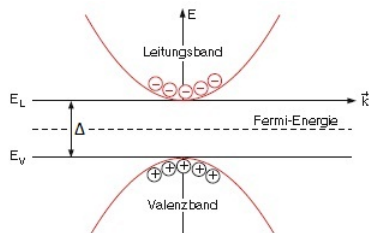


Exziton exciton

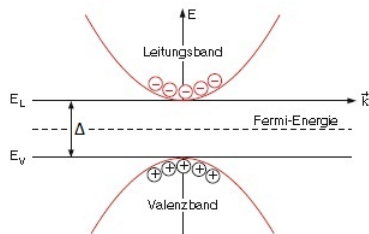
Jean Diehl Kai Ackermann

09.02.2011

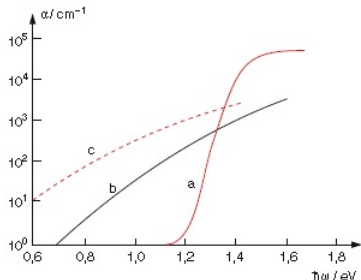
- Valenzbandoberkante E_V
- Leitungsbandunterkante E_L
- Bandlücke Δ



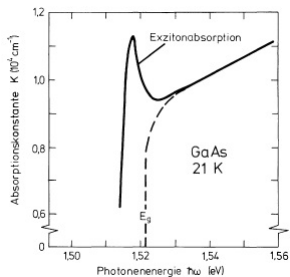
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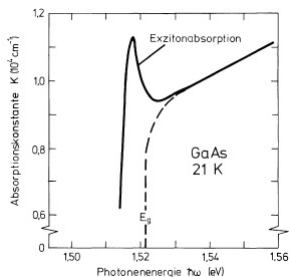
- GaAs
- Kristallines Si
- Amorphes Si



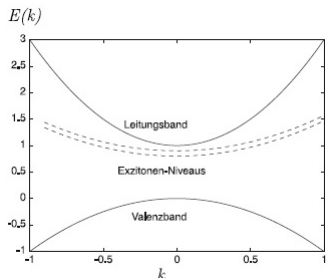
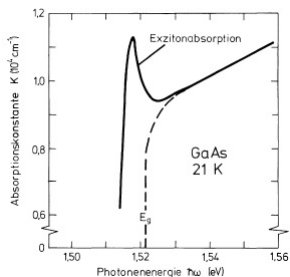
- Experimentell ermittelter Absorptionskoeffizient



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- Photoabsorption bereits bei Energien $E < \Delta$



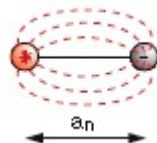
- Experimentell ermittelter Absorptionskoeffizient
- Photoabsorption bereits bei Energien $E < \Delta$
- Energieniveaus unterhalb der Leitungsbandunterkante E_L



- Energieabsenkung durch gebundenes Elektron-Loch Paar

Energieabsenkung

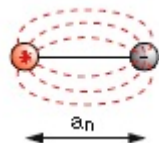
$$E_E = \Delta - E_B + E_{kin}$$



- Energieabsenkung durch gebundenes Elektron-Loch Paar
- Entspricht effektiven Wasserstoffproblem

Energieabsenkung

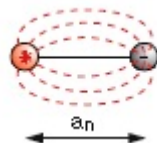
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- Energieabsenkung durch gebundenes Elektron-Loch Paar
- Entspricht effektiven Wasserstoffproblem
- Unterscheidung in stark gebundene Frenkel - Exzitonen und schwach gebundene Wannier- Mott- Exzitonen

Energieabsenkung

$$E_E = \Delta - E_B + E_{kin}$$



Nur zwei Bänder: Valenz- und Leitungsband sowie Wechselwirkung zwischen Valenz- und Leitungselektron (keine Wechselwirkung von Valenz- bzw. Leitungselektronen untereinander):

$$H = \sum_{\mathbf{k}} \left(E(\mathbf{k}) c_{v,\mathbf{k}}^\dagger c_{v,\mathbf{k}} + E_l(\mathbf{k}) c_{l,\mathbf{k}}^\dagger c_{l,\mathbf{k}} \right) + H_1$$

$$H_1 = \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} u_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} c_{v, \mathbf{k}_1}^\dagger c_{l, \mathbf{k}_2}^\dagger c_{l, \mathbf{k}_3} c_{v, \mathbf{k}_4}$$

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Bandstruktur hat Extrema bei Bandlücke, d.h. quadratische Näherung durch effektive Massen:

$$E_v(\mathbf{k}) = -\frac{\hbar^2 k^2}{2m_v}, \quad E_l(\mathbf{k}) = \Delta + \frac{\hbar^2 k^2}{2m_{lv}}$$

Grundzustand: $|\Psi_0\rangle = \prod_{\mathbf{k}} c_{v,\mathbf{k}}^\dagger |0\rangle$

Angeregter Zustand: $|\Psi\rangle = \sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k},\mathbf{k}'} c_{l,\mathbf{k}}^\dagger h_{\mathbf{k}'}^\dagger |\Psi_0\rangle$

$$a_{\mathbf{k},\mathbf{k}'} (E_0 - E + E_l(\mathbf{k}) - E_v(\mathbf{k}')) - \sum_{\mathbf{k}_1, \mathbf{k}_3} u_{\mathbf{k}_1, \mathbf{k}, \mathbf{k}_3, \mathbf{k}'} a_{\mathbf{k}_1 \mathbf{k}_2} = 0$$

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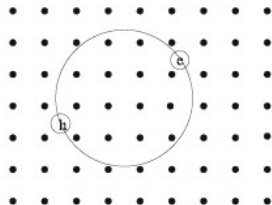
$$a_{\mathbf{k},\mathbf{k}'} (E_0 - E + E_l(\mathbf{k}) - E_v(\mathbf{k}')) - \sum_{\mathbf{k}_1, \mathbf{k}_3} u_{\mathbf{k}_1, \mathbf{k}, \mathbf{k}_3, \mathbf{k}'} a_{\mathbf{k}_1 \mathbf{k}_2} = 0$$

Wechselwirkungselemente mit freien Teilchen berechnen
 (Wannier-Mott-Exzitonen):

$$\tilde{E} a_{\mathbf{k},\mathbf{k}'} = \left(\frac{\hbar^2 k^2}{2m_l} + \frac{\hbar^2 k'^2}{2m_v} \right) a_{\mathbf{k},\mathbf{k}'} - \frac{4\pi e^2}{\epsilon V} \sum_{\mathbf{q}} \frac{1}{q^2} a_{\mathbf{k}'+\mathbf{q}, \mathbf{k}+\mathbf{q}}$$

$$\left(-\frac{\hbar^2}{2m_I} \Delta_{\mathbf{r}_1} - \frac{\hbar^2}{2m_V} \Delta_{\mathbf{r}_2} - \frac{e^2}{\epsilon |\mathbf{r}_1 - \mathbf{r}_2|} - \tilde{E} \right) \psi(\mathbf{r}_1, \mathbf{r}_2) = 0$$

$$\left(-\frac{\hbar^2}{2(m_V + m_I)} \Delta_{\mathbf{r}_{CM}} - \frac{\hbar^2}{2\mu} \Delta_{\mathbf{r}} - \frac{e^2}{\epsilon r} - \tilde{E} \right) \psi = 0$$

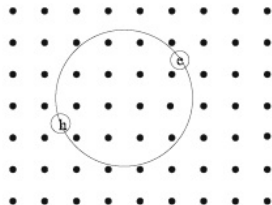


$$\left(-\frac{\hbar^2}{2m_I} \Delta_{\mathbf{r}_1} - \frac{\hbar^2}{2m_V} \Delta_{\mathbf{r}_2} - \frac{e^2}{\epsilon |\mathbf{r}_1 - \mathbf{r}_2|} - \tilde{E} \right) \psi(\mathbf{r}_1, \mathbf{r}_2) = 0$$

$$\left(-\frac{\hbar^2}{2(m_V + m_I)} \Delta_{\mathbf{r}_{CM}} - \frac{\hbar^2}{2\mu} \Delta_{\mathbf{r}} - \frac{e^2}{\epsilon r} - \tilde{E} \right) \psi = 0$$

$$\psi_{\mathbf{k},n}(\mathbf{r}_{CM}, r) = F_n(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}_{CM}}$$

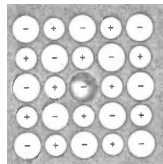
$$\tilde{E}_{\mathbf{k},n} = \frac{\hbar^2 k^2}{2(m_V + m_I)} - \frac{\mu e^4}{2\epsilon^2 \hbar^2} \cdot \frac{1}{n^2}$$



$$H_1 = \sum_{\mathbf{R}, \mathbf{R}'} \left(u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, l\nu} c_{\nu, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}'} c_{\nu, \mathbf{R}} - u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, \nu l} c_{\nu, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}} c_{\nu, \mathbf{R}'} \right)$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, l\nu} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_l(\mathbf{r}' - \mathbf{R}') w_\nu(\mathbf{r} - \mathbf{R})$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, \nu l} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_\nu(\mathbf{r}' - \mathbf{R}') w_l(\mathbf{r} - \mathbf{R})$$



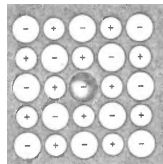
$$H_1 = \sum_{\mathbf{R}, \mathbf{R}'} \left(u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, l\nu} c_{\nu, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}'} c_{\nu, \mathbf{R}} - u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, \nu l} c_{\nu, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}} c_{\nu, \mathbf{R}'} \right)$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, l\nu} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_l(\mathbf{r}' - \mathbf{R}') w_\nu(\mathbf{r} - \mathbf{R})$$

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Frenkel- Exzitonen

- Starke Bindungsenergie (1eV)



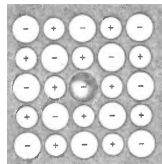
$$H_1 = \sum_{\mathbf{R}, \mathbf{R}'} \left(u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, l\nu} c_{\nu, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}'} c_{\nu, \mathbf{R}} - u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, \nu l} c_{\nu, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}} c_{\nu, \mathbf{R}'} \right)$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, l\nu} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_l(\mathbf{r}' - \mathbf{R}') w_\nu(\mathbf{r} - \mathbf{R})$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{\nu l, \nu l} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_\nu(\mathbf{r}' - \mathbf{R}') w_l(\mathbf{r} - \mathbf{R})$$

Frenkel- Exzitonen

- Starke Bindungsenergie (1eV)
- Treten beispielsweise in Ionenkristallen mit großer Bandlücke auf



$$H_1 = \sum_{\mathbf{R}, \mathbf{R}'} \left(u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{v_l, l\nu} c_{v, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}'} c_{v, \mathbf{R}} - u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{v_l, v_l} c_{v, \mathbf{R}}^\dagger c_{l, \mathbf{R}'}^\dagger c_{l, \mathbf{R}} c_{v, \mathbf{R}'} \right)$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{v_l, l\nu} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_l(\mathbf{r}' - \mathbf{R}') w_\nu(\mathbf{r} - \mathbf{R})$$

$$u_{\mathbf{R}\mathbf{R}', \mathbf{R}'\mathbf{R}}^{v_l, v_l} = \int d^3 r \int d^3 r' w_\nu^*(\mathbf{r} - \mathbf{R}) w_l^*(\mathbf{r}' - \mathbf{R}') \frac{e^2}{\epsilon |\mathbf{r} - \mathbf{r}'|} w_\nu(\mathbf{r}' - \mathbf{R}') w_l(\mathbf{r} - \mathbf{R})$$

Frenkel- Exzitonen

- Starke Bindungsenergie (1eV)
- Treten beispielsweise in Ionenkristallen mit großer Bandlücke auf
- Nachweis über optische Absorption

