Selection rules

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Optical transitions selection rules

- CB and VB symmetry and optical selection rules
- Optical transitions with linearly polarized light
- Optical transitions with circularly polarized light
- Optical spin orientation

$$W_{if} = \frac{2\pi}{\hbar} \left(\frac{e E_0}{m_0 \omega} \right)^2 \left| \langle f | \vec{e} \cdot \vec{p} | i \rangle \right|^2 \delta (E_i - E$$

$E_0 \Rightarrow$ AMPLITUDE ELECTRIC FIELD

FINAL STATE INITIAL STATE

$$\langle f | \vec{e} \cdot \vec{p} | i \rangle$$

POL VECTOR $\vec{p} = -i\hbar \vec{\nabla}$

$$f = e^{i k_f \cdot r} u_f(r) \qquad i = e^{i k_i \cdot r} u_i(r)$$

$$\vec{e}\cdot\langle f|\vec{p}|i\rangle = \vec{e}\cdot\int e^{-ik_f \bar{r}} u_f^*(r)\, \underline{-i\hbar\vec{\nabla}}\,(e^{i}$$

$$= \vec{e}\cdot\int e^{-ik_f r} u_f^*(r)\, \hbar\vec{k}_i\, e^{ik_i r} u_i(r)\, d^3r \; +$$

$$\parallel$$

$$\emptyset$$

$$\vec{e}\cdot\int e^{-ik_f r} e^{ik_i r} u_f^*(r)\, -i\hbar\vec{\nabla}(u_i(r))($$

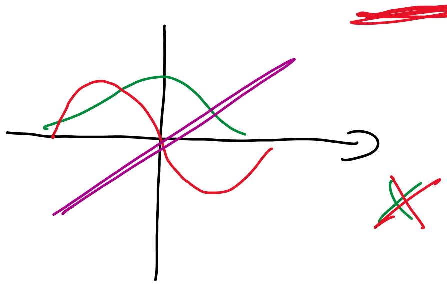
For direct transitions $k_f = k_i$

$$\vec{e}\cdot\int u_f^*(r)\, -i\hbar\vec{\nabla}\,(u_i(r))\,d^3r$$

$f \to$ S-LIKE initial HH, LH, SO

$$\vec{e}\,\langle S\uparrow|-i\hbar\vec{\nabla}|-\frac{1}{\sqrt{2}}(P_x+iP_y)\uparrow\rangle =$$

$$\langle S\uparrow|-i\hbar\frac{\partial}{\partial x}|-\frac{1}{\sqrt{2}}(P_x\; +iP_y)\uparrow\rangle$$



$$\langle S\,|-i\hbar\frac{\partial}{\partial x}|P_x\rangle = P_c$$

$$\langle S|-i\hbar\frac{\partial}{\partial x}|P_y\rangle = \emptyset$$

VB CB

$HH \to S \quad \left|\vec{e}\cdot\langle i|\vec{p}|f\rangle\right| = e_x \cdot \left(-\underline{\frac{1}{\sqrt{2}} P_{cv}}\right) + e_y$

$e_z \to$

$HH \to S \quad \left|\vec{e}\cdot\langle i|\vec{p}|f\rangle\right|^2 =$

x - POLARIZED LIGHT $\quad \frac{1}{2} P_{cv}^2$

y - POLARIZED LIGHT $\quad \frac{1}{2} P_{cv}^2$

z - POLARIZED LIGHT $\quad \emptyset$

$LH \to S \quad \langle \underline{S}(\downarrow\uparrow)| -i\hbar\vec{\nabla}| \underline{\frac{1}{\sqrt{6}}} (\underline{P_x} - iP_y)\uparrow$

x - POL $\quad \frac{1}{6} P_{cv}^2$

y - POL $\quad \frac{1}{6} P_{cv}^2$

z - POL $\quad \frac{4}{6} P_{cv}^2 = \frac{2}{3} P_{cv}^2$

Selection rules for interband transitions

The relevant matrix element is:

$$\boldsymbol{p}_{\mathrm{if}} = -i\hbar \int \psi^*_{\mathbf{k}_f\ell'} \nabla \psi_{\mathbf{k}_i\ell}\, d^3r$$

$$
\begin{aligned}
|i\rangle &= \psi_{\mathbf{k}_i \ell} \\
&= e^{i\mathbf{k}_i\cdot\mathbf{r}} u_{\mathbf{k}_i \ell} \\
|f\rangle &= \psi_{\mathbf{k}_f \ell'} \\
&= e^{i\mathbf{k}_f\cdot\mathbf{r}} u_{\mathbf{k}_f \ell'}
\end{aligned}
$$

$$
\boldsymbol{p}_{\mathrm{if}} = \hbar \boldsymbol{k}_i \int \psi^*_{\mathbf{k}_f \ell'}\, \psi_{\mathbf{k}_i \ell}\, d^3r - i\hbar \int u^*_{\mathbf{k}_f \ell'} \left(\nabla u_{\mathbf{k}_i \ell}\right) e^{i(\mathbf{k}_i - \mathbf{k}_f)\cdot\mathbf{r}}\, d^3r
$$

Zero since Bloch states are orthogonal

Selection rules for interband transitions

- Conduction band:

$$u_{c0} = |s\rangle$$

where $|s\rangle$ is a spherically symmetric state.

- Valence band:

Heavy hole states:
$$|3/2, 3/2\rangle = \frac{-1}{\sqrt{2}}\left(|p_x\rangle + i|p_y\rangle\right)\uparrow$$
$$|3/2, -3/2\rangle = \frac{1}{\sqrt{2}}\left(|p_x\rangle - i|p_y\rangle\right)\downarrow$$

Light hole states:
$$|3/2, 1/2\rangle = \frac{-1}{\sqrt{6}}\left[\left(|p_x\rangle + i|p_y\rangle\right)\downarrow -2|p_z\rangle \uparrow\right]$$
$$|3/2, -1/2\rangle = \frac{1}{\sqrt{6}}\left[\left(|p_x\rangle - i|p_y\rangle\right)\uparrow +2|p_z\rangle >\downarrow\right]$$

From symmetry we see that *only* the matrix elements of the form

$$-\hbar\langle s|\frac{\partial}{\partial x}|p_x\rangle = -\hbar\langle s|\frac{\partial}{\partial y}|p_y\rangle = -\hbar\langle s|\frac{\partial}{\partial z}|p_z\rangle = p_{cv}$$

are different from zero.

Selection rules for interband transitions

VB HH → CB S	VB LH → CB S

X pol	$\hbar^2 \lvert \langle s \lvert \frac{\partial}{\partial x} \rvert HH \rangle \rvert^2 = \frac{1}{2} p_{cv}^2$	$\hbar^2 \lvert \langle s \lvert \frac{\partial}{\partial x} \rvert LH \rangle \rvert^2 = \frac{1}{6} p_{cv}^2$
Y pol	$\hbar^2 \lvert \langle s \lvert \frac{\partial}{\partial y} \rvert HH \rangle \rvert^2 = \frac{1}{2} p_{cv}^2$	$\hbar^2 \lvert \langle s \lvert \frac{\partial}{\partial y} \rvert LH \rangle \rvert^2 = \frac{1}{6} p_{cv}^2$
Z pol	0	$\hbar^2 \lvert \langle s \lvert \frac{\partial}{\partial y} \rvert LH \rangle \rvert^2 = \frac{2}{3} p_{cv}^2$

Optical matrix element for HH and LH

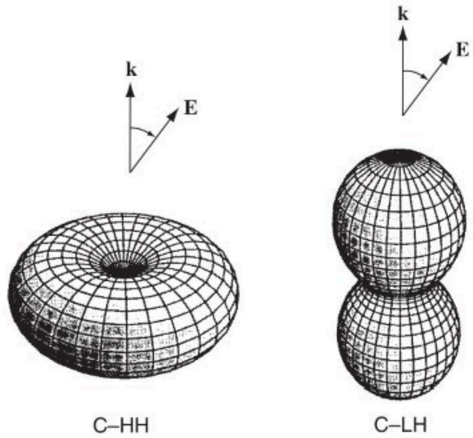
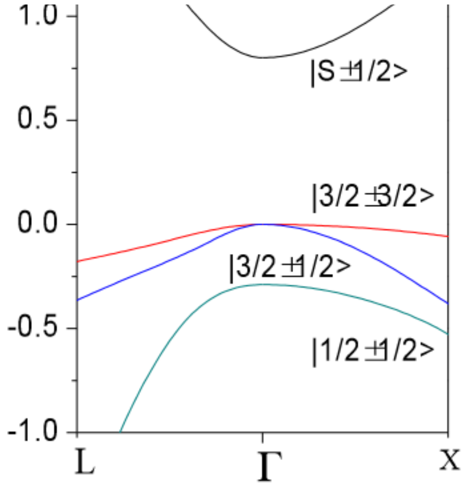


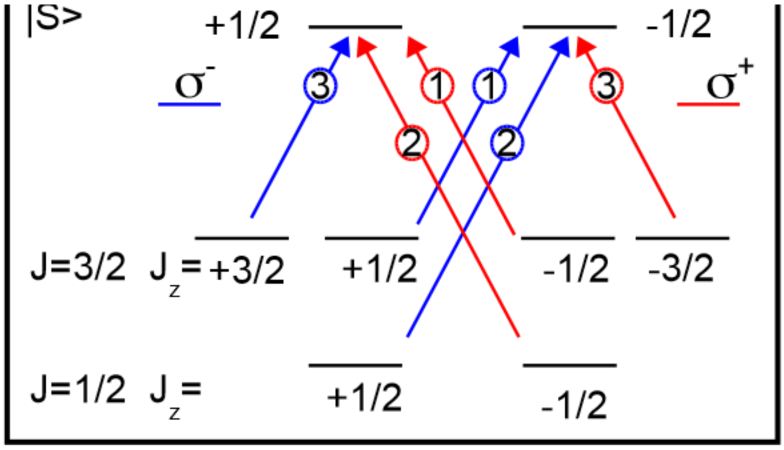
FIGURE A10.2: Dependence of the transition strength, $|M_T|^2$, on angle between the electron's k-vector and the incident electric field vector, **E**, for C–HH and C–LH transitions (C–SO transitions are independent of angle). For C–HH transitions, $|M_T|^2$ is zero when $\mathbf{E} \parallel \mathbf{k}$ and becomes a maximum of $\frac{1}{2} \times |M|^2$ when $\mathbf{E} \perp \mathbf{k}$. For C–LH transitions, when $\mathbf{E} \parallel \mathbf{k}$, $|M_T|^2$ has a peak value of $\frac{2}{3} \times |M|^2$ and is reduced to $\frac{1}{6} \times |M|^2$ when $\mathbf{E} \perp \mathbf{k}$.

HH states can be excited only by x,y polarized light

LH states can be excited by x,y and (predominantly) z polarized light

Optical Spin Orientation





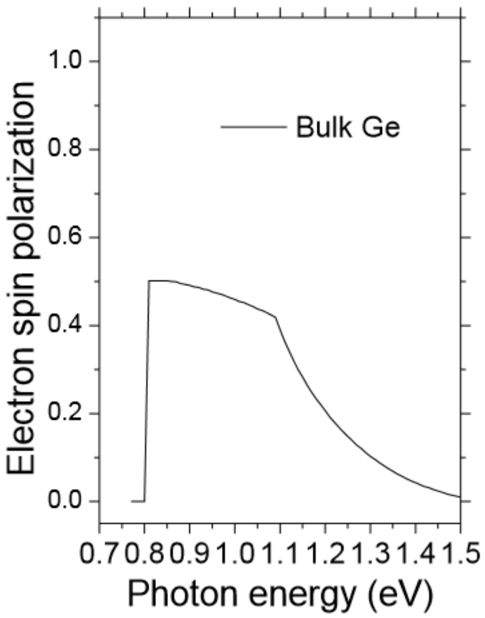
$$P = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}}$$

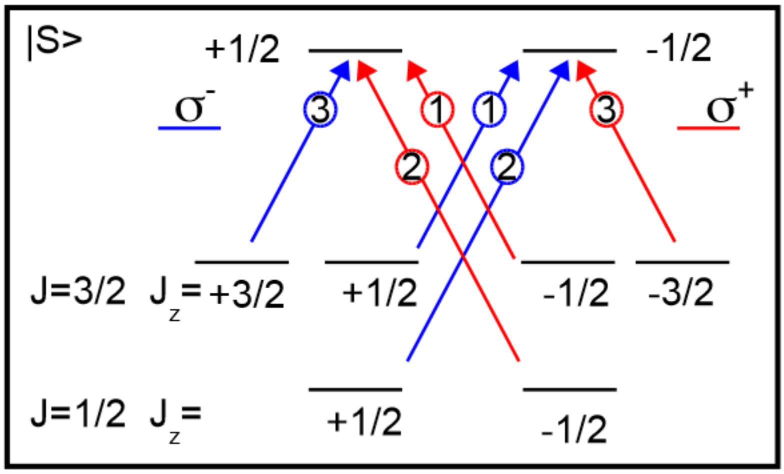
σ^- excitation

at Γ

$$P = 0.5$$

Optical Spin Orientation





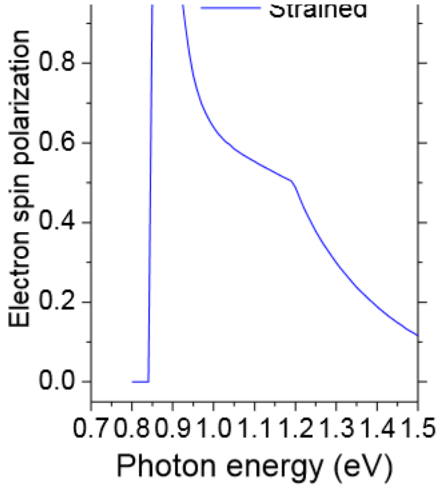
$$P = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}}$$

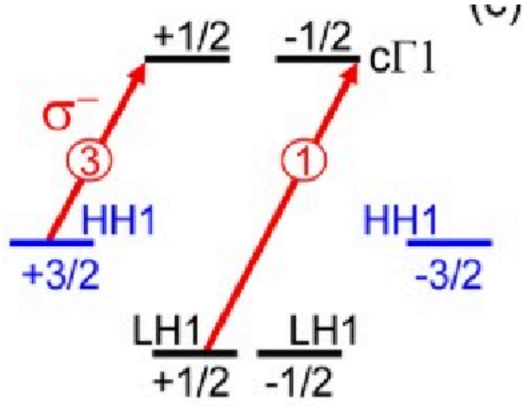
σ^- excitation

at Γ

$$P = 0.5$$

Optical Spin Orientation





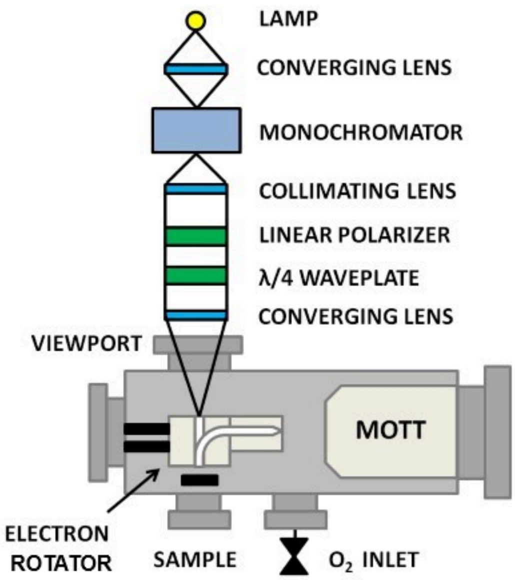
$$P = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}$$

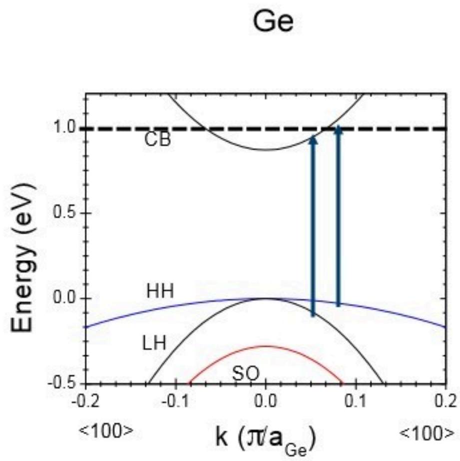
σ^- excitation

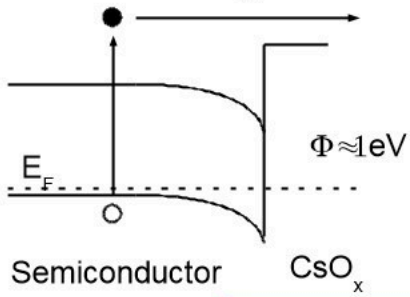
at Γ

$$P = 1$$

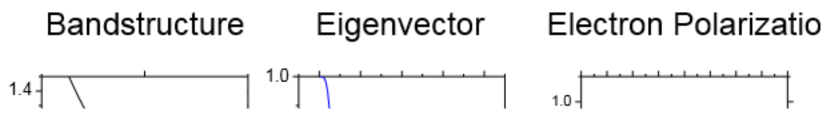
Optical Spin Orientation: spin polarized photoemission







Optical Spin Orientation: spin polarized photoemission



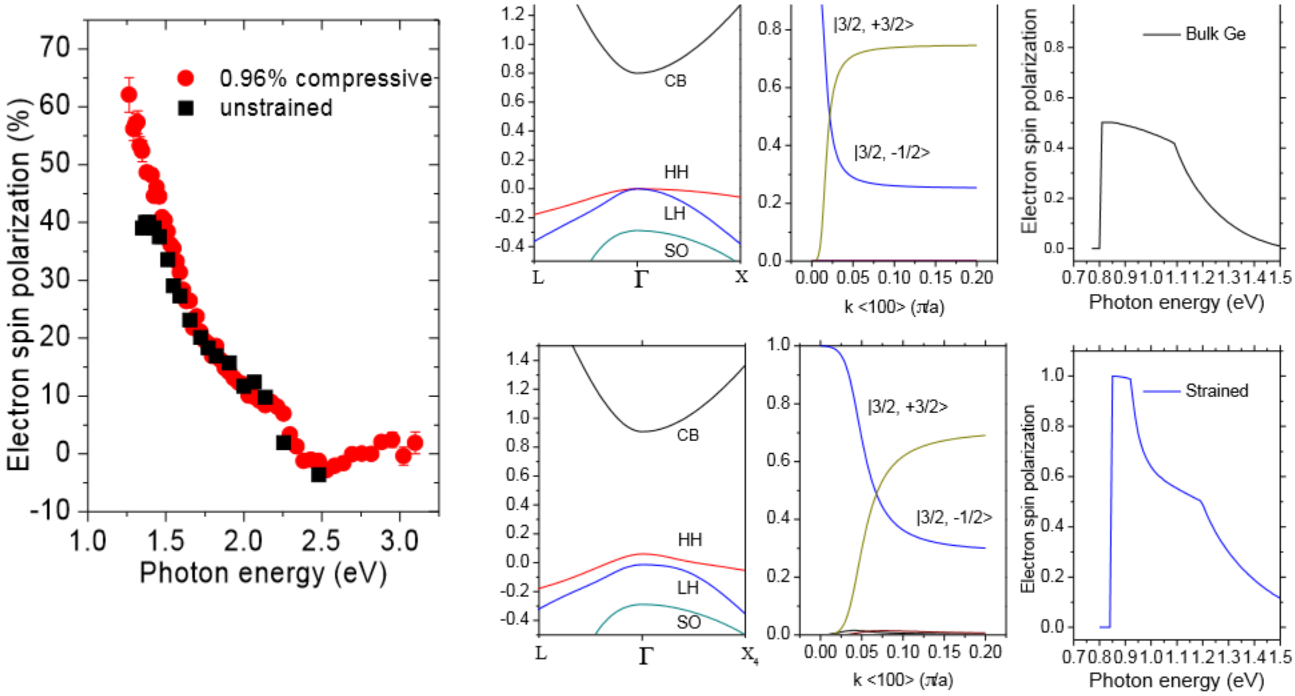


Photo induced inverse spin Hall effect

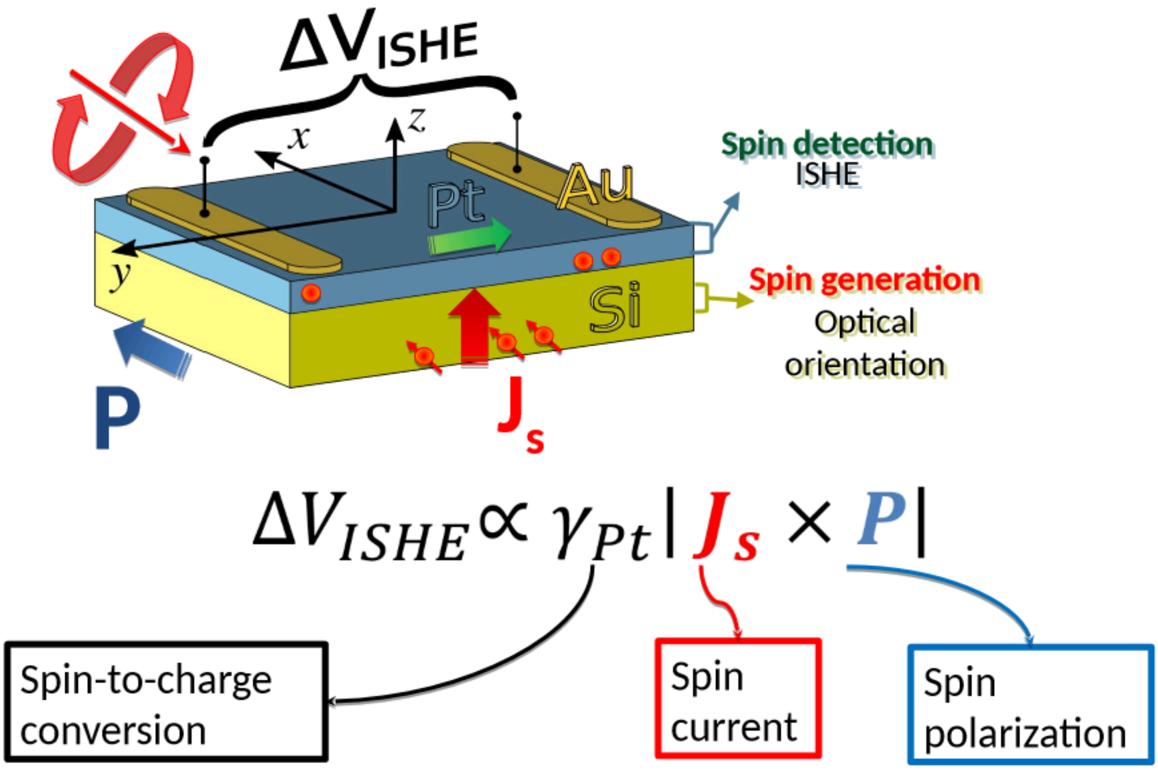


Photo induced inverse spin Hall effect

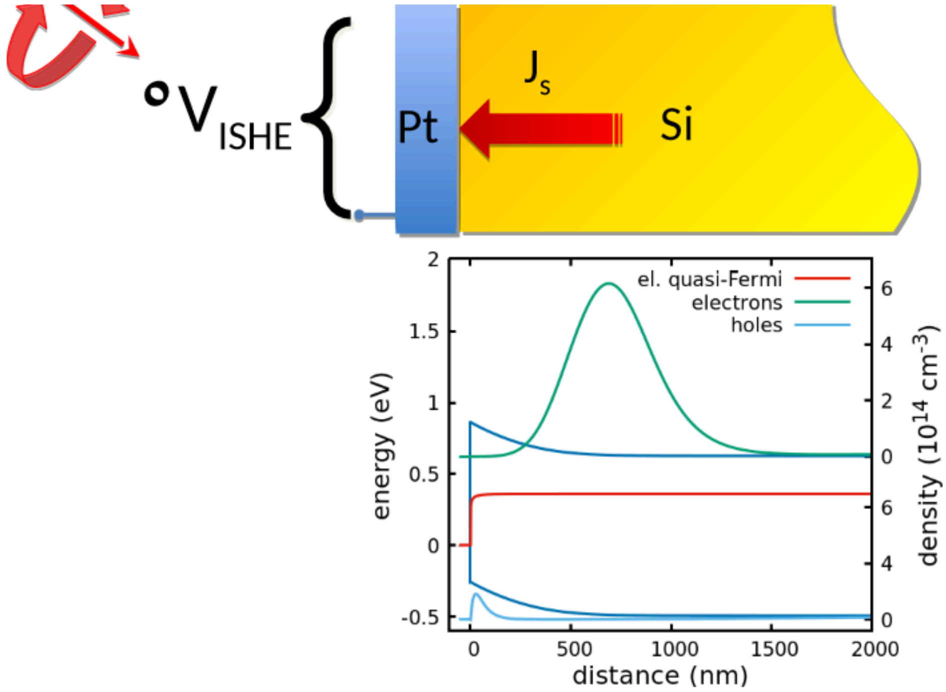


Photo induced inverse spin Hall effect

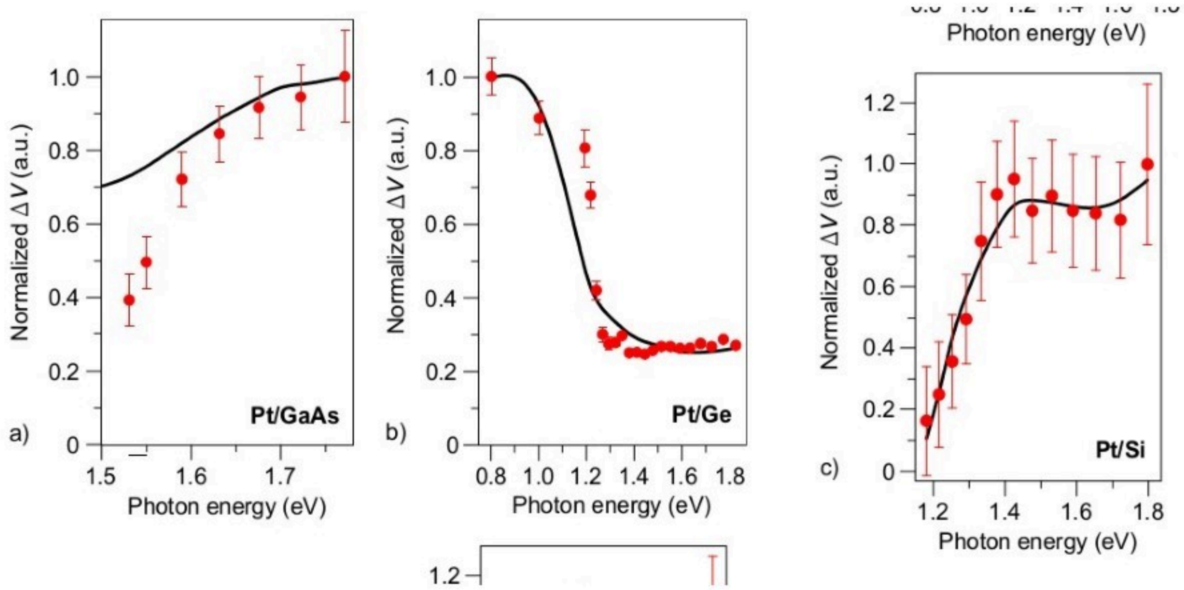
Charge drift-diffusion equations

Current eq.	Continuity eq.	Poisson
$J_n = -D_n \frac{\partial n}{\partial x} - \mu_n n E$	$\frac{\partial J_n}{\partial x} = SRH + \Phi_0 \alpha e^{-\alpha x}$	$\frac{\partial E}{\partial x} = \frac{q}{\epsilon}(p + N_d - n)$
$J_p = -D_p \frac{\partial p}{\partial x} + \mu_p p E$	$\frac{\partial J_p}{\partial x} = SRH + \Phi_0 \alpha e^{-\alpha x}$	$SRH = w(x)(n_i^2 - np)$

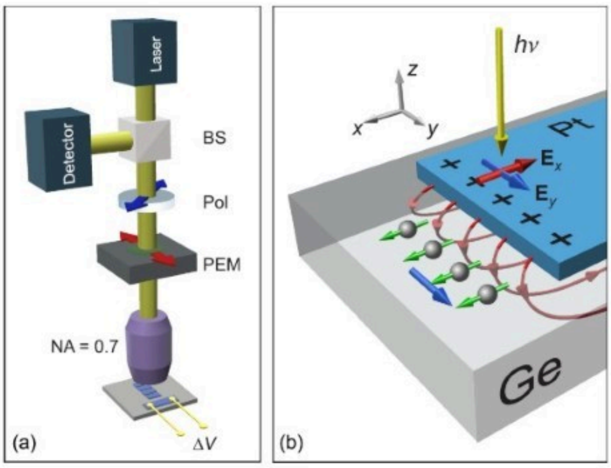
Spin drift-diffusion equations

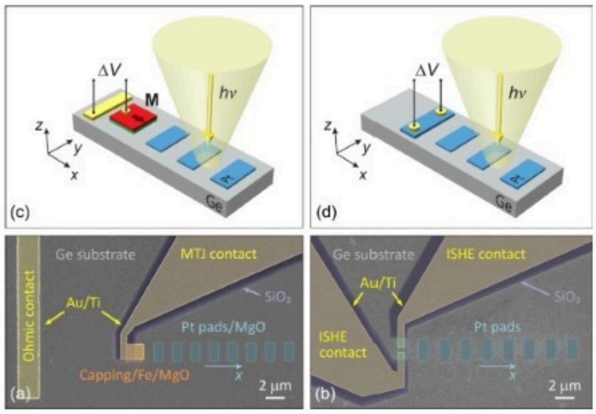
Definitions	Current eq.	Continuity eq.
$s = n_+ - n_-$ $J_s = J_{n+} - J_{n-}$	$J_s = -D_n \frac{\partial s}{\partial x} - \mu_n s E$	$\frac{\partial J_s}{\partial x} = \frac{-s}{\tau_s} - w(sp) + P \Phi_0 \alpha e^{-\alpha x}$

Photo induced inverse spin Hall effect



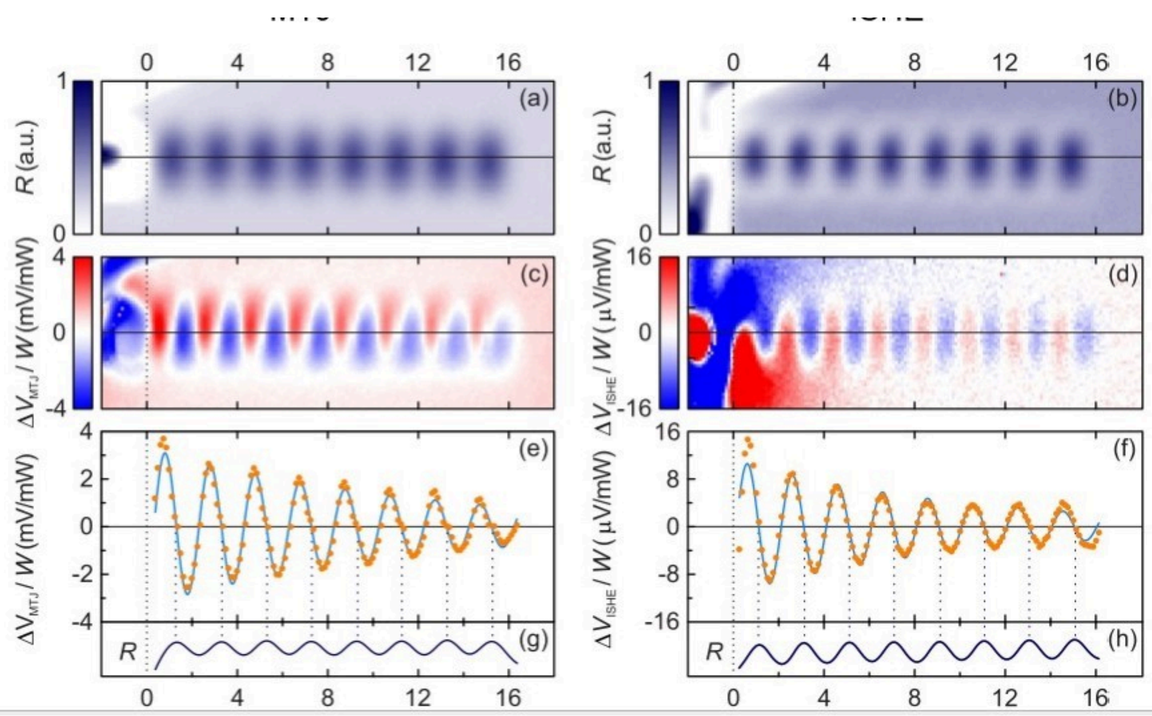
Imaging spin diffusion





Imaging spin diffusion

MTJ ISHE



(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
R (a.u.)
ΔV_{MTJ} / W (mV/mW)
ΔV_{ISHE} / W (μV/mW)
R