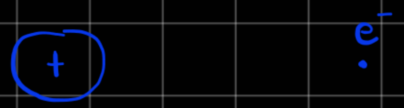
Moderna fizika - vaje

Nastanek NaCl

1. Ionizacija Na

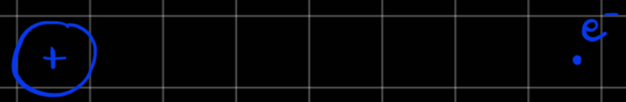


jedro z notranjimi e^-

// vezan sistem

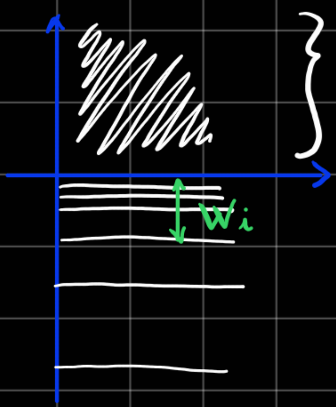
atom ioniziramo (e^- dalč stran)

$\downarrow$ ionizacija



// nevezan sistem, prost e^-

Pri vezanem sistemu so dovoljena diskretna stanja energije

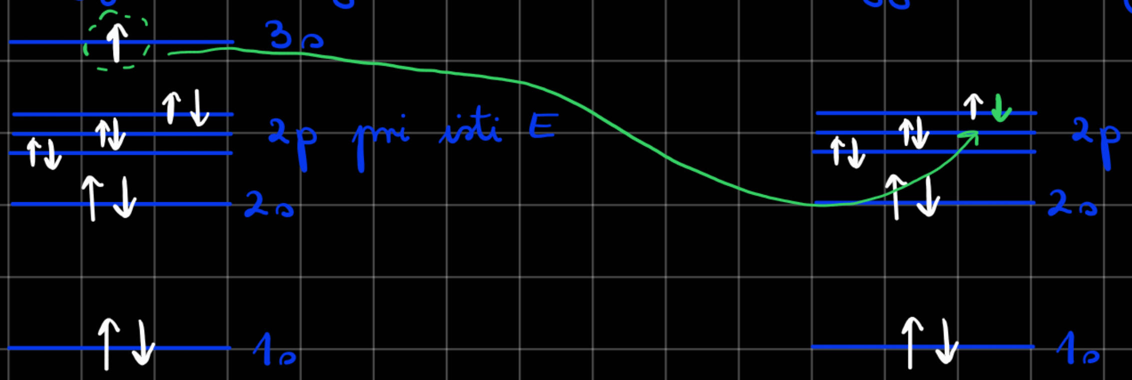


$E > 0$ nevezan sistem kontinuum stanj

$E < 0$ vezana stanja, diskretna

W_i ... ionizacijska energija (en. potrebna za to, da damo e^- dovolj dalč od jedra z notranjimi e^-)

Energijska stanja Na Energijska stanja Cl



2. Vezava z Na in Cl

Sprosti E → W_a ... elektronska afiniteta

$$W_i - W_a > 0$$

Da nastane ion, mora biti osnovno stanje iona nižje od tega, ko sta atoma nevezana.
Ion se ne sesede zaradi Paulijevega izključitvenega načela.

$$W_v = W_k(r_0) + W_c(r_0) + W_i - W_a$$

W_v ↓ vezavna en.

W_k ↓ odb. pot. kratkega dosega → Pauli (prekrivanje e^- oblakov)

W_c ↓ Coulombska energija

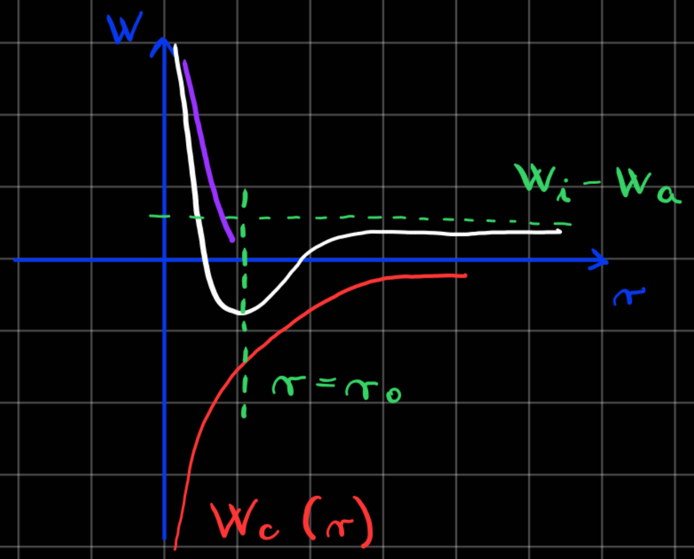
r_0 ... ravnovesna lega

$Z_1 e_0$ (+) $-Z_2 e_0$ (−)

$$\vec{F} = \frac{e}{4\pi\varepsilon_0 r^2}\frac{\vec{r}}{|\vec{r}|}$$

$$\vec{F} = -\nabla V \Rightarrow V(r) = \frac{e}{4\pi\varepsilon_0 r}$$

$$W_c(r) = eV(r) = \frac{-Z_1 Z_2 e_0^2}{4\pi\varepsilon_0 r}$$

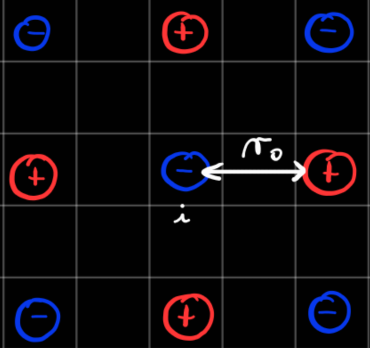


Ionski kristal

število ⊕ oz. ⊖ ionov (vs skupaj 2N gradnikov)

$$W_V = N\left(\tilde{V}_k(r_0) + \tilde{W}_c\right) + NW_i - NW_a$$

$\hat{V}_k, \tilde{W}_c$ ... fji nista enaki kot pri 1 ionu NaCl



$\hat{V}_k$ ima enako funkcijsko odvisnost, drugačni predfaktor

$\to$ Madelungova konst.

$$W_c = \underbrace{z_i e_0}_{\text{naboj centralnega iona}} \cdot \underbrace{V_{c,i}}_{\text{potencial na mestu centralnega iona}} = z_i e_0 \frac{\alpha_{M,i}\, e_0}{4\pi \varepsilon_0 r_0}$$

parska interakcija, za kristal pomnožimo z N

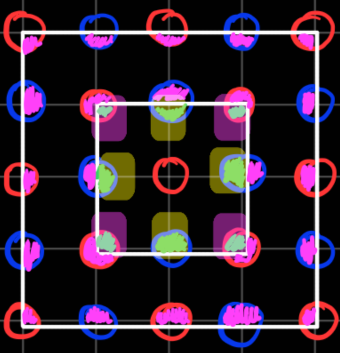
$\alpha_{M,i}$ porazdelitev naboja v okolici centralnega atoma

$$\alpha_{M,i} = \sum_j \frac{z_j}{\frac{r_j}{r_0}}$$

↘ po sosedih

$z_{Na} = +1, \quad z_{Cl} = -1$

Skripta Žorko 4.1



$$\alpha_{M,i} = \sum_j \frac{z_j}{\frac{r_j}{r_0}}$$

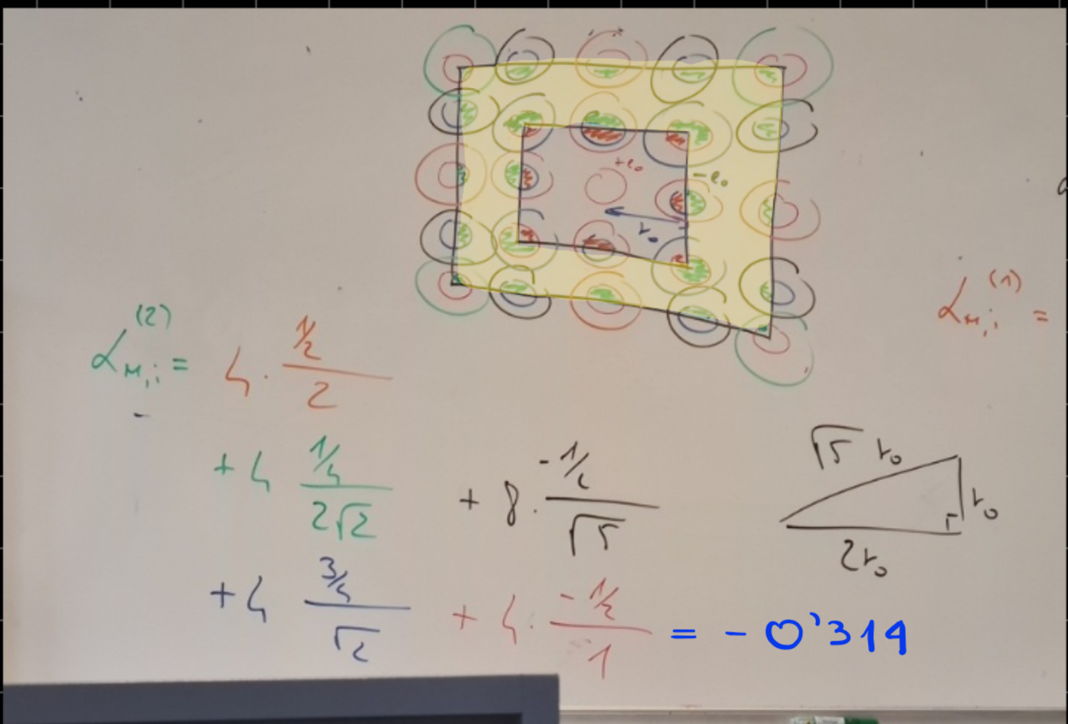
$$\alpha_{M,i} = \alpha_{M,i}^{(1)} + \alpha_{M,i}^{(2)} + \dots$$

↱ modri, 1/2, negativni naboj

(1) $\alpha_{M,i}^{(1)} = 4 \cdot \frac{-\frac{1}{2}}{\underset{\searrow \frac{r}{r_0}}{1}} + 4 \frac{\frac{1}{4}}{1} = -1'293$

$\Rightarrow \alpha = -1'607$

(2) $\alpha_{M,i}$ // seštejš naboje na notranji strani 2. kvadrata in naboje na zunanji strani 1. kvadrata



$\alpha_{M,i} = -1'6155$

$W_v = 2N \cdot 5\,eV$

$W_i = 1'5\,eV$

$W_a = 1'0\,eV$

$W_k(r) \propto \frac{1}{r^{12}} \Rightarrow V_r = \frac{K}{r^{12}}$ ne poznamo

$$W_v = N\left(V_k(r) + W_c(r)\right) + N(W_i - W_a) \quad \text{// osnovna enačba}$$

$$\Rightarrow -2W_0 = V_K(r) + W_c(r) + W_i - W_a$$

Imamo dve neznanki: r_0 in K

Pri r_0 je minimum → odvajamo

$$\left.\frac{\partial W_r}{\partial r}\right|_{r=r_0} = 0 = -12\frac{K}{r^{13}} - \frac{\alpha_M e_0^2}{4\pi\varepsilon_0 r^2}$$

$$\frac{\partial W_c}{\partial r} = \frac{\partial}{\partial r}\left(\frac{\alpha_M e_0^2}{4\pi\varepsilon_0 r}\right)$$

$$\Rightarrow K = \frac{\alpha_M e_0^2 r_0^{11}}{48\pi\varepsilon_0}$$

$$-2W_0 = \frac{\alpha_M e_0^2}{48\pi\varepsilon_0 r_0} + \frac{\alpha_M e_0^2}{4\pi\varepsilon_0 r} + W_i - W_a$$

Zanima nas r_0:

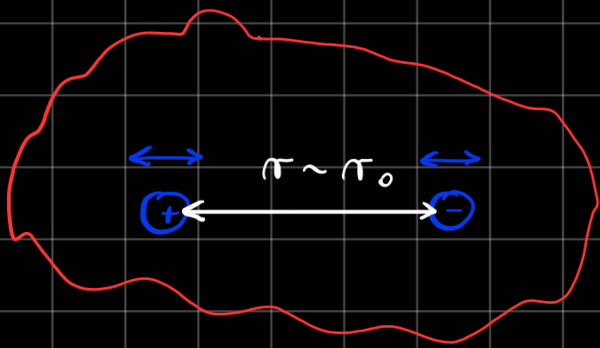
$$r_0 = \frac{11\alpha_M e_0^2}{48\pi\varepsilon_0(-2W_0 - W_i + W_a)} = 0'20\,nm$$

4.2

$r_0 = 0'281$

$V_k(r) = \frac{c}{r^{7'7}}$

$\alpha_M = 1'75$

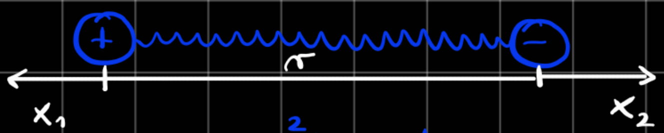


Kako se spreminja E, če se par premika v levo in desno?

$$W_p(r) = V_k(r) - W_c(r) = \frac{c}{r^{7,7}} - \frac{\alpha_M e_0^2}{4\pi \varepsilon_0 r}$$

Konstanto c določimo z odvodom po r, glej prejšnjo nalogo

$$c = \frac{\alpha_M e_0^2 r_0^{6'7}}{30'8 \pi \varepsilon_0}$$



$$k = \frac{\partial^2 W_p}{\partial r^2}\Big|_{r=r_0}$$ nihanje okrog tč. r_0

x… raztezek, $x = x_1 + x_2$

II N.Z.

(1) $m_{Na} \ddot{x}_1 = -kx$ // izpostavimo $\ddot{x}_1$

(2) $m_{Cl} \ddot{x}_2 = -kx$ // izpostavimo $\ddot{x}_2$

(3) $\frac{\partial^2}{\partial t^2}(x) = \ddot{x}_1 + \ddot{x}_2$

$$\ddot{x} = \ddot{x}_1 + \ddot{x}_2$$

$$\ddot{x} = -k\left(\frac{1}{m_{Na}} + \frac{1}{m_{Cl}}\right)x$$

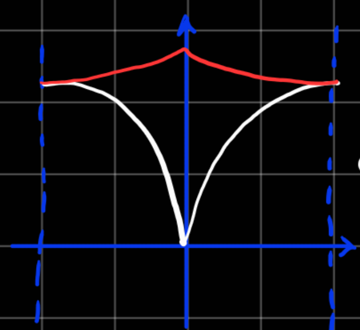
$$\ddot{x} + \underbrace{k\left(\frac{1}{m_{Na}} + \frac{1}{m_{Cl}}\right)}_{\omega_0^2} x = 0$$

$$\omega_0 = \sqrt{\frac{k}{m^*}}\ , \quad m^* = \frac{m_{Na}\, m_{Cl}}{m_{Na} + m_{Cl}}$$

Podatki: $m_{Na} = 23'0\,u$, $u = \dfrac{M(^{12}C)}{12 N_A} = 1'66\cdot10^{-23}\,kg$

$m_{Cl} = 35'45\,u$

$\Rightarrow \omega_0 = 7'3\cdot10^{13}/s\ , \quad \nu = 11'6\ THz$



optična nihanja

akustična nihanja

$k = \frac{2\pi}{\lambda}$