Intrinsic spin Hall effect
in semiconductors and metals:
Ab initio calculations and model studies

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Plan of this Talk

I. Introduction
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   3. Motivations

II. Theory and computational method
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   2. \textit{Ab initio} relativistic band structure method.

III. Spin and orbital-angular-momentum Hall effects in \textit{p}-type zincblende semiconductors

IV. Strain dependence of spin Hall effect in \textit{n}-type wurtzite semiconductors

V. Intrinsic spin Hall effect in platinum metal
I. Introduction

1. Basic elements of spintronics (spin electronics)

Spin currents:

generation,
detection,
manipulation (control).
Usual spin current generations:

**Ferromagnetic leads especially half-metals**

Schematic band pictures of (a) non-magnetic metals, (b) ferromagnetic metals and (c) half-metallic metals.

**Spin filter**

[Slobodsky, et al., PRL 2003]

Problems: magnets and/or magnetic fields needed, and difficult to integrate with semiconductor technologies.
2. Spin Hall effect

1) The Hall Effect

Ordinal Hall Effect (1879)

\[ \rho_{\text{Hall}} = R_0 B \]

Anomalous Hall Effect (Hall, 1880 & 1881)  
(Extraordinary or spontaneous Hall effect)

\[ \rho_{\text{Hall}} = R_0 B + R_s M \]
Zoo of the Hall Effects

Ordinary Hall effect (1879);

Anomalous Hall effect (1880 & 1881);

Integer quantum Hall effect (von Klitzing, et al., 1980);

Fractional quantum Hall effect (Tsui, et al., 1982);

(Extrinsic) spin Hall effect (Dyakonov+Perel, 1971; Hirsch, 1999);

Intrinsic spin Hall effect (Murakami, et al., 2003, Sinova, et al., 2004).

Hall effect of light (Nagaosa, et al., 2004)

Thermal Hall effect (??)
2) (Extrinsic) Spin Hall Effect

(Extrinsic) spin Hall effect

\[ V = V_c(r) + V_{so}(r) \sigma \cdot L \]

3) Intrinsic spin Hall effect

(1) In p-type bulk semiconductors

\[ H_0 = \frac{\hbar^2}{2m}\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2(k\cdot S)^2 \]
Spin current

\[ j_j^i = \sigma_s \epsilon^{ijk} E_k \]  

(1)

\[ j_y^x = \frac{e E_z}{12 \pi^2 (3 k^H_F - k^L_F)} = \frac{\hbar}{2e} \sigma_s E_z \]  

(10)

\[ n_h = 10^{19} \text{ cm}^{-3}, \quad \mu = 50 \text{ cm/Vs}, \quad \sigma = e \mu n_h = 80 \ \Omega^{-1}\text{cm}^{-1}; \]
\[ \sigma_s = 80 \ \Omega^{-1}\text{cm}^{-1} \]

\[ n_h = 10^{16} \text{ cm}^{-3}, \quad \mu = 50 \text{ cm/Vs}, \quad \sigma = e \mu n_h = 0.6 \ \Omega^{-1}\text{cm}^{-1}; \]
\[ \sigma_s = 7 \ \Omega^{-1}\text{cm}^{-1} \]
(2) In a 2-D electron gas in n-type semiconductor heterostructures

**Rashba Hamiltonian**

\[ H = \frac{p^2}{2m} - \frac{\lambda}{\hbar} \vec{\sigma} \cdot (\hat{z} \times \vec{p}) \]  \hspace{1cm} (1)

contributes to the spin current. In this case we find that the spin current in the \( \hat{y} \) direction is [23]

\[ j_{s,y} = \int_{\text{shells}} \frac{d^3 \vec{p}}{(2\pi \hbar)^3} \left\{ \frac{\hbar}{m} \right\} \frac{e}{2} \frac{E_\parallel}{16\pi \alpha m} (p_{F,+} - p_{F,-}). \]  \hspace{1cm} (6)

where \( p_{F,+} \) and \( p_{F,-} \) are the Fermi momenta of the majority and minority spin Rashba bands. We find that when both bands are occupied, i.e., when \( n_{3D} > m^2 \lambda^2 / \pi \hbar^2 = n_{3D}^0, \) \( p_{F,+} - p_{F,-} = 2m \lambda / \hbar \) and then the spin Hall (sH) conductivity is

\[ \sigma_{sH} = -j_{s,y} \frac{E_\parallel}{E_s} = \frac{e}{8\pi}. \]  \hspace{1cm} (7)

independent of both the Rashba coupling strength and of the 2DES density. For \( n_{3D} < n_{3D}^0 \) the upper Rashba band is depopulated. In this limit \( p_{F,-} \) and \( p_{F,+} \) are the interior and exterior Fermi radii of the lowest Rashba split band, and \( \sigma_{sH} \) vanishes linearly with the 2DES density:

\[ \sigma_{sH} = \frac{e}{8\pi} \frac{n_{3D}}{n_{3D}^0}. \]  \hspace{1cm} (8)

**Universal spin Hall conductivity**

**FIG. 1** (color online). (a) The 2D electronic eigenstates in a Rashba spin-orbit coupled system are labeled by momentum (green or light gray arrows). For each momentum the two eigenspinors point in the azimuthal direction (red or dark gray arrows). (b) In the presence of an electric field the Fermi surface (circle) is displaced an amount \( \pm eE_t \delta / \hbar \) at time \( t_0 \) (shorter than typical scattering times). While moving in momentum space, electrons experience an effective torque which tilts the spins up for \( p_{x} > 0 \) and down for \( p_{x} < 0 \), creating a spin current in the \( y \) direction.
(3) Significances of these theoretical discoveries of intrinsic spin Hall effects

Among other things, it would enable us to generate spin current electrically in semiconductor microstructures without applied magnetic fields or magnetic materials, and hence make possible pure electric driven spintronics in semiconductors which could be readily integrated with conventional electronics.
4) Experiments on spin Hall effect

(a) in n-type 3D GaAs and InGaAs thin films

Attributed to extrinsic SHE because of weak crystal direction dependence.

(b) in p-type 2D semiconductor quantum wells

Attributed to intrinsic SHE.
3. Motivations

In this work, we study intrinsic spin Hall effect in semiconductors and metals by performing *ab initio* calculations.

(1) Will the intrinsic spin Hall effect exactly cancelled by the intrinsic orbital-angular-momentum Hall effect?

\[
\mathcal{J}^{\text{spin}}_{\text{int}} = \frac{e}{8\pi} E; \\
\mathcal{J}^{\text{orbit}}_{\text{int}} = -\frac{e}{8\pi} E.
\]

[S. Zhang and Z. Yang, PRL 2005]

In conclusion, we have constructed a general framework for calculating intrinsic linear response coefficients. We have shown that the intrinsic spin Hall effect is accompanied by the intrinsic orbital-angular-momentum Hall effect so that the total angular momentum spin current is zero in a spin-orbit coupled system. The intrinsic spin Hall effect is not a source of spin currents because the intrinsic spin current is not transportable. Most of the proposed experimental detections of the intrinsic spin Hall effect are the artifact of the boundary conditions that are not valid for the intrinsic spin Hall current.
(2) To go beyond the spherical 4-band Luttinger Hamiltonian.

(3) To understand the effects of epitaxial strains.

(4) To determine Rashba and Dresselhaus spin-orbit couplings in polar semiconductors, e. g., wurtzite.
(5) Spin Hall effect in transition metals

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**Direct electronic measurement of the spin Hall effect**

S. O. Valenzuela & M. Tinkham

fcc Al

$\sigma_{SH} = 27\sim34 \ (\Omega \text{ cm})^{-1}$

$(T= 4.2 \text{ K})$
II. Theory and Computational Method

1. Berry phase and semiclassical transport theory

(1) Berry phase

Parameter dependent system:
\[ \{ \epsilon_n(\lambda), \psi_n(\lambda) \} \]

Adiabatic theorem:
\[ \Psi(t) = \psi_n(\lambda(t)) e^{-it \int_0^t dt' \epsilon_n / \hbar} e^{-i\gamma_n(t)} \]

Geometric phase:
\[ \gamma_n = \int_{\lambda_0}^{\lambda_1} d\lambda \langle \psi_n | i \frac{\partial}{\partial \lambda} | \psi_n \rangle \]
Well defined for a closed path

\[ \gamma_n = \oint_C d\lambda \langle \psi_n | i \frac{\partial}{\partial \lambda} | \psi_n \rangle \]

Stokes theorem

\[ \gamma_n = \int \int d\lambda_1 d\lambda_2 \Omega \]

Berry Curvature

\[ \Omega = i \frac{\partial}{\partial \lambda_1} \langle \psi | \frac{\partial}{\partial \lambda_2} | \psi \rangle - i \frac{\partial}{\partial \lambda_2} \langle \psi | \frac{\partial}{\partial \lambda_1} | \psi \rangle \]
Analogies

Berry curvature
\[ \Omega(\tilde{\lambda}) \]
Berry connection
\[ \langle \psi | i \frac{\partial}{\partial \lambda} | \psi \rangle \]
Geometric phase
\[ \oint d\lambda \langle \psi | i \frac{\partial}{\partial \lambda} | \psi \rangle = \iint d^2 \lambda \ \Omega(\tilde{\lambda}) \]
Chern number
\[ \iiint d^2 \lambda \ \Omega(\tilde{\lambda}) = \text{integer} \]

Magnetic field
\[ B(\vec{r}) \]
Vector potential
\[ A(\vec{r}) \]
Aharonov-Bohm phase
\[ \oint dr \ A(\vec{r}) = \iint d^2 r \ B(\vec{r}) \]
Dirac monopole
\[ \iiint d^2 r \ B(\vec{r}) = \text{integer } h/e \]
Symmetry properties

Time reversal: \[ \Omega(-\mathbf{k}) = -\Omega(\mathbf{k}) \]

Space inversion: \[ \Omega(-\mathbf{k}) = \Omega(\mathbf{k}) \]

Both: \[ \Omega(\mathbf{k}) = 0 \]

Violation: e.g., ferromagnets, zincblende crystal
(2) Semiclassical dynamics of Bloch electrons

Old version [e.g., Aschroft, Mermin, 1976]

\[ \dot{x}_c = \frac{1}{\hbar} \frac{\partial \varepsilon_n (k)}{\partial k}, \]

\[ \dot{k} = -\frac{e}{\hbar} E - \frac{e}{\hbar} \dot{x}_c \times B = \frac{e}{\hbar} \frac{\partial \varphi (r)}{\partial r} - \frac{e}{\hbar} \dot{x}_c \times B. \]

Berry phase correction [e.g., Chang & Niu, PRL (1995), PRB (1996)]

New version [Marder, 2000]

\[ \dot{x}_c = \frac{1}{\hbar} \frac{\partial \varepsilon_n (k)}{\partial k} - \dot{k} \times \Omega_n (k), \]

\[ \dot{k} = \frac{e}{\hbar} \frac{\partial \varphi (r)}{\partial r} - \frac{e}{\hbar} \dot{x}_c \times B, \]

\[ \Omega_n (k) = - \text{Im} \left\langle \frac{\partial u_{nk}}{\partial k} \big| \times \big| \frac{\partial u_{nk}}{\partial k} \right\rangle. \text{ (Berry curvature)} \]
(3) Semiclassical transport theory

\[ j = \int d^3k (-e \dot{x}) g(r, k) \]

\[ \dot{x} = \frac{\partial \varepsilon_n(k)}{\hbar \partial k} + \frac{e}{\hbar} E \times \Omega \]

\[ g(r, k) = f(k) + \delta f(r, k) \]

\[ j = -\frac{e^2}{\hbar} E \times \int d^3k f(k) \Omega - \frac{e}{\hbar} \int d^3k \delta f(k, r) \frac{\partial \varepsilon_n(k)}{\partial k} \]

(Anomalous Hall conductance) (ordinary conductance)
Anomalous Hall conductivity [Yao, et al., PRL 2004]

\[
\sigma_{xy} = \frac{e^2}{\hbar} \int d^3k \sum_n f(\varepsilon_n(k)) \Omega^z_n(k)
\]

\[
\Omega^z_n(k) = -\sum_{n' \neq n} \frac{2 \text{Im} \langle kn | v_x | kn' \rangle \langle kn' | v_y | kn \rangle}{(\omega_{kn'} - \omega_{kn})^2}
\]

FM bcc Fe
The Anomalous Hall Effect and Magnetic Monopoles in Momentum Space

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Atsushi Asamitsu,1,6 Roland Mathieu,1 Takeshi Ogasawara,3
Hiroyuki Yamada,3 Masashi Kawasaki,3,7 Yoshinori Tokura,1,3,4
Kiyoyuki Terakura8

Efforts to find the magnetic monopole in real space have been made in cosmic rays and in particle accelerators, but there has not yet been any firm evidence for its existence because of its very heavy mass, \( \sim 10^{16} \) giga-electron volts. We show that the magnetic monopole can appear in the crystal momentum space of solids in the accessible low-energy region (\( \sim 0.1 \) to 1 electron volts) in the context of the anomalous Hall effect. We report experimental results together with first-principles calculations on the ferromagnetic crystal \( \text{SrRuO}_3 \) that provide evidence for the magnetic monopole in the crystal momentum space.
(4) Berry phase formalism for Hall effects

\[ \sigma_{xy} = \frac{e}{\hbar} \int d^3k \sum_n f(\varepsilon_n(k)) \Omega_n^z(k) \]

\[ \Omega_n^z(k) = \sum_{n' \neq n} \frac{2 \text{Im} \langle kn | j_x | kn' \rangle \langle kn' | v_y | kn \rangle}{(\omega_{kn} - \omega_{kn'})^2} \]

Current operator \( j_x = -e v_x \) (AHE),

\[ j_x = \hbar \{ L_z, v_x \}/4 \] (SHE),

\[ j_x = \hbar \{ L_z, v_x \}/4 \] (OHE).
2. *Ab initio* relativistic band structure method

Calculations must be based on a relativistic band theory because all the intrinsic Hall effects are caused by spin-orbit coupling.

Fully relativistic extension of linear muffin-tin orbital (LMTO) method. [Ebert, PRB 1988; Guo, Ebert, PRB 1995]

Dirac Hamiltonian

velocity operator \( \mathbf{v} = c \gamma \),
current operator \( \mathbf{j} = -ec \gamma \) (AHE),
\[
\mathbf{j} = \frac{\hbar}{4} \{ \beta \Sigma, c \alpha \} \text{(SHE)},
\]
\[
\mathbf{j} = \frac{\hbar}{2} \{ \beta L_z, c \alpha \} \text{(OHE)}.
\]

\( \gamma, \alpha, \beta \) are 4x4 Dirac matrices.
Density functional theory with generalized gradient approximation (DFT-GGA).

The number of $k$-points in the IW (3/48 of BZ) for Si and Ge used is 49395 and for AlAl and GaAs is 98790 (6/48) (56 divisions of Γ-X).

TABLE 1: Experimental lattice constant $a$ (see [20] and references therein), average atomic sphere radius $R_{\text{avg}}$ and band gap $E_g$ (see [21] and references therein) of the semiconductors studied. The calculated band gaps $E_g^{\text{the}}$ and spin-orbit splitting $\Delta_{so}$ of the top valence bands at $\Gamma$ are also listed.

<table>
<thead>
<tr>
<th></th>
<th>$a$ (Å)</th>
<th>$R_{\text{avg}}$ (Å)</th>
<th>$E_g$ (eV)</th>
<th>$E_g^{\text{the}}$ (eV)</th>
<th>$\Delta_{so}$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>5.431</td>
<td>2.526</td>
<td>1.17</td>
<td>0.81</td>
<td>47</td>
</tr>
<tr>
<td>Ge</td>
<td>5.630</td>
<td>2.632</td>
<td>0.74</td>
<td>0.28</td>
<td>278</td>
</tr>
<tr>
<td>AlAs</td>
<td>5.620</td>
<td>2.615</td>
<td>2.23</td>
<td>1.52</td>
<td>301</td>
</tr>
<tr>
<td>GaAs</td>
<td>5.654</td>
<td>2.632</td>
<td>1.52</td>
<td>0.76</td>
<td>336</td>
</tr>
</tbody>
</table>

Scizzor’s approximation.
III. Spin and orbital-angular-momentum Hall effects in $p$-type zincblende semiconductors

[Guo, Yao, Niu, PRL 94, 226601 (2005)]

1. dc Hall conductivity

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_{xy}^{SH} (\hbar/\Omega \text{cm})$</th>
<th>$\sigma_{xy}^{OH} (\hbar/\Omega \text{cm})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_h = 0.0$</td>
<td>0.4</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>-0.2</td>
</tr>
<tr>
<td>Si</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ge</td>
<td>9.0</td>
<td>63.1</td>
</tr>
<tr>
<td>GaAs</td>
<td>10.6</td>
<td>117.1</td>
</tr>
<tr>
<td>AlAs</td>
<td>2.5</td>
<td>111.5</td>
</tr>
<tr>
<td>$n_h = 0.0$</td>
<td>0.0</td>
<td>4.7</td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>1.4</td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>0.5</td>
</tr>
</tbody>
</table>
Spin Hall insulators
[Murakami, Nagaosa, Zhang, 2004 PRL93, 156804]

Undoped PbS
$\sigma_{xy}^s = 57.5 \ (\hbar/e) \ \Omega^{-1} cm^{-1}$

cubic zincblende structure

Spin-orbit gap
2. Effects of lattice mismatch strains

![Graph showing strained GaAs with different percentages of strain]

- For +2% strain:
  - 15nm Zn$_{0.95}$Be$_{0.05}$Se ($10^{19}$)
  - 10nm ZnSe (i)
  - 5nm Zn$_{0.7}$Be$_{0.3}$Se (i)
  - 5nm Zn$_{0.7}$Mn$_{0.3}$Se (i)
  - 10nm ZnSe (i)
  - 10nm Zn$_{0.35}$Be$_{0.65}$Se ($10^{15}$)

- For -2% strain:
  - 30nm ZnSe ($1.5 \times 10^{19}$)
  - Metal
  - 100nm ZnSe ($1.5 \times 10^{19}$)
  - 300nm Zn$_{0.79}$Be$_{0.15}$Se ($8 \times 10^{18}$)
  - GaAs Substrate
3. *ac* Hall conductivity

![Graph showing ac Hall conductivity for GaAs with different energy levels and carrier densities.](image)
IV. Strain dependence of spin Hall effect in \( n \)-type wurtzite semiconductors

[Chang, Chen, Chen, Hong, Tsai, Chen, Guo, PRL 98, 136403 (2007); 98, 239902 (2007) (Erratum)]

\( n \)-type (5nm \( \text{In}_x\text{Ga}_{1-x}\text{N}/3\text{nm GaN} \) superlattice (\( x=0.15 \))
FIG. 4. The degree of circular polarization as a function of excitation density and corresponding strain. The strain is calculated by the Raman spectra in Fig. 5. The in-plane electric field is applied in $-y$ direction.

$$P = \frac{I_{\sigma+} - I_{\sigma-}}{I_{\sigma+} + I_{\sigma-}}.$$  \hspace{1cm} (1)

$$\epsilon = \frac{\Delta \omega}{2a - 2b \frac{C_{13}}{C_{33}}},$$  \hspace{1cm} (2)
For wurtzite structures

\[
H_0 = \frac{\hbar^2 k^2}{2m^*} + (\alpha_e + \beta k^2)(\sigma_x k_y - \sigma_y k_x)
\]

\[
E_{\pm k} = \frac{\hbar^2 k^2}{2m^*} \mp (\alpha_e k + \beta k^3), \quad \alpha_e = \lambda + \alpha
\]
Linear response Kubo formalism

\[ \sigma_{xy}^{SH} = \frac{e}{8\pi} \left[ 1 + \frac{2}{3} \alpha_e \beta \left( \frac{2m^*}{h^2} \right)^2 \right] \approx \frac{e}{8\pi} \frac{2}{3} \alpha_e \beta \left( \frac{2m^*}{h^2} \right)^2 \]

\[ \square \]

\[ \Box (\text{exp}) \sim 0.06 \text{ (eVA)} \]

zero due to any disorder [Sinova, et al., SSC138 (2006) 214]
V. Large intrinsic spin Hall effect in platinum

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fcc Al

$\sigma_{\text{SH}} = 27\sim34 \; (\Omega \text{cm})^{-1} \; (T=4.2 \text{ K})$
Conversion of spin current into charge current at room temperature: Inverse spin-Hall effect

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Room Temperature Reversible Spin Hall Effect

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$\sigma_{sh} = 240 \text{ (}\Omega\text{ cm})^{-1}$

$(T= 290 \text{ K})$

Assumed to be extrinsic!
*Ab initio* relativistic band structure calculations

Pt: $\sigma_{sH} = 2200 \ (\Omega\ cm)^{-1} \ (T = 0 \ K)$

Al: $\sigma_{sH} = 17 \ (\Omega\ cm)^{-1} \ (T = 0 \ K)$

\[
\sigma_{xy} = \frac{e}{\hbar} \sum_k \Omega_z^\ell (k) = \frac{e}{\hbar} \sum_k \sum_n f(\varepsilon_n(k)) \Omega_z^\ell (k)
\]
\[
\Omega_z^\ell (k) = \sum_{n' \neq n} \frac{2 \text{Im} \langle kn | j_z^\ell | kn' \rangle \langle kn' | v_y | kn \rangle}{(\omega_{kn} - \omega_{kn'})^2}
\]

Pt: \( \sigma_{sh} (300K) = 240 \left( \frac{\Omega}{\text{cm}} \right)^{-1} \)
\( \sigma_{sh} \) (exp., RT) = 240 \( \left( \frac{\Omega}{\text{cm}} \right)^{-1} \)

Al: \( \sigma_{sh} (4.2 K) = 17 \left( \frac{\Omega}{\text{cm}} \right)^{-1} \)
\( \sigma_{sh} (300 K) = 6 \left( \frac{\Omega}{\text{cm}} \right)^{-1} \)
\( \sigma_{sh} \) (exp., 4.2K) = 27, 34 \( \left( \frac{\Omega}{\text{cm}} \right)^{-1} \)
Effect of impurity scattering and two band model analysis

Intrinsic SHE is robust against short-ranged impurity scattering!
Acknowledgements:

Collaborators:

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[on \(p\)-type zincblende semiconductors, PRL 94, 226601 (2005)]

Yang-Fang Chen + his exp. team (Nat’l Taiwan U.)

Tsung-Wei Chen (Nat’l Taiwan U.)
[on \(n\)-type wurtzite nitride semiconductors, PRL 98, 136403 (2007)]

Shuichi Murakami, Naoto Nagaosa (Tokyo U.)

Tsung-Wei Chen [on platinum, arXiv: 0705.0409]

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