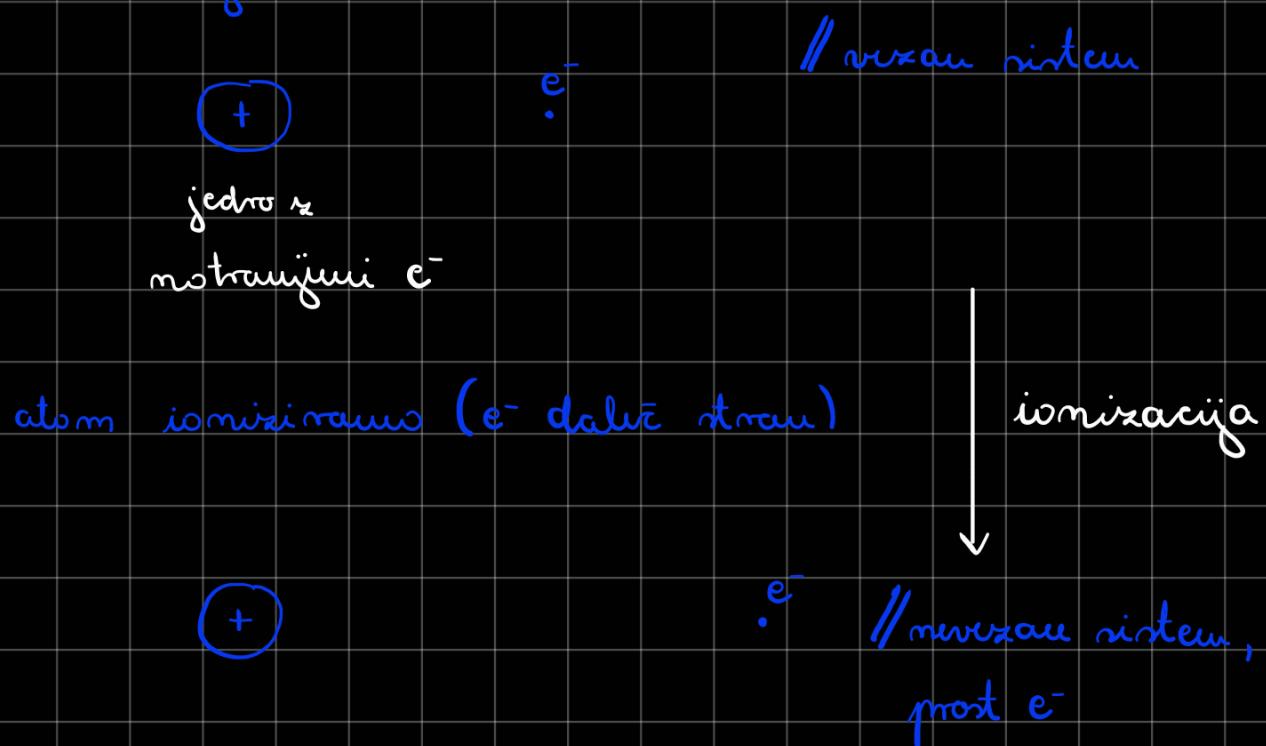


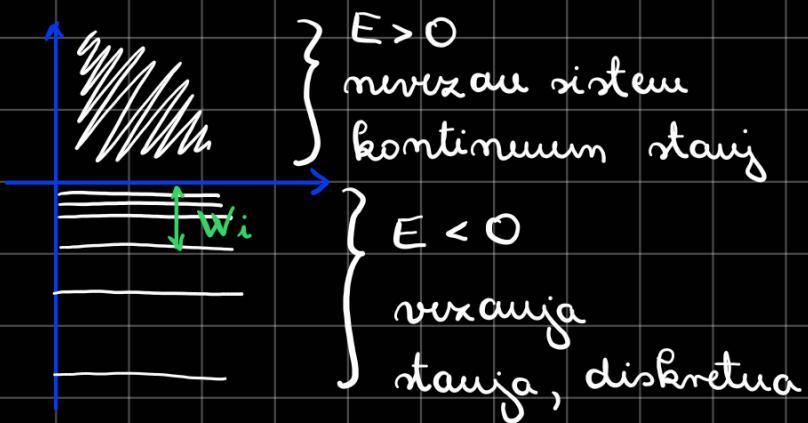
Moderna fizika - vajf

Naturalk NaCl

1. Ionizacija Na



Pri vezanem sistemu so dovoljne diskretna stanja energije



w_i ... ionizacijska energija (en. potrebna za to, da danas e^- dovolj daleč od jedra x motrajući e^-)

Energijška stanja Na



Energijška stanja Cl



2. Veržuta \propto Na in Cl

Uprnosti $E \rightarrow W_a \dots$ elektronska afiniteta

$$W_i - W_a > 0$$

Da nastane ion, mora biti omočno stanje iona nižje od tega, ko sta atoma nevzvraša.

Ion \propto ne zende zaradi Paulijevoga vzklopjutivnega načila.

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

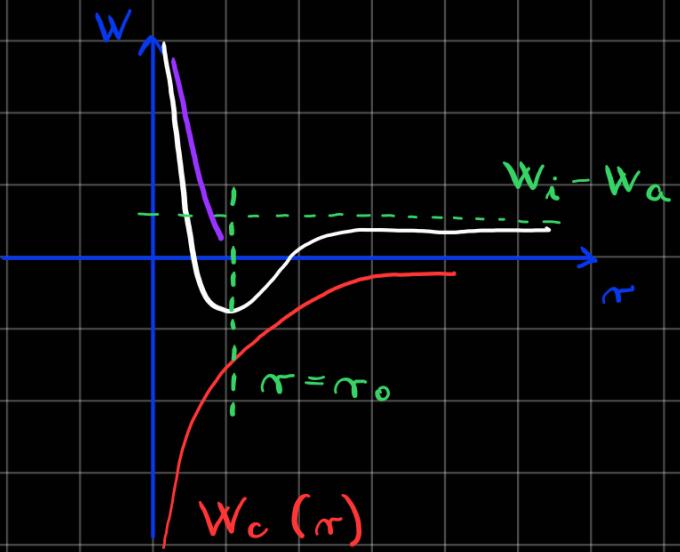
↓
 nevzvrašna
 en.
 ↓ odb. pot.
 bratkega doseganja
 r_0 ... nizovsredna lega
 Z_1 e.
 +
 Z_2 e.
 -
 Pauli (prenaravnje e- oblakov)

Coulumbova
 energija

$$\vec{F} = \frac{e}{4\pi\epsilon_0 r^2} \frac{\vec{r}}{|\vec{r}|}$$

$$\vec{F} = -\nabla V \Rightarrow V(r) = \frac{e}{4\pi\epsilon_0 r}$$

$$W_c(r) = eV(r) = -\frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r}$$

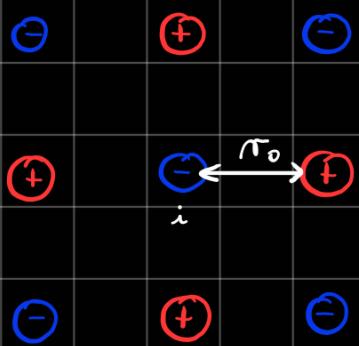


Ionski kristal

število \oplus oz. \ominus ionov (vsi skupaj $2N$ gradnikov)

$$W_V = \underbrace{N(\tilde{V}_k(r_0) + \tilde{W}_c)}_{\uparrow} + NW_i - NW_a$$

$\tilde{V}_k, \tilde{W}_c \dots$ jiji mista enaki kot pri 1 ionu NaCl



\tilde{V}_k je ena enake funkcijosko odvivnost, drugaciu predfaktor

naboj centralnega iona

→ Madlunova komst.

$$\tilde{W}_c = \underbrace{\alpha_{M,i}}_{\text{potencial}} e_0 \cdot \underbrace{V_{C,i}}_{\text{na mestu centralnega iona}} = \alpha_{M,i} e_0 \frac{q \pi \epsilon_0 r_0}{4 \pi \epsilon_0 r_0}$$

parска
interakcija,
za kristal pomnozimo s N

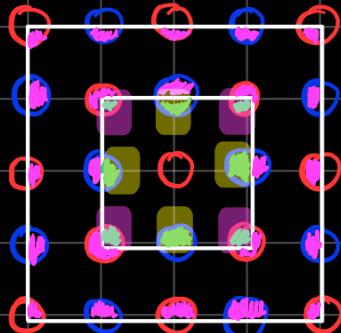
$\alpha_{M,i}$ porazdelitev nabaja v okoli centralnega atoma

$$\alpha_{M,i} = \sum_{\delta} \frac{\chi_{\delta}}{\frac{r_i}{r_0}}$$

$\chi_{Na} = +1, \chi_{Ce} = -1$

↓ porządku

Skrypta Zorko 4.1



$$\alpha_{M,i} = \sum_{\delta} \frac{\chi_{\delta}}{\frac{r_i}{r_0}}$$

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

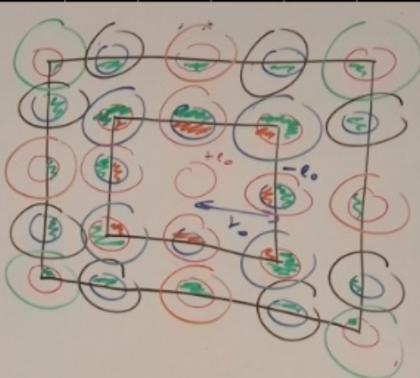
→ miedzi, $1/2$, negatywna mądrość

$$(1) \quad \alpha_{M,i}^{(1)} = 4 \cdot \left[\frac{-\frac{1}{2}}{\frac{1}{1}} \right] + 4 \cdot \left[\frac{\frac{1}{4}}{\frac{1}{1}} \right] = -1'293$$

↓ $\frac{\pi}{r_0}$

$$\Rightarrow \alpha = -1'607$$

$$(2) \quad \alpha_{M,i}$$



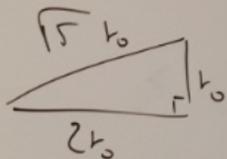
$$\alpha_{M,i}^{(2)} = \zeta \cdot \frac{\chi}{2}$$

$$+ \zeta \cdot \frac{\frac{1}{2}}{2\sqrt{2}}$$

$$+ \zeta \cdot \frac{\frac{3}{2}}{\sqrt{2}}$$

$$+ 8 \cdot \frac{-\frac{1}{2}}{\sqrt{2}}$$

$$+ \zeta \cdot \frac{-\frac{1}{2}}{1}$$



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

$$= -0'314$$

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

$$W_v = 2N \cdot 5 \text{ eV}$$

$$W_i = 15 \text{ eV}$$

$$W_a = 10 \text{ eV}$$

$$W_k(\tau) \propto \frac{1}{\tau^{12}} \Rightarrow V_\tau = \frac{K}{\tau^{12}}$$

$$W_v = N(V_k(\tau) + W_c(\tau)) + N(W_i - W_a) \quad \text{Homomorfna enačba}$$

$$\Rightarrow -2W_0 = V_k(\tau) + W_c(\tau) + W_i - W_a$$

Imamo dve neizvanki: τ_0 in K

Pri τ_0 je minimum \rightarrow odvajamo

$$\frac{\partial W_\tau}{\partial \tau} \Big|_{\tau=\tau_0} = 0 = -12 \frac{K}{\tau^{13}} - \frac{\alpha_m e_0^2}{9\pi \epsilon_0 \tau^2}$$

$$\frac{\partial W_c}{\partial \tau} = \frac{\partial}{\partial \tau} \left(\frac{\alpha_m e_0^2}{9\pi \epsilon_0 \tau} \right)$$

$$\Rightarrow K = \frac{\alpha_m e_0^2 \tau_0^{11}}{48\pi \epsilon_0}$$

$$-2W_0 = \frac{\alpha_m e_0^2}{98\pi \epsilon_0 \tau_0} + \frac{\alpha_m e_0^2}{9\pi \epsilon_0 \tau} + W_i - W_a$$

Zavima nas τ_0 :

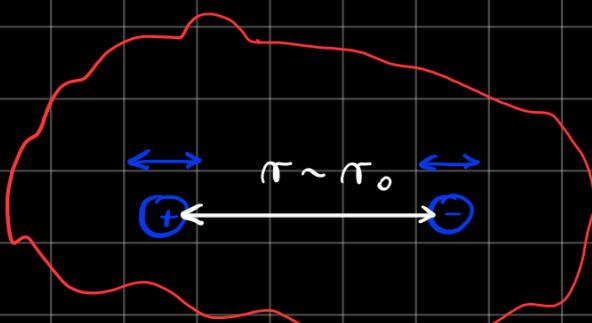
$$\tau_0 = \frac{11\alpha_m e_0^2}{48\pi \epsilon_0 (-2W_0 - W_i + W_a)} = 0.20 \text{ mm}$$

4.2

$$\pi_0 = 0'281$$

$$V_R(\pi) = \frac{C}{\pi^{7,7}}$$

$$\alpha_M = 1'75$$



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

$$W_p(\pi) = V_R(\pi) - W_C(\pi) = \frac{C}{\pi^{7,7}} - \frac{\alpha_M \epsilon_0^2}{4\pi \epsilon_0 \pi}$$

Konstanto C določimo s odvodom po π , ali je prejšnjo mogoče

$$C = \frac{\alpha_M \epsilon_0^2 \pi_0^{6,7}}{30'8 \pi \epsilon_0}$$



$$k = \left. \frac{\partial^2 W_p}{\partial \pi^2} \right|_{\pi=\pi_0} \text{ mehanični okrovki k. } \pi_0$$

x ... razstrelk., $x = x_1 + x_2$

II N.Z.

$$\textcircled{1} \quad m_{Na} \ddot{x}_1 = -kx \quad // \text{izpostavimo } \ddot{x}_1$$

$$\textcircled{2} \quad m_{cl} \ddot{x}_2 = -kx \quad // \text{izpostavimo } \ddot{x}_2$$

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

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

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

$$\ddot{x} + k \left(\frac{1}{m_{Na}} + \frac{1}{m_{Cl}} \right) x = 0$$

$\underbrace{\qquad\qquad\qquad}_{\omega_0^2}$

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

Podatki: $m_{Na} = 23'0 \mu$, $m_{Cl} = 35'45 \mu$, $u = \frac{M(^{12}C)}{12 N_A} = 1'66 \cdot 10^{-23} \text{ kg}$

$$\Rightarrow \omega_0 = 7'3 \cdot 10^{13} / \text{s}, \quad \gamma = 11'6 \text{ THz} \rightarrow \leftarrow \begin{array}{c} \oplus \\ \ominus \end{array}$$

