ELEKTRONI V SNOVI

$Q_2 = Ze_0$ $\quad Q_1 = +2e_0$ $\quad \frac{1}{2}mv^2 = \frac{Q_1 Q_2}{4\pi\varepsilon_0 r} \rightarrow r = 10^{-15}\,m = 1\,fm$

$0{,}1\,nm \simeq 10^{-10}\,m$

Rutherford (1911)

1) BOHROV MODEL ATOMA (1913)

$F_{gra} \sim \frac{1}{r^2}$ $\quad F_{el} \sim \frac{1}{r^2}$

$F = \frac{e_0^2}{4\pi\varepsilon_0 r^2}$

$x = r\cos\omega t$ $\quad \ddot{x} = -r\omega^2\cos\omega t$

$y = r\sin\omega t$ $\quad \ddot{y} = -r\omega^2\sin\omega t$

$a_r = r\omega^2$

$F = ma$

$\omega = \frac{v}{r}$ $\quad T = \frac{2\pi r}{v}$ $\quad \omega = 2\pi\nu = \frac{2\pi}{T} = \frac{v}{r}$

$mr\frac{v^2}{r} = \frac{e_0^2}{4\pi\varepsilon_0 r^2} \rightarrow$ ① $mrv^2 = \frac{e_0^2}{4\pi\varepsilon_0}$

$2\pi r = n\lambda$ $\quad \lambda = \frac{h}{p}$ $\quad 2\pi r = n\frac{h}{mv}$ ② $mrv = n\hbar$ $\quad n = 1, 2, 3, \ldots$

$v = \frac{n\hbar}{mr}$ $\quad mr\frac{n^2\hbar^2}{m^2r^2} = \frac{e_0^2}{4\pi\varepsilon_0}$

$$r_n = n^2\frac{4\pi\varepsilon_0\hbar^2}{e_0^2 m_e}$$

$$E_n = \frac{1}{2}mv^2 - \frac{e_0^2}{4\pi\varepsilon r} = \frac{-1}{n^2}E_I$$

$a_B = \frac{4\pi\varepsilon_0\hbar^2}{e_0^2 m_e}$ Bohrov radij $\quad a_B = 0{,}052\,nm$

$1\,\text{Å} = 0{,}1\,nm \quad a_B = 0{,}5\,\text{Å}$

Rydbergova konstanta $E_I = 1\,Ry = \frac{e_0^4 m_e}{2(4\pi\varepsilon_0\hbar)^2} = 13{,}6\,eV$

$\hbar\omega = E_{n'} - E_n = E_I\left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$

2) ATOMSKE ORBITALE

$$-\frac{\hbar^2}{2m_e}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) - \frac{e_0^2}{4\pi\varepsilon_0 r}\psi = E\psi$$

$\psi = \psi(x, y, z)$

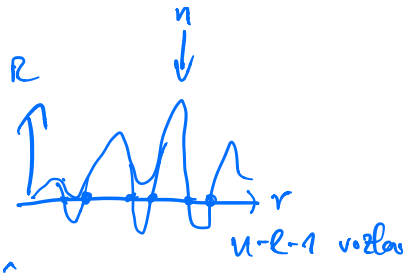
$\psi = \psi(r, \theta, \varphi)$ — radialna, azimutni, polarni kot

$\psi_{nlm} = R_{nl}(r)\,Y_{lm}(\theta, \varphi)$

radialni del, lastna funkcija, krogelna funkcija

n glavno kv. število
l tirno (orbitalno) kv. število
m magnetno kv. število

$R_{nl} \sim e^{-r}(r^3 + 2r^2 + \dots)$



$n-l-1$ vozlov

$Y_{lm}(\theta, \varphi)$

$\hat{\vec{l}} = \hat{\vec{r}} \times \hat{\vec{p}}$

$\hat{l}_x, \hat{l}_y, \hat{l}_z$

$\hat{l}^2 = \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2$

$[\hat{l}_x, \hat{l}_y] = i\hbar\,\hat{l}_z$

$[\hat{l}^2, \hat{l}_i] = 0 \quad i = x, y, z$

$\hat{l}^2, \hat{l}_z$

$$\begin{cases} \hat{l}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm} \\ \hat{l}_z Y_{lm} = \hbar m Y_{lm} \end{cases}$$

$l = 0, 1, 2, \dots, n-1$

$m = -l, -l+1, -l+2, \dots, l-1, l$ $\quad (2l+1)$

$$E_n = -\frac{E_I}{n^2}$$

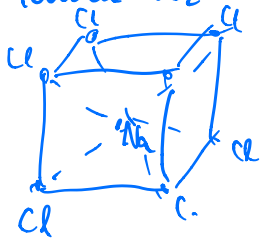
1) $x, y, z \longrightarrow r, \theta, \varphi \longrightarrow n, l, m$
2) $m_s = +1/2 \quad m_s = -1/2$
3) $\rho = |\psi|^2$
4) $n = 1\ 2\ 3\ 4$ $\quad l = 0\ 1\ 2\ 3$
   K L M N $\quad$ s p d f
   lupine $\quad$ podlupine

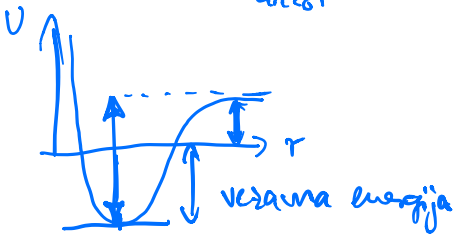
D.N.
Rok 14. 5.

3) PERIODNI SISTEM

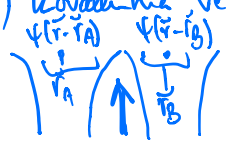
4) KEMIJSKE VEZI

a) Ionska vez: Na^+ Cl^- $\quad F = \frac{k q_1 q_2}{4\pi\varepsilon_0 r}$



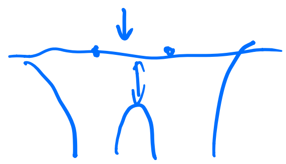


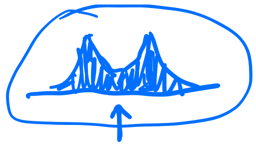
b) Kovalentna vez

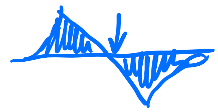


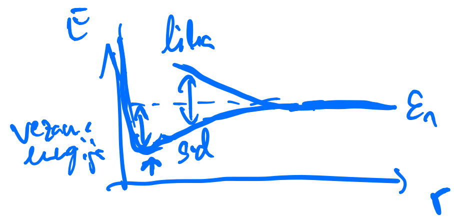
$\psi_{sod} = A(\psi(\vec{r} - \vec{r}_A) + \psi(\vec{r} - \vec{r}_B))$

$\psi_{ods} = A(\psi(\vec{r} - \vec{r}_A) - \psi(\vec{r} - \vec{r}_B))$

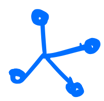


ψ_{sod}  energijsko ugodno

ψ_{lih}  energijsko neugodno

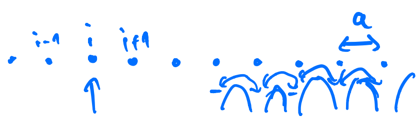


razcep

C 4 valenčni elektroni  CH_4

5) KRISTALI

6) ELEKTRONSKI PASOVI



$|i\rangle \quad i \in \mathbb{Z} \qquad \varepsilon_0 \qquad H|i\rangle = E|i\rangle \qquad E = \varepsilon_0$

$|i\rangle \to |i+1\rangle$
$\searrow |i-1\rangle \qquad t$

$$H = \underbrace{\sum_{i=-\infty}^{\infty} \varepsilon_0 |i\rangle\langle i|}_{H_0} - t\big(\underbrace{|i+1\rangle\langle i|}_{H_D} + \underbrace{|i-1\rangle\langle i|}_{H_L}\big)$$

$$H_0|i\rangle = \sum_{j=-\infty}^{\infty} \varepsilon_0 |j\rangle \underbrace{\langle j||i\rangle}_{\delta_{ij}} = \varepsilon_0 |i\rangle$$

$$H_D|i\rangle = -t\sum_{j=-\infty}^{\infty} |j+1\rangle \underbrace{\langle j||i\rangle}_{\delta_{ij}} = -t|i+1\rangle$$

$k = \frac{2\pi}{\lambda} \qquad x_n = na$

$$|\psi_k\rangle = \sum_{n=-\infty}^{\infty} e^{ik\overbrace{na}} |n\rangle$$

$$H|\psi_k\rangle = \left[\sum_{i=-\infty}^{\infty} \varepsilon_0 |i\rangle\langle i| - t\big(|i+1\rangle\langle i| + |i-1\rangle\langle i|\big)\right] \sum_{n=-\infty}^{\infty} e^{ikna} |n\rangle$$

$$= \sum_{n=-\infty}^{\infty} e^{ikna} \left(\sum_{i=-\infty}^{\infty} -ii- \right) |n\rangle$$

$$= \sum_{n=-\infty}^{\infty} e^{ikna} \left(\varepsilon_0 |n\rangle - t|n+1\rangle - t|n-1\rangle \right)$$

$$= \sum_{n=-\infty}^{\infty} e^{ikna} \varepsilon_0 |n\rangle - t \sum_{\substack{n=-\infty \\ m=n+1}}^{\infty} e^{ikna} |n+1\rangle - t \sum_{\substack{n=-\infty \\ m=n-1}}^{\infty} e^{ikna} |n-1\rangle$$

$$= \sum_{n=-\infty}^{\infty} e^{ikna} \varepsilon_0 |n\rangle - t \sum_{m \to n} e^{ik(m-1)a} |m\rangle - t \sum_{m \to n} e^{ik(m+1)a} |m\rangle$$

$$= \sum_{n=-\infty}^{\infty} e^{ikna} \underbrace{\left(\varepsilon_0 - t e^{ika} - t e^{-ika} \right)}_{} |n\rangle$$

$$= \left[\varepsilon_0 - 2t \cos(ka) \right] \sum_n e^{ikna} |n\rangle$$

$$H|\psi_k\rangle = \left[\varepsilon_0 - 2t \cos(ka) \right] |\psi_k\rangle \qquad \varepsilon(k) = \varepsilon_0 - 2t\cos(ka)$$

k majhen $\quad \cos(ka) = 1 - \frac{(ka)^2}{2}$ $\qquad \varepsilon(k) \approx \varepsilon_0 - 2t + \frac{2ta^2}{2} k^2$

$$E = \frac{1}{2} \frac{p^2}{m} = \frac{\hbar^2}{2m} k^2$$

$$\frac{\hbar^2}{2m} = \frac{2ta^2}{2}$$

$$\boxed{m = \frac{\hbar^2}{2ta^2}}$$

efektivna masa

t majhen $\Rightarrow$ m visoka masa

Težki fermioni $m \sim 1000\, m_e$

Ce, Yb, U, Pu
↑ ↑

k $\quad$ $\overset{a}{\leftrightarrow}$ $\quad$ $\frac{2\pi}{a}$ $\quad$ $\bullet\,[\,\bullet\,]\,\bullet$ $2\pi/a$

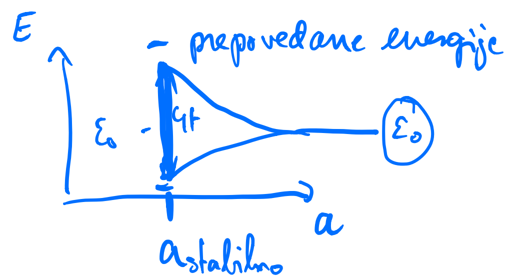
Brillouinova cona: $[-\pi/a\,;\,\pi/a]$.

$$\varepsilon_k = \varepsilon_0 - 2t\cos(ka)$$

ε_0+2t

ε_0 $\quad$ $4t$ $\quad$ elektronski pas.

ε_0-2t



$N_A \sim 10^{23}$