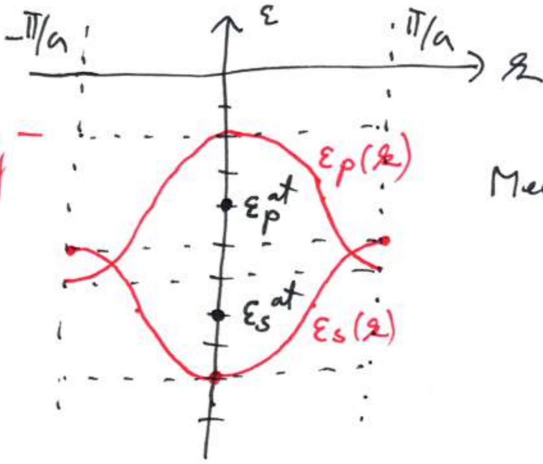
① a) $\varepsilon_s(k) = \varepsilon_s^{at} - 2\gamma_{ss}\cos ka$ 1/4

$\varepsilon_p(k) = \varepsilon_p^{at} - 2\gamma_{pp}\cos ka$

$\varepsilon_s^{at} = -7\,\mathrm{eV}$
$\varepsilon_p^{at} = -4\,\mathrm{eV}$
$\gamma_{ss} = 1\,\mathrm{eV}$
$\gamma_{pp} = -1\,\mathrm{eV}$
$\gamma_{sp} = -1.5\,\mathrm{eV}$

1/4 –



Med pasovoma ni energijske reže. +

b) $\gamma_{sp}(-a) = -\int d\vec{r}\, \psi_s^*(\vec{r})\, \Delta V(\vec{r})\, \psi_{px}(\vec{r} + a\hat{x}) = -\gamma_{sp}(a)$, ker ima orbitala px liho parnost. +

$$\psi(\vec{r}) = \sum_{m,\alpha\in\{s,px\}} c_{m\alpha}\psi_\alpha(\vec{r} - ma\hat{x})$$

$$\varepsilon c_{ms} = \varepsilon_s^{at} c_{ms} - \gamma_{ss} c_{m+1,s} - \gamma_{ss} c_{m-1,s} - \gamma_{sp} c_{m+1,px} + \gamma_{sp} c_{m-1,px}$$

$$\varepsilon c_{mp} = \varepsilon_p^{at} c_{mp} - \gamma_{pp} c_{m+1,px} - \gamma_{pp} c_{m-1,px} + \gamma_{sp} c_{m+1,s} - \gamma_{sp} c_{m-1,s}$$

++

$$c_{ms} = c_s e^{ikma}$$

$$c_{mpx} = c_{px} e^{ikma}$$

+

$$\varepsilon c_s = \varepsilon_s^{at} c_s - 2\gamma_{ss}\cos ka\, c_s - 2i\gamma_{sp}\sin ka\, c_{px}$$

$$\varepsilon c_{px} = \varepsilon_p^{at} c_{px} - 2\gamma_{pp}\cos ka\, c_{px} + 2i\gamma_{sp}\sin ka\, c_s$$

$$\begin{bmatrix} \varepsilon_s^{at} - 2\gamma_{ss}\cos ka - \varepsilon, & -2i\gamma_{sp}\sin ka \\ 2i\gamma_{sp}\sin ka, & \varepsilon_p^{at} - 2\gamma_{pp}\cos ka - \varepsilon \end{bmatrix} \begin{bmatrix} c_s \\ c_{px} \end{bmatrix} = 0$$

+

$$\varepsilon^2 - \varepsilon\left[\varepsilon_s^{at} + \varepsilon_p^{at} - 2(\gamma_{ss} + \gamma_{pp})\cos ka\right] + (\varepsilon_s^{at} - 2\gamma_{ss}\cos ka)(\varepsilon_p^{at} - 2\gamma_{pp}\cos ka) - 4\gamma_{sp}^2\sin^2 ka = 0$$

$$\varepsilon_\pm(k) = \frac{\varepsilon_s^{at} + \varepsilon_p^{at}}{2} - (\gamma_{ss} + \gamma_{pp})\cos ka \pm \sqrt{\left(\frac{\varepsilon_s^{at} - \varepsilon_p^{at}}{2} - (\gamma_{ss} - \gamma_{pp})\cos ka\right)^2 + 4\gamma_{sp}^2\sin^2 ka}$$

+

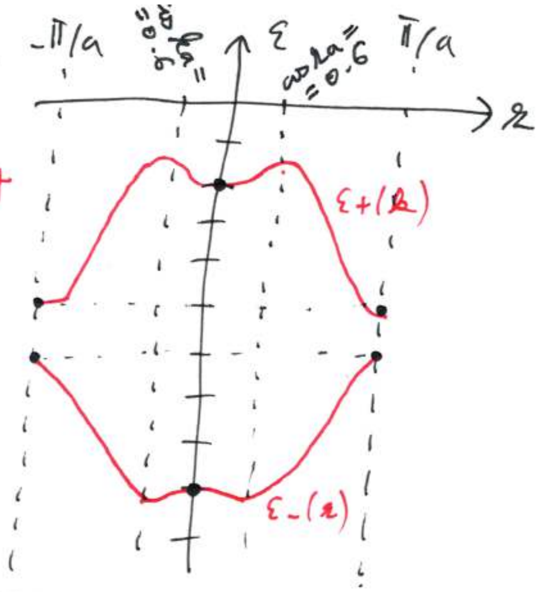
$$\varepsilon_\pm(k) = -5.5\,\mathrm{eV} \pm \sqrt{11.25\,\mathrm{eV}^2 + 6\,\mathrm{eV}^2\cos ka - 5\,\mathrm{eV}^2\cos^2 ka}$$

$k = 0 \rightarrow \varepsilon_\pm(k) = -5.5\,\mathrm{eV} \pm 3.5\,\mathrm{eV}$

$k = \pm\pi/a \rightarrow \varepsilon_\pm(k) = -5.5\,\mathrm{eV} \pm 0.5\,\mathrm{eV} \Longrightarrow$ širina energijske reže je 1 eV. +

$\max(11.25\,\mathrm{eV}^2 + 6\,\mathrm{eV}^2\cos ka - 5\,\mathrm{eV}^2\cos^2 ka)$ je pri $\cos ka = 0.6$

① b) ...



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② a) $n_c = N_p = N_c e^{-\beta(\varepsilon_c - \mu)}$

$$\mu = \varepsilon_c - k_B T \ln \frac{N_c}{N_p} = \underline{\underline{\varepsilon_c - 0.3066\,\mathrm{eV}}}$$ +++

b) $$\frac{p_p}{N_p} = \frac{1}{1+2e^{-\beta(\varepsilon_p - \mu)}} = \frac{1}{1+2e^{-\beta(-\Delta\varepsilon_p + \varepsilon_c - \mu)}} =$$

$$= \frac{1}{1+2\frac{N_p}{N_c}e^{\beta\Delta\varepsilon_p}} = \underline{\underline{0.99992}}$$

$$\frac{p_s}{N_s} = \frac{1}{1+2e^{-\beta(\varepsilon_s - \mu)}} = \frac{1}{1+2\frac{N_p}{N_c}e^{\beta\Delta\varepsilon_s}} = \underline{\underline{0.2295}}$$

Predpostavka, da so vsi globoki donorji nevtralni, ni upravičena. +++

c) Obdržimo samo predpostavko, da so plitvi donorji vsi ionizirani:

$$n_c = N_c e^{-\beta(\varepsilon_c - \mu)} = N_p + \frac{N_s}{1+2e^{-\beta(\varepsilon_s - \mu)}}$$ +++

$$e^{-\beta(\varepsilon_c - \mu)} = \frac{N_p}{2N_c} - \frac{1}{4}e^{-\beta\Delta\varepsilon_s} + \sqrt{\left(\frac{N_p}{2N_c} - \frac{1}{4}e^{-\beta\Delta\varepsilon_s}\right)^2 + \frac{N_p + N_s}{2N_c}e^{-\beta\Delta\varepsilon_s}}$$

$$\mu = \underline{\underline{\varepsilon_c - 0.3002\,\mathrm{eV}}}$$

$$\frac{p_p}{N} = \underline{\underline{0.99990}}$$ +++

$$\frac{p_s}{N_s} = \underline{\underline{0.1885}}$$

$k_B = 1.38 \times 10^{-23}\,\mathrm{J/K}$
$\mathrm{eV} = 1.6 \times 10^{-19}\,\mathrm{J}$
$N_p = 2 \times 10^{14}\,\mathrm{cm}^{-3}$
$N_s = 3 \times 10^{14}\,\mathrm{cm}^{-3}$
$N_c = 2.8 \times 10^{19}\,\mathrm{cm}^{-3}$
$\Delta\varepsilon_p = 0.045\,\mathrm{eV}$
$\Delta\varepsilon_s = 0.32\,\mathrm{eV}$