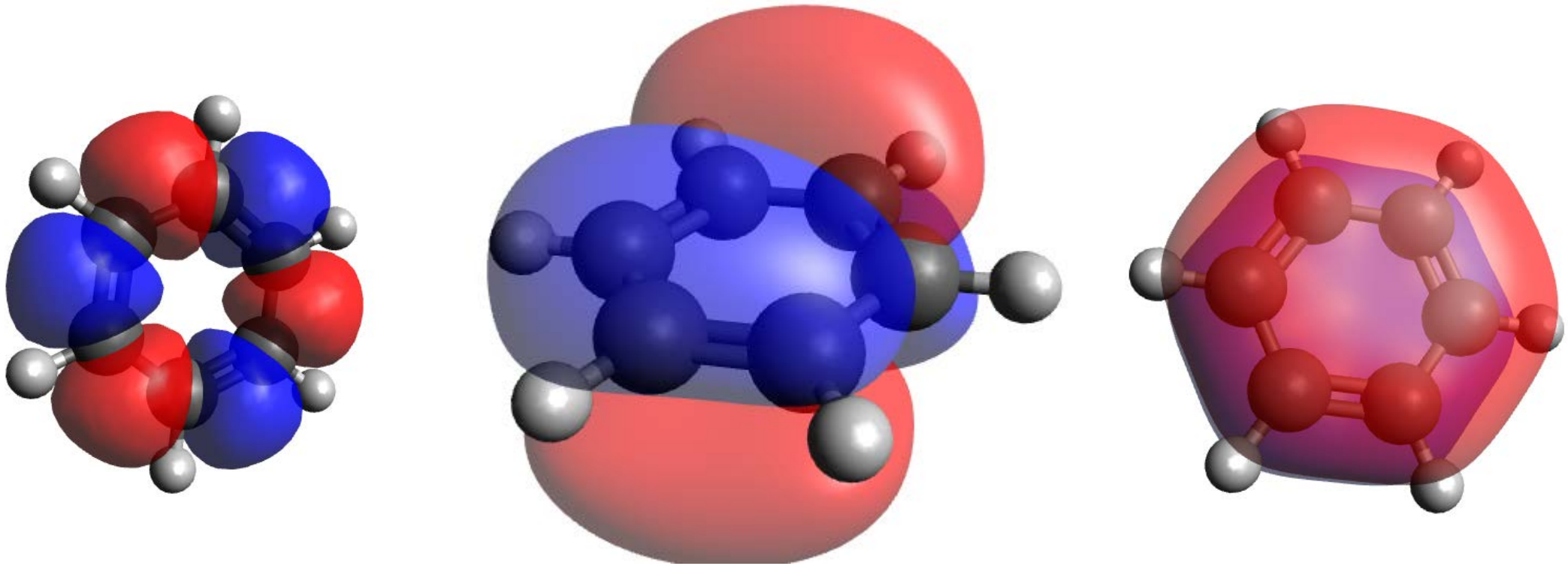

−
+
−




pz
pz
+
−
±
+
−
π*z
ψpz − ψpz
ψpz + ψpz
πz
+
−
−
+
+
−

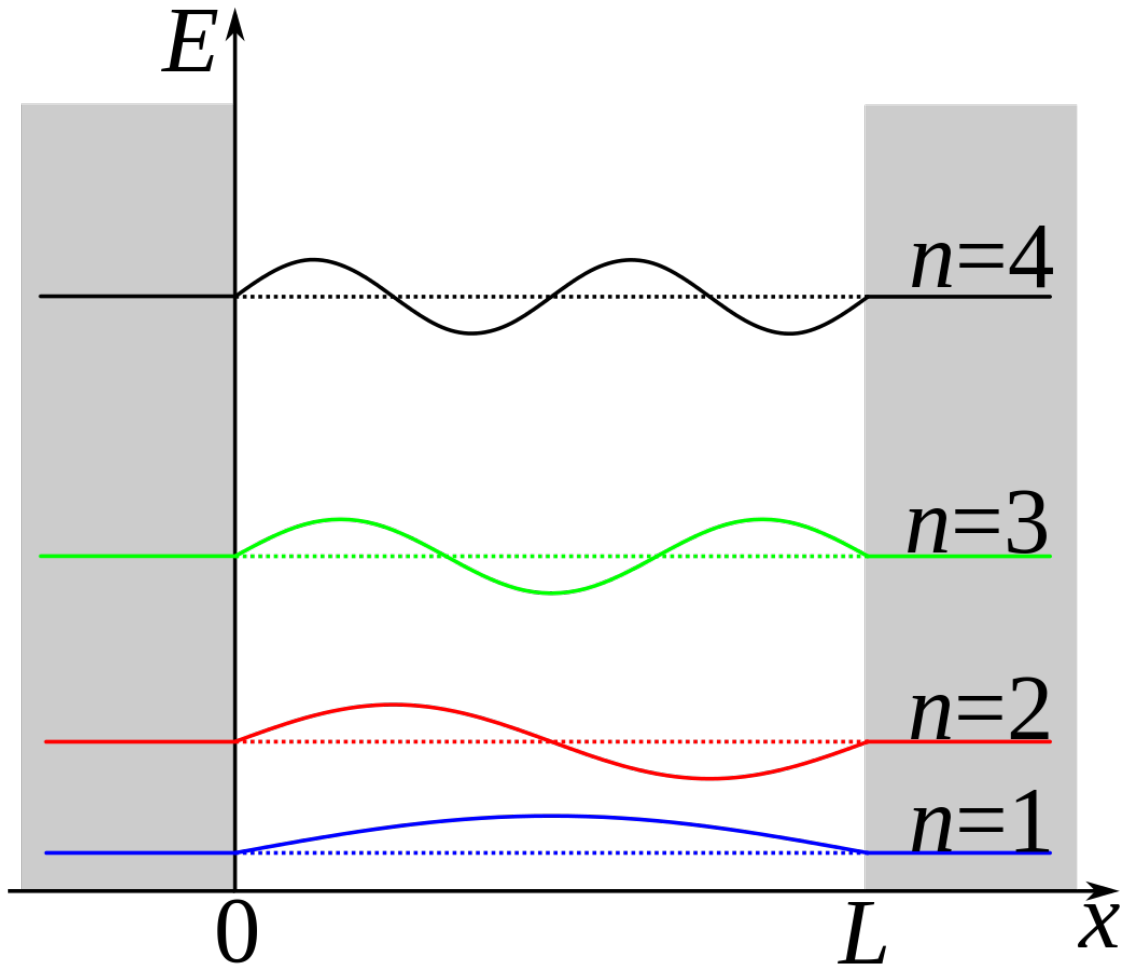


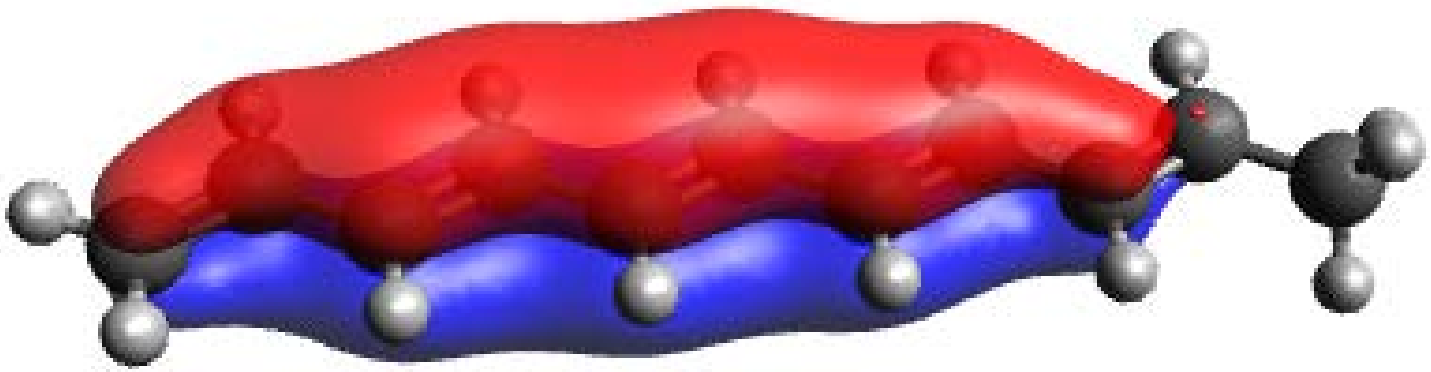


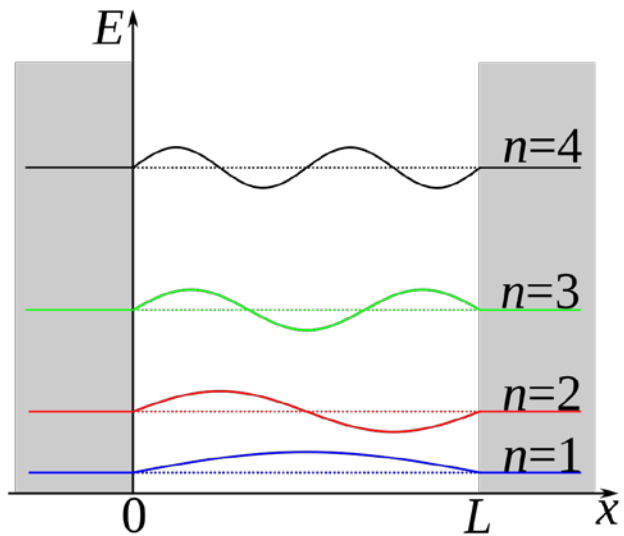


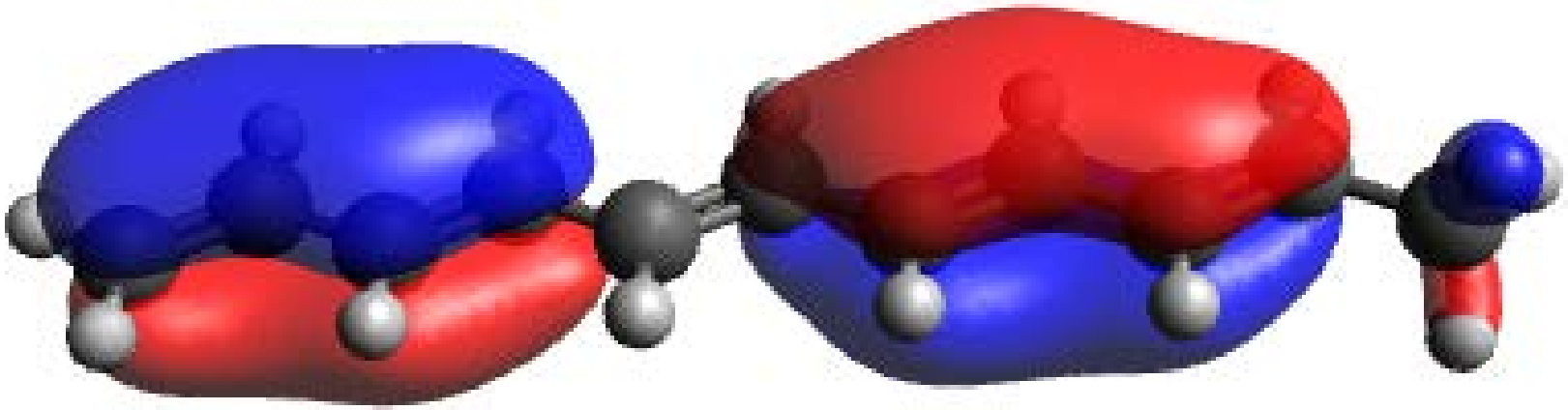
$$\hat{H}\Psi = E\Psi$$

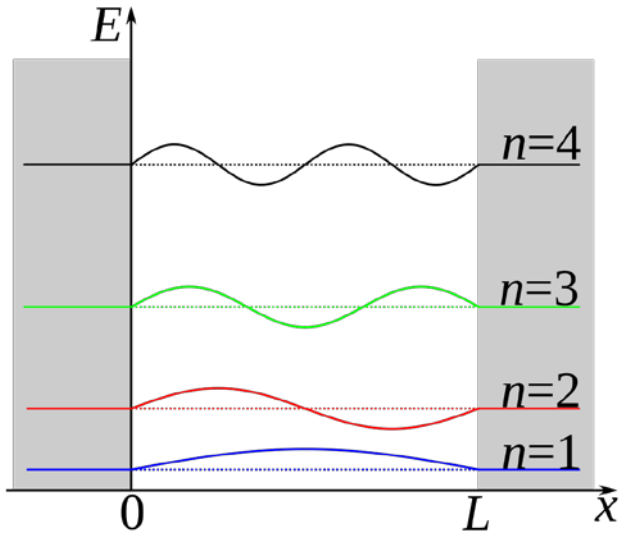
Částice v nekonečné jámě

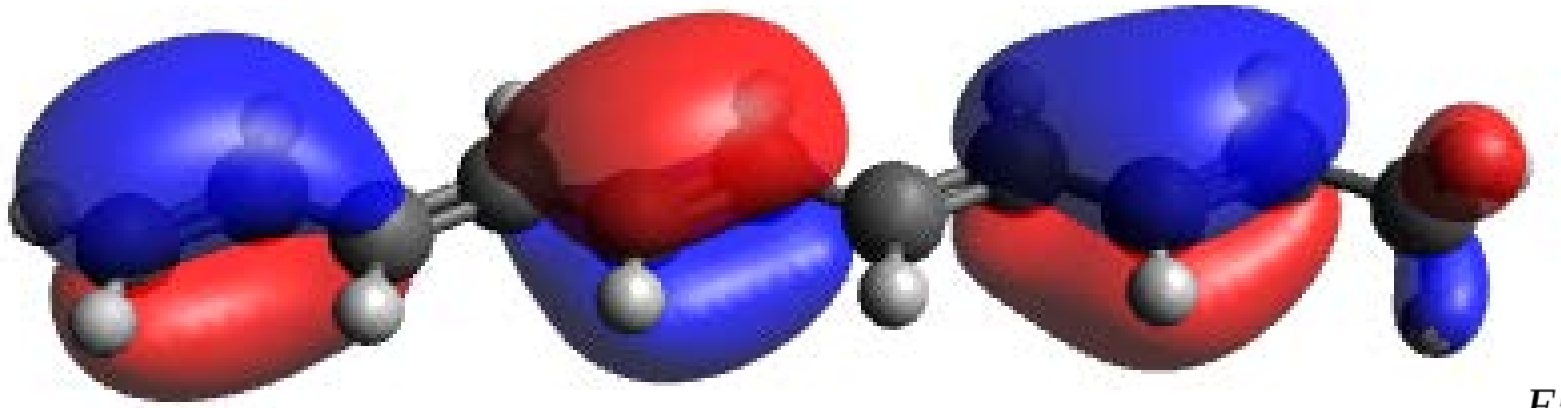


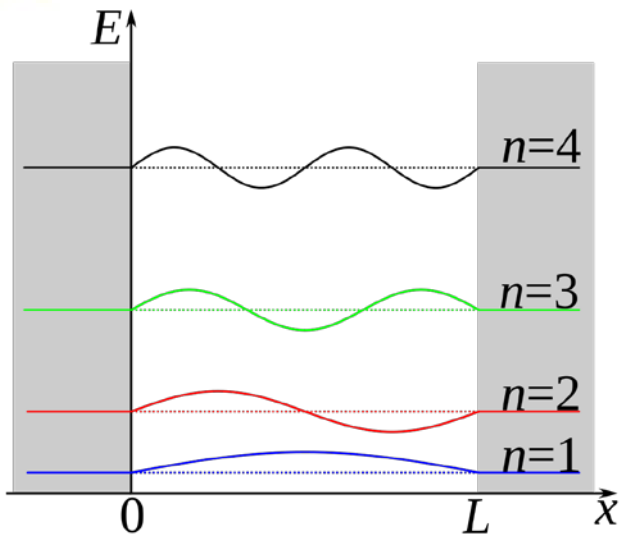


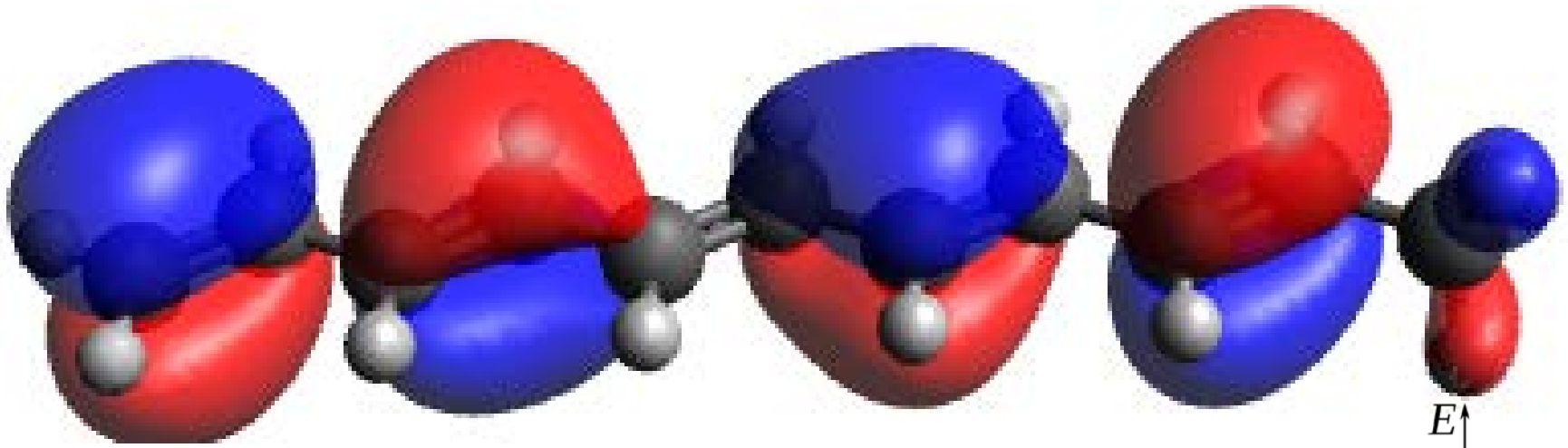

E
n=4
n=3
n=2
n=1
0
L
x

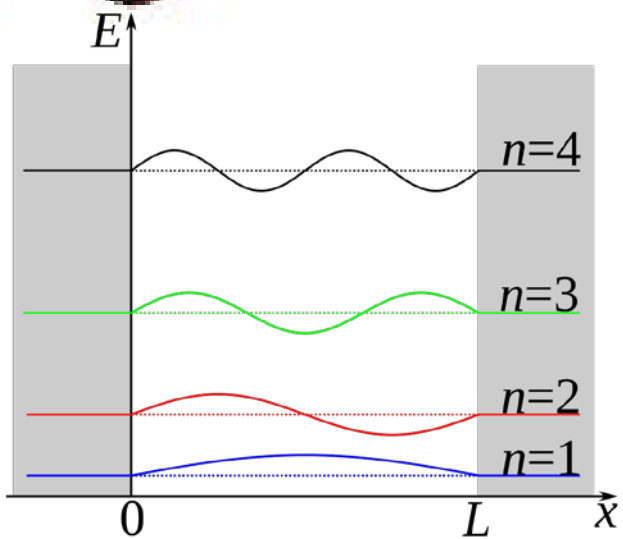


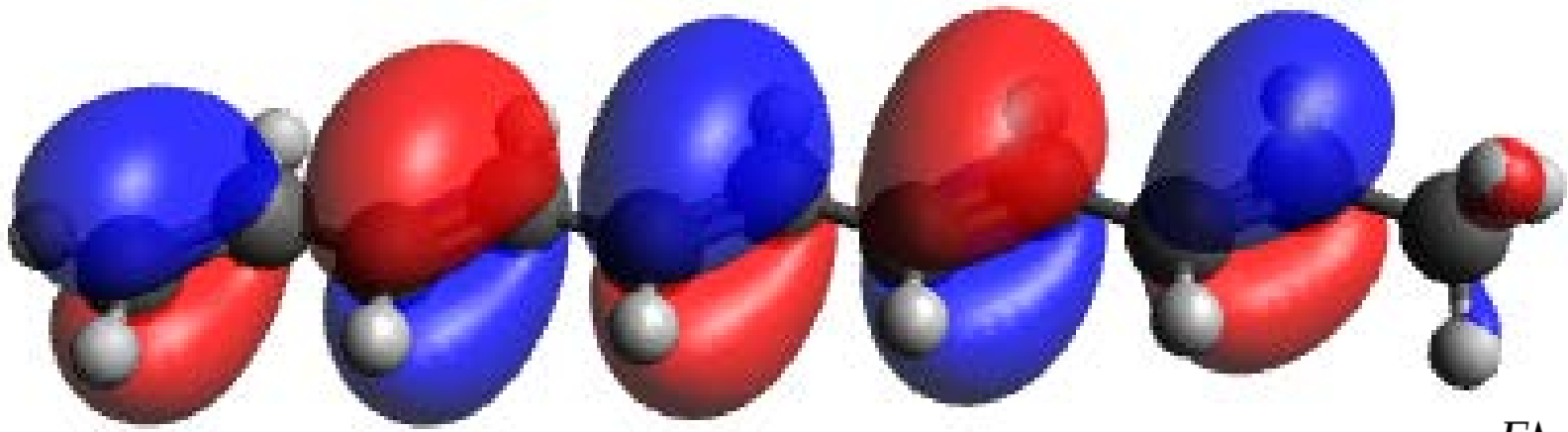

E
n=4
n=3
n=2
n=1
0
L
x

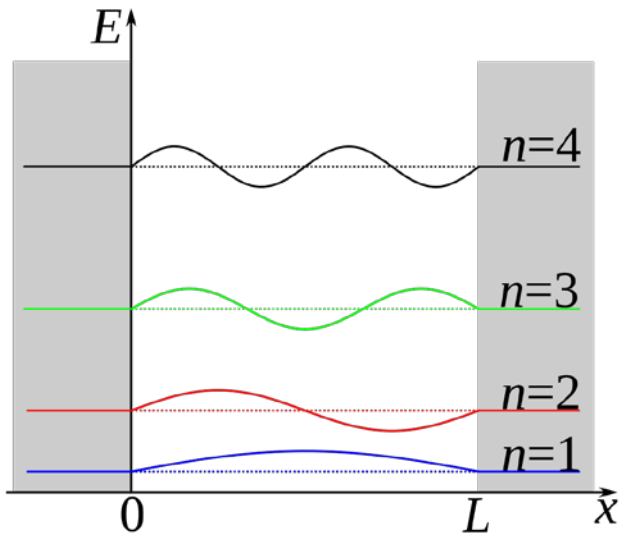



E
n=4
n=3
n=2
n=1
0
L
x



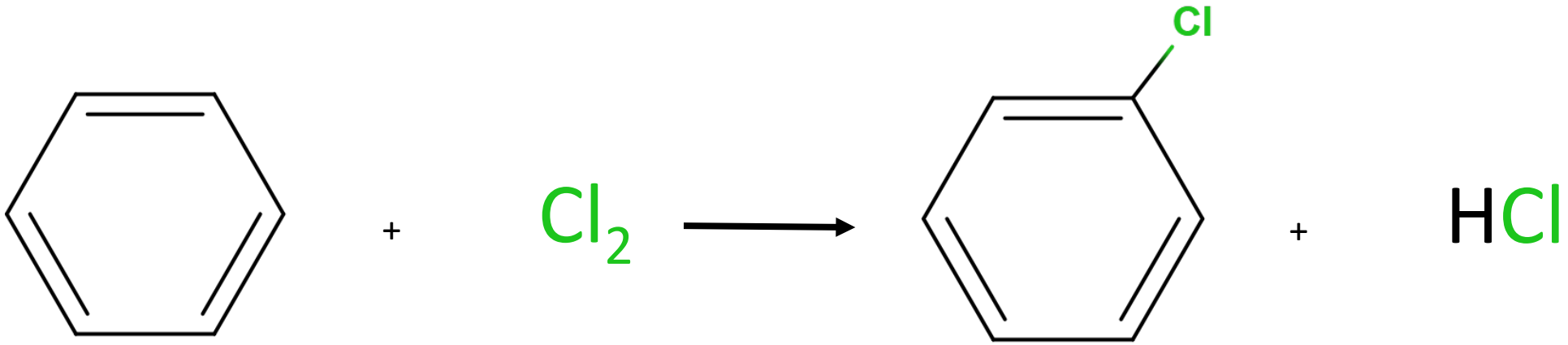

E
n=4
n=3
n=2
n=1
0
L
x




E
n=4
n=3
n=2
n=1
0
L
x

Reakční teplo

$$\hat{H}\Psi = E\Psi$$


Cl
+
Cl_2
+
HCl

```
Nuclear Repulsion Energy =            204.2549728329875620
One-Electron Energy =                -714.7502316437271475
Two-Electron Energy =                 279.7672557484565914
DFT Exchange-Correlation Energy =       0.0000000000000000
Empirical Dispersion Energy =           0.0000000000000000
PCM Polarization Energy =               0.0000000000000000
EFP Energy =                            0.0000000000000000
Total Energy =                       -230.7280030622829941
```

Cl_2	-918,9640159785 Ha	Chlorbenzen	-689,6503230681 Ha
Benzen 	-230,7280030369 Ha	HCl	-460,0916379704 Ha

$$\Delta E = E_{chlorbenzen} + E_{Cl_2} - E_{HCl} - E_{benzen}$$

$$\Delta E = -0{,}0499420231 \text{ Ha}$$

$$\Delta E = -\ 131.1227916375 \text{ kJ} \cdot \text{mol}^{-1}$$

By formula: $C_6H_6 + Cl_2 = C_6H_5Cl + HCl$

Quantity	Value	Units	Method	Reference	Comment
$\Delta_r H°$	-134.	kJ/mol	Cm	Kirkbride, 1956	liquid phase; *ALS*


2 H2 + O2
2 H2O

O_2	-149,5360807 Ha	H_2O	-76,04182372 Ha
H_2	-1,128826547 Ha		

$$2\Delta E = 2E_{H_2O} - 2E_{H_2} - E_{O_2}$$

$$\Delta E = -0,14495683495 \text{ Ha}$$

$$\Delta E = -380,58419915259 \text{ kJ} \cdot \text{mol}^{-1}$$

$$2\ H_2 + O_2 \longrightarrow 2\ H_2O$$

Výsledky

Vlastnost	**Měřená hodnota**	**Teoretická hodnota**
Reakční energie chlorbenzenu	131,123 kJ· mol^{-1}	134,000 kJ· mol^{-1}
Reakční energie H_2O	380,580 kJ· mol^{-1}	241,300 kJ· mol^{-1}