Ab Initio Studies of Intrinsic Spin Hall Effect and Magnetic Nanostructures

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(A talk in Physics Dept., Natl. Tsing-Hua Univ., April 13, 2005)

Plan of this Talk

Part I. Intrinsic Spin Hall Effect in Semiconductors

Part II. Magnetic Nanostructures

Part I: *Ab Initio* Calculation of Intrinsic Spin Hall Effect in Semiconductors

-- spin current generation without magnetic field or magnetic materials --

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Outline of this first part of the talk

I. Introduction
   1. Basic elements in spintronics.
   2. Spin Hall effect.
   3. Motivations

II. Theory and Computational Method
   1. Kubo linear response theory.
   2. Relativistic band structure methods.

III. Calculated Spin and Orbital-Angular-Momentum Hall Effects in Semiconductors

   1. *dc* spin Hall effect.
   2. Effects of epitaxial strain.
   3. *ac* spin Hall effect.

IV. Conclusions

I. Introduction

1. Basic elements of spintronics

Spin currents:

Generation,
detection,
manipulation (control).

Usual spin current generations:

Ferromagnetic leads
especially half-metals

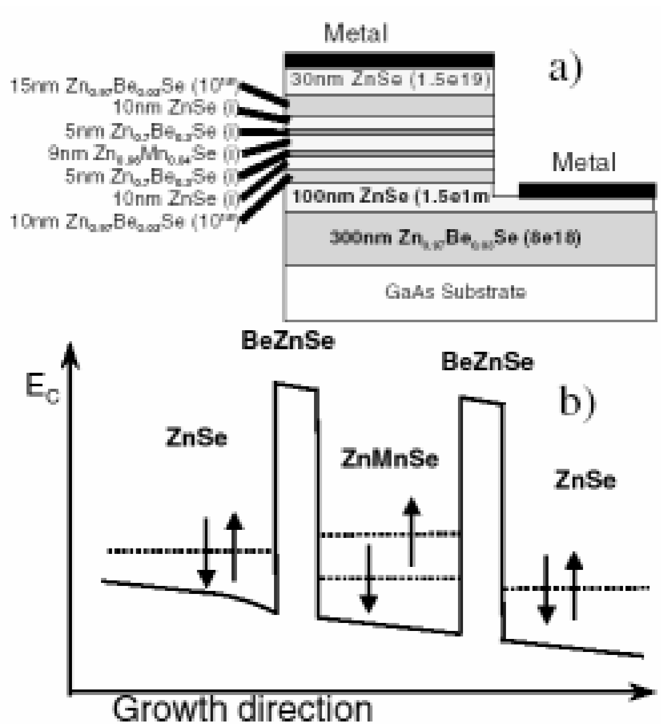
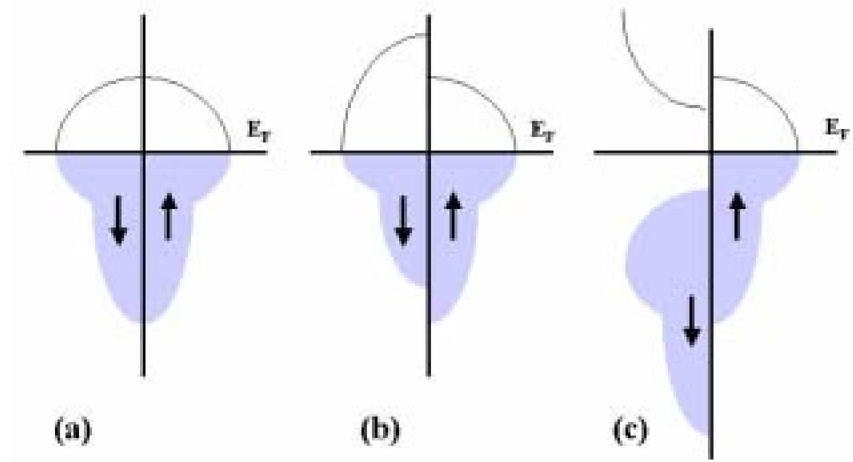


FIG. 1. (a) Layer structure of the device and (b) schematic view of resonant tunnel diode band structure under bias.



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

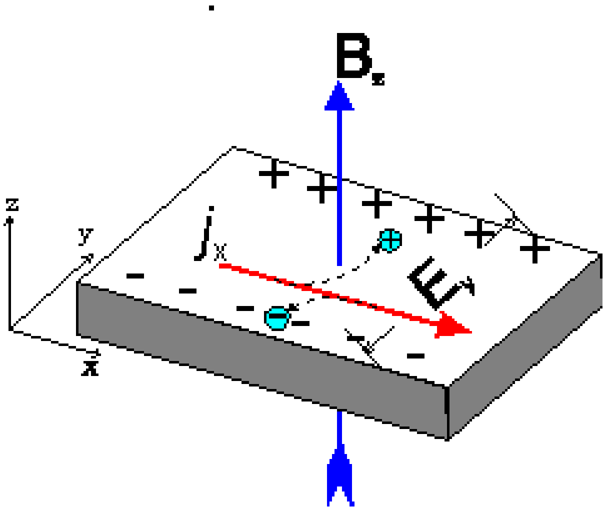
Spin filter

[Slobodskyy, 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)

$$\rho_{\mathrm{Hall}} = R_0 B$$

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

$$\rho_{\mathrm{Hall}} = R_0 B + R_S M$$

Zoo of the Hall Effects

Ordinary Hall effect (1879);

Anomalous Hall effect (1880 & 1881);

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

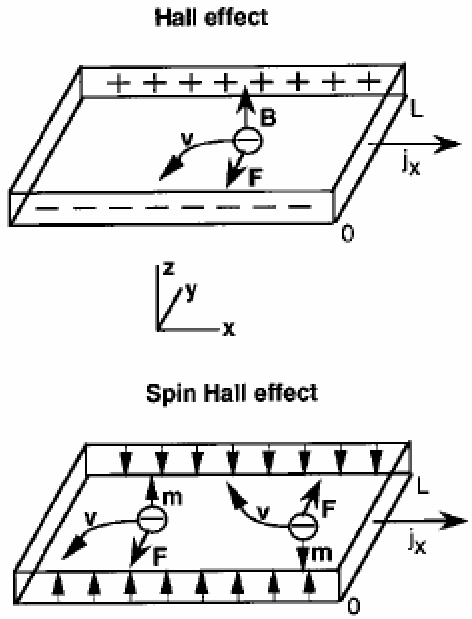
Fractional quantum Hall effect (Tsui, et al., 1982);

(Extrinsic) spin Hall effect (Hirsch, 1999);

Intrinsic spin Hall effect (Murakami, et al., 2003).
(Spontaneous and dissipationless)

2) (Extrinsic) Spin Hall Effect

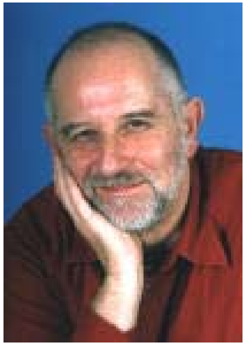
(Extrinsic) spin Hall effect



[Dyakonov & Perel, JETP 1971; Hirsch, PRL 1999; Zhang, PRL 2000]

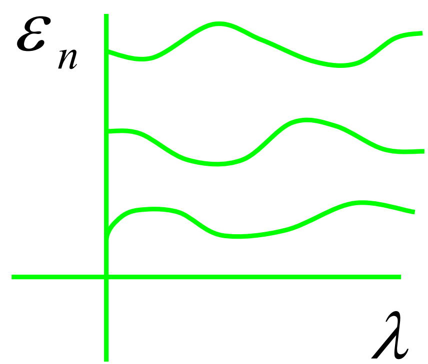
$$V = V_c(r) + V_{so}(r)\boldsymbol{\sigma}\cdot\mathbf{L}$$

3) Berry phase and semiclassical dynamics of electrons



(1) Berry phase

[Berry, Proc. Roy. Soc. London A 392, 451 (1984)]

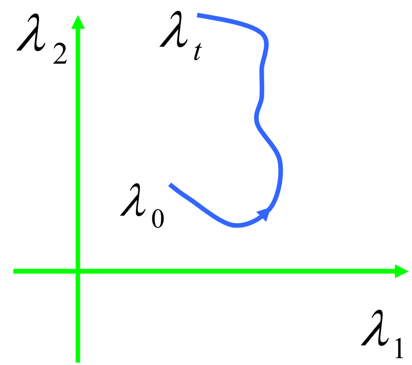


Parameter dependent system:

$$\{ \varepsilon_n(\lambda), \ \psi_n(\lambda) \}$$

Adiabatic theorem:

$$\Psi(t) = \psi_n(\lambda(t)) \ e^{-i\int_0^t dt \, \varepsilon_n/\hbar} \ e^{-i\gamma_n(t)}$$

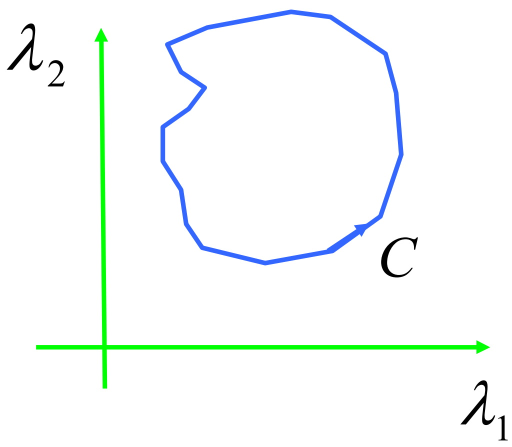


Geometric phase:

$$\gamma_n = \int_{\lambda_0}^{\lambda_t} d\lambda \, \langle \psi_n | i \frac{\partial}{\partial \lambda} | \psi_n \rangle$$

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

$$\gamma_n = \iint d\lambda_1 d\lambda_2 \, \Omega$$

Berry Curvature

$$\Omega = i \frac{\partial}{\partial \lambda_1} \langle \psi | \frac{\partial}{\partial \lambda_2} | \psi \rangle - i \frac{\partial}{\partial \lambda_2} \langle \psi | \frac{\partial}{\partial \lambda_1} | \psi \rangle$$

(2) Semiclassical dynamics of Bloch electrons

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

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

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

Berry phase correction [Chang & Niu, PRB (1996)]

New version [Marder, 2000]

$$\dot{\mathbf{x}}_c = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}_n(\mathbf{k}),$$

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

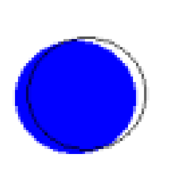
$$\mathbf{\Omega}_n(\mathbf{k}) = -\,\mathrm{Im}\left\langle \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \middle| \times \middle| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right\rangle.$$ (Berry curvature)

(3) Semiclassical transport theory

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

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

$$g(\mathbf{r},\mathbf{k}) = f(\mathbf{k}) + \delta f(\mathbf{r},\mathbf{k})$$



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

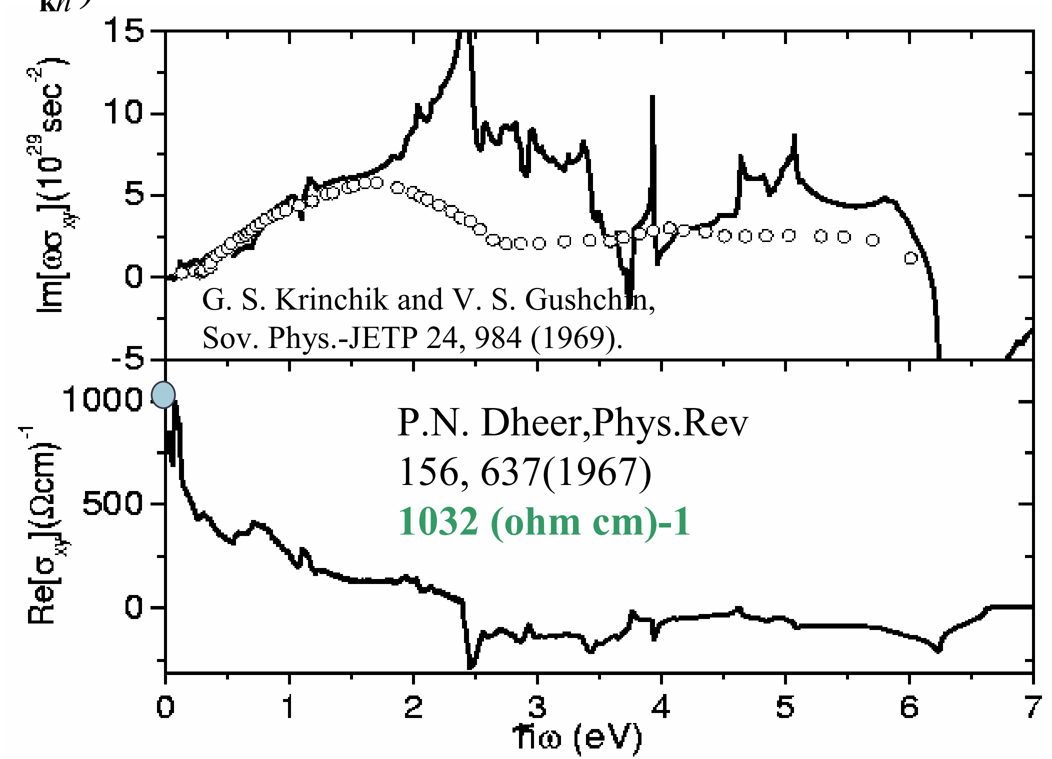
(Anomalous Hall conductance) (ordinary conductance)

Anomalous Hall conductivity [Yao, et al., PRL 2004]

$$\sigma_{xy} = -\frac{e^2}{\hbar}\int d^3\mathbf{k}\sum_n f(\varepsilon_n(\mathbf{k}))\Omega_n^z(\mathbf{k})$$

$$\Omega_n^z(\mathbf{k}) = -\sum_{n'\neq n}\frac{2\,\mathrm{Im}\langle \mathbf{k}n|v_x|\mathbf{k}n'\rangle\langle \mathbf{k}n'|v_y|\mathbf{k}n\rangle}{(\omega_{\mathbf{k}n'}-\omega_{\mathbf{k}n})^2}$$

FM bcc Fe



3) Intrinsic spin Hall effect

(1) In p-type bulk semiconductors

1348 5 SEPTEMBER 2003 VOL 301 SCIENCE www.sciencemag.org

Dissipationless Quantum Spin Current at Room Temperature

Shuichi Murakami,[1*] Naoto Nagaosa,[1,2,3] Shou-Cheng Zhang[4]

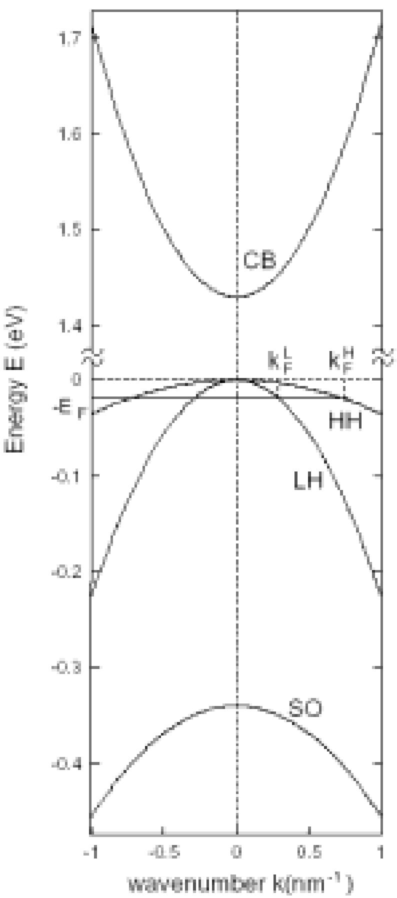
Luttinger Hamiltonian

$$H_0 = \frac{\hbar^2}{2m}\left(\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2(\mathbf{k}\cdot\mathbf{S})^2\right) \quad (2)$$

Spin current

$$j_j^i = \sigma_s \varepsilon^{ijk} E_k \quad (1)$$

$$j_y^x = \frac{eE_z}{12\pi^2}(3k_F^{\mathrm{H}} - k_F^{\mathrm{L}}) = \frac{\hbar}{2e}\sigma_s E_z \quad (10)$$



$n_h = 10^{19}$ cm^{-3}, $\mu = 50$ cm /V·s, $\sigma = e\,\mu\,n_h = 80\ \Omega^{-1}\mathrm{cm}^{-1}$; $\sigma_s = 80\ \Omega^{-1}\mathrm{cm}^{-1}$

$n_h = 10^{16}$ cm^{-3}, $\mu = 50$ cm /V·s, $\sigma = e\,\mu\,n_h = 0.6\ \Omega^{-1}\mathrm{cm}^{-1}$; $\sigma_s = 7\ \Omega^{-1}\mathrm{cm}^{-1}$

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(2) In a 2-D electron gas in n-type semiconductor heterostructures

Universal Intrinsic Spin Hall Effect

Jairo Sinova,[1,2] Dimitrie Culcer,[2] Q. Niu,[2] N. A. Sinitsyn,[1] T. Jungwirth,[2,3] and A. H. MacDonald[2]
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(Received 27 July 2003; published 25 March 2

Rashba Hamiltonian

$$H = \frac{p^2}{2m} - \frac{\lambda}{\hbar}\vec{\sigma}\cdot(\hat{z}\times\vec{p}), \qquad (1)$$

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

$$j_{s,y} = \int_{\text{annulus}} \frac{d^2\vec{p}}{(2\pi\hbar)^2}\frac{\hbar n_{z,\vec{p}}}{2}\frac{p_y}{m} = \frac{-eE_x}{16\pi\lambda m}(p_{F+} - p_{F-}), \qquad (6)$$

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 $n_{2D} > m^2\lambda^2/\pi\hbar^4 \equiv n_{2D}^*$, $p_{F+} - p_{F-} = 2m\lambda/\hbar$ and then the spin Hall (sH) conductivity is

Universal spin Hall conductivity

$$\sigma_{sH} \equiv -\frac{j_{s,y}}{E_x} = \frac{e}{8\pi}, \qquad (7)$$

independent of both the Rashba coupling strength and of the 2DES density. For $n_{2D} < n_{2D}^*$ 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 σ_{sH} vanishes linearly with the 2DES density:

$$\sigma_{sH} = \frac{e}{8\pi}\frac{n_{2D}}{n_{2D}^*}. \qquad (8)$$

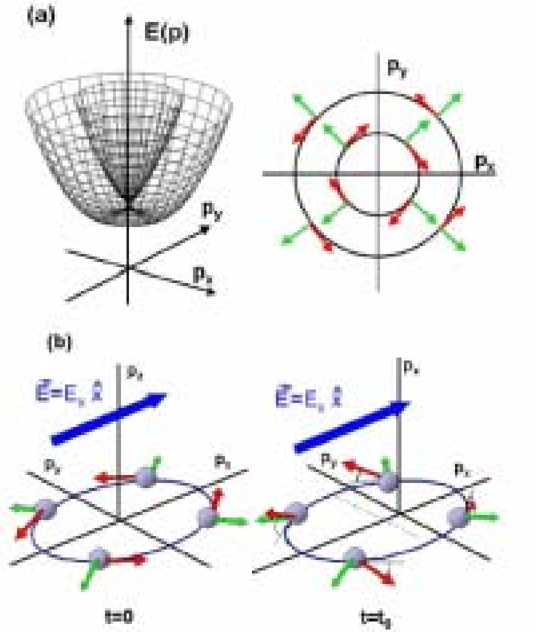


FIG. 1 (color online). (a) The 2D electronic eigenstates in a Rashba spin-orbit coupled system are labeled by momentum (green or light gray arrows). For each momentum the two eigenspinors point in the azimuthal direction (red or dark gray arrows). (b) In the presence of an electric field the Fermi surface (circle) is displaced an amount $|eE_xt_0/\hbar|$ 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 $p_y > 0$ and down for $p_y < 0$, 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 integated with conventional electronics.

3. Motivations

1) Questions concerning the intrinsic spin Hall Effects?

(1) Non-existence of intrinsic spin Hall effect in bulk *p*-type semiconductor?

[X. Wang and X.-G. Zhang, cond-mat/0407699]

In conclusion, we have shown that at least for a class of semiconductors described by the Luttinger Hamiltonian, spin symmetry of the eigenstates rules out the possibility of a spontaneous spin current in these materials. Thus, any attempt to produce such a spin current must include symmetry breaking terms in the Hamiltonian. This should provide important guidance to future attempts of finding a mechanism for spin currents in semiconductors.

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

[S. Zhang and Z. Yang, cond-mat/0407704]

$$\mathcal{J}_{int}^{spin} = \frac{e}{8\pi}E;$$

$$J_{int}^{orbit} = -\frac{e}{8\pi}E.$$

for Rashba Hamiltonian.

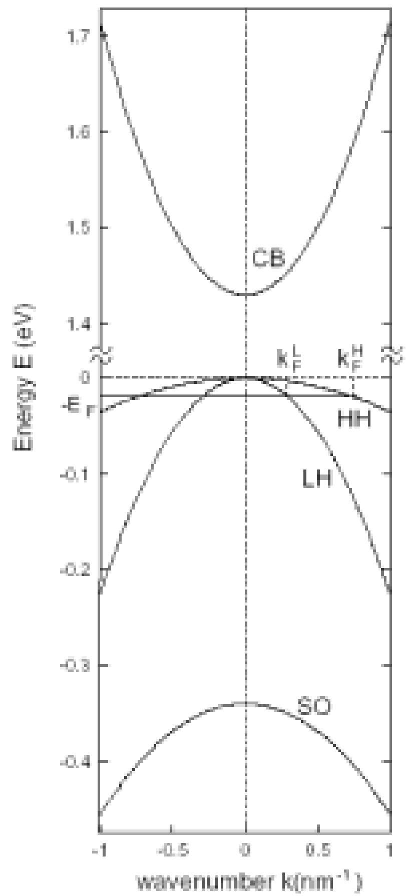
In conclusion, we have constructed a general framework for calculating intrinsic linear response coefficients. We have shown that the intrinsic spin Hall effect is accompanied by the intrinsic orbital-angular-momentum Hall effect so that the total angular momentum spin current is zero in a spin-orbit 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.

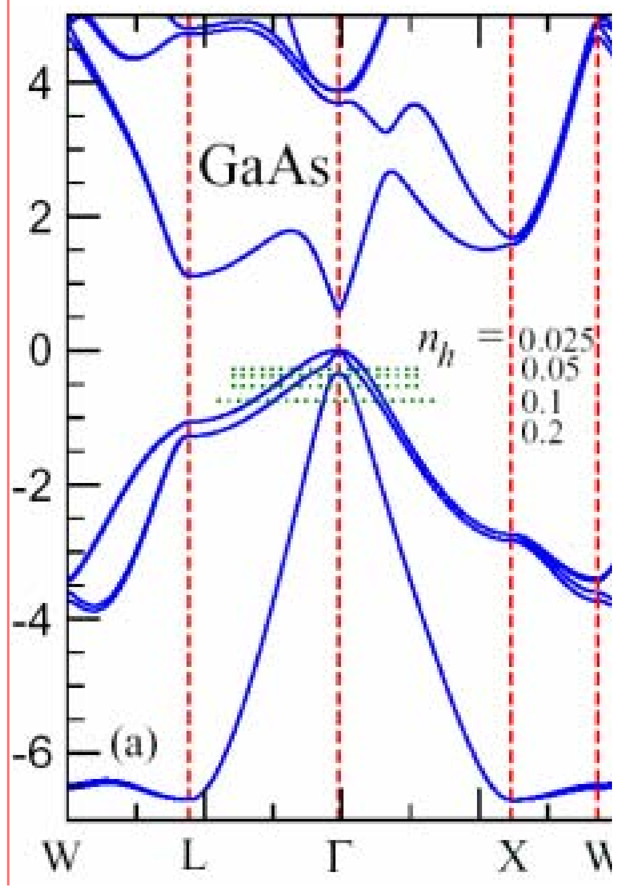
2) Motivations for the present work

(1) Try to resolve the above two important problems.

(2) To go beyond the spherical 4-band Luttinger Hamiltonian.

(3) To understand the effects of epitaxial strains.





II. Theory and Computational Method

1. Linear-response-theory Kubo formalism

Assume E-field along *x*-axis and spin or H-field along *z*-axis, the Hall conductivity (off-diagonal element) is [e.g., Marder, 2000]

$$\sigma_{xy}^{q}(\omega) = -\frac{e}{iV_c}\sum_{\mathbf{k}}\sum_{n\neq n'}\frac{f_{\mathbf{k}n}-f_{\mathbf{k}n'}}{\varepsilon_{\mathbf{k}n}-\varepsilon_{\mathbf{k}n'}}\frac{\langle \mathbf{k}n|v_x|\mathbf{k}n'\rangle\langle \mathbf{k}n'|j_y^q|\mathbf{k}n\rangle}{\varepsilon_{\mathbf{k}n}-\varepsilon_{\mathbf{k}n'}+\hbar\omega+i\eta} \qquad (1)$$

where V_c is the cell volume, |**k***n*> is the *n*th Bloch state with crystal momentum **k**, $\hbar\omega$ is the photon energy.

The intrinsic Hall effect comes from the static $\omega = 0$ limit:

$$\sigma_{xy}^{q} = -\frac{e}{V_c}\sum_{\mathbf{k}}\sum_{n\neq n'}(f_{\mathbf{k}n}-f_{\mathbf{k}n'})\frac{\mathrm{Im}[\langle \mathbf{k}n|v_x|\mathbf{k}n'\rangle\langle \mathbf{k}n'|j_y^q|\mathbf{k}n\rangle]}{(\varepsilon_{\mathbf{k}n}-\varepsilon_{\mathbf{k}n'})^2} \qquad (2)$$

current operator $j_y = -ev_y$ (AHE),

$j_y = \hbar\{\sigma_z, v_y\}/4$ (SHE),

$j_y = \hbar\{L_z, v_y\}/4$ (OHE).

Setting η to zero and using $\lim_{\eta\to 0}\frac{1}{\omega \pm i\eta} = \mathrm{P}\frac{1}{\omega} \mp i\pi\delta(\omega)$ (3),

Imaginary (part) Hall conductivity

$$\sigma''^{q}_{xy}(\omega) = \frac{\pi e}{\omega V_c}\sum_{\mathbf{k}}\sum_{n\neq n'}(f_{\mathbf{k}n} - f_{\mathbf{k}n'})\,\mathrm{Im}[\langle \mathbf{k}n \,|\, v_x \,|\, \mathbf{k}n'\rangle\langle \mathbf{k}n' |\, j^{q}_{y} \,|\, \mathbf{k}n\rangle]\delta(\varepsilon_{\mathbf{k}n'} - \varepsilon_{\mathbf{k}n} - \hbar\omega) \qquad (4).$$

Real (part) Hall conductivity is (Kramers-Kronig transformation)

$$\sigma'_{xy}(\omega) = \frac{2}{\pi}\mathrm{P}\int_0^\infty d\omega' \frac{\omega'\sigma''_{xy}(\omega')}{\omega'^2 - \omega^2} \qquad (5).$$

2. 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.

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

Dirac Hamiltonian $H_D = c\boldsymbol{\alpha}\cdot\mathbf{p} + mc^2(\beta - I) + v(\mathbf{r})$

velocity operator $\mathbf{v} = c\,\alpha$,
current operator $\mathbf{j} = -ec\,\alpha$ (AHE), $\mathbf{j} = \frac{\hbar}{4}\{\beta\Sigma_z, c\alpha\}$ (SHE), $\mathbf{j} = \frac{\hbar}{2}\{\beta L_z, c\alpha\}$ (OHE)
α, β, Σ are 4×4 Dirac matrices.

Density functional theory with generalized gradient approximation (DFT-GGA).

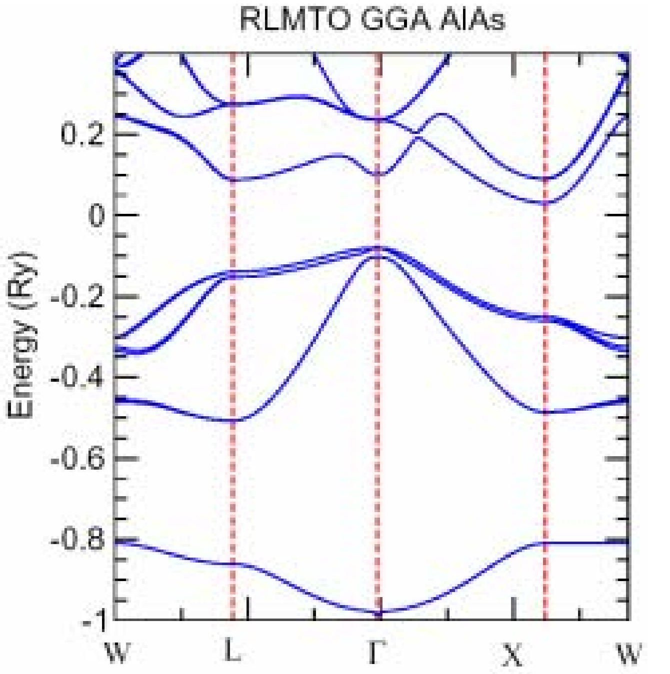
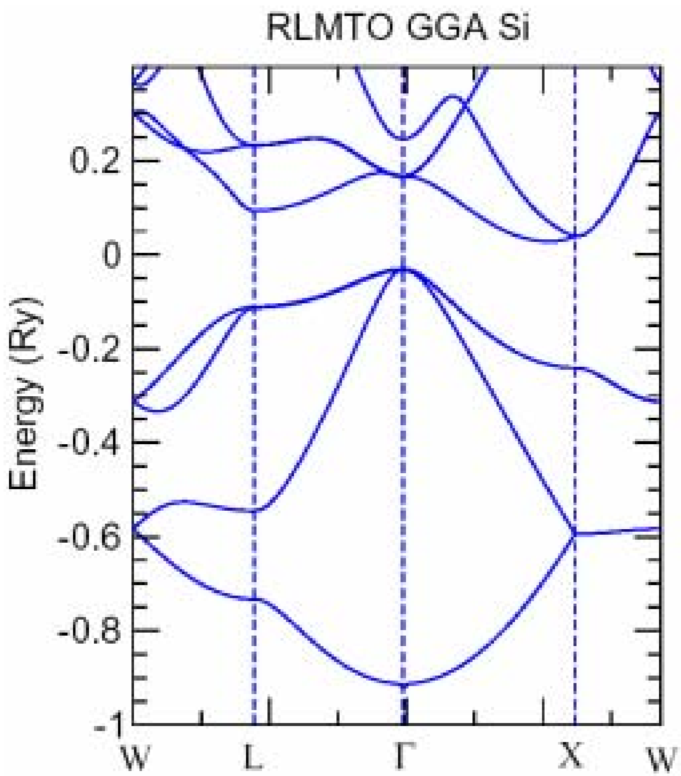
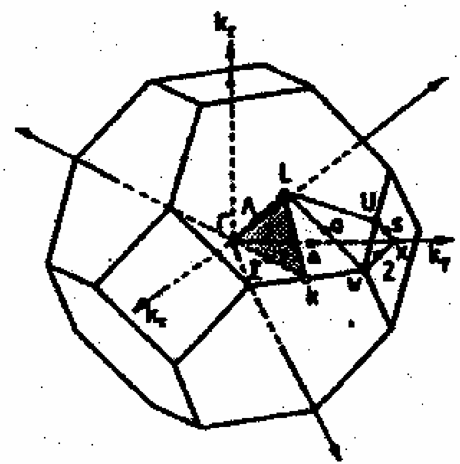
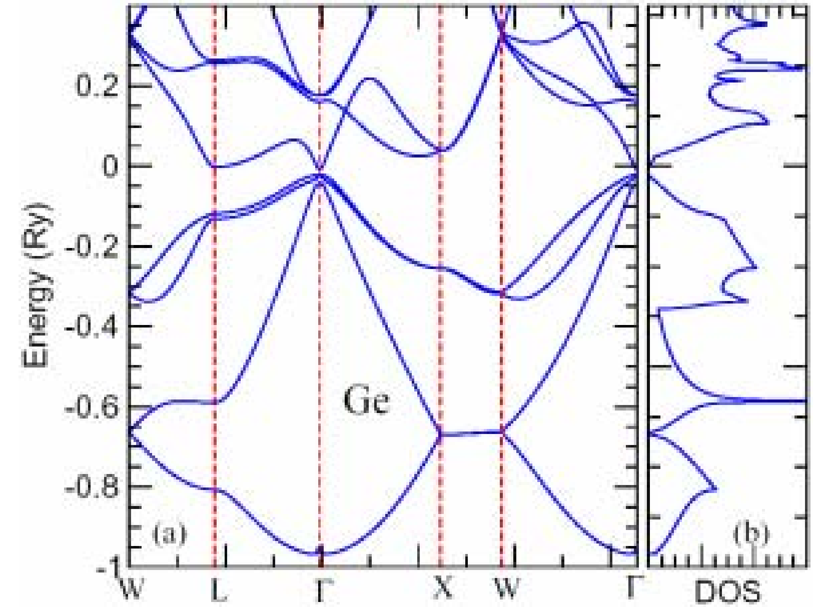


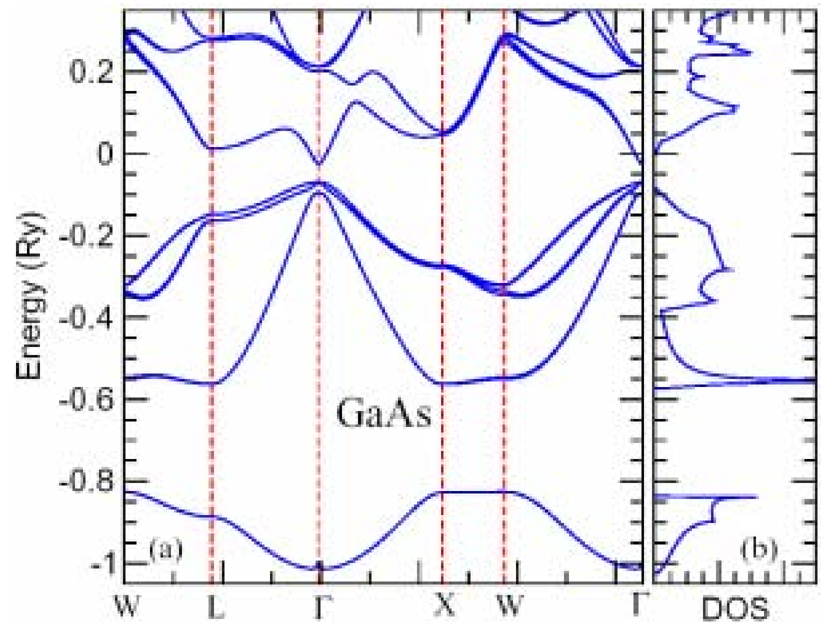
TABLE I: Experimental lattice constant a (see [20] and references therein), average atomic sphere radius R_{ws} and band gap E_g (see [21] and references therein) of the semiconductors studied. The calculated band gaps E_g^{the} and spin-orbit splitting Δ_{so} of the top valence bands at Γ are also listed.

	a (Å)	$R_{ws}(a.u.)$	E_g (eV)	E_g^{the} (eV)	Δ_{so} (meV)
Si	5.431	2.526	1.17	0.81	47
Ge	5.650	2.632	0.74	0.28	278
AlAs	5.620	2.615	2.23	1.52	301
GaAs	5.654	2.632	1.52	0.76	336


RLMTO GGA Si
Energy (Ry)
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
W
L
Γ
X
W


L
U
X
W


Energy (Ry)
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
Ge
(a)
(b)
W
L
Γ
X
W
Γ
DOS

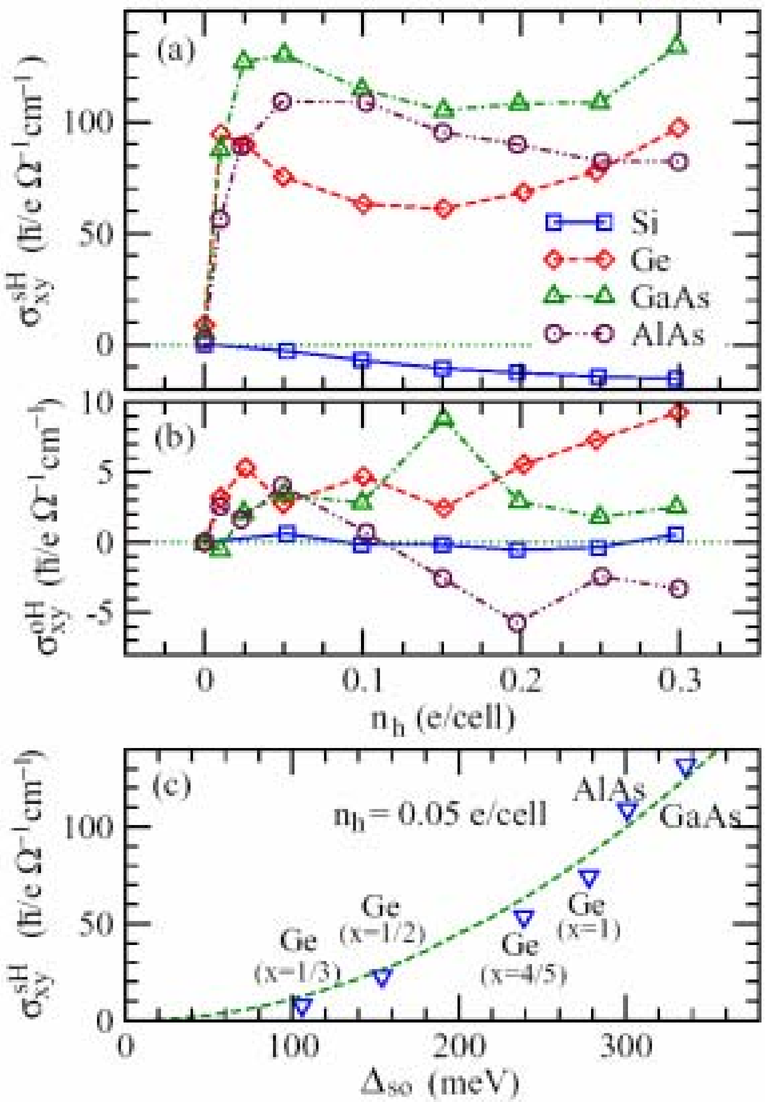

Energy (Ry)
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
GaAs
(a)
(b)
W
L
Γ
X
W
Γ
DOS

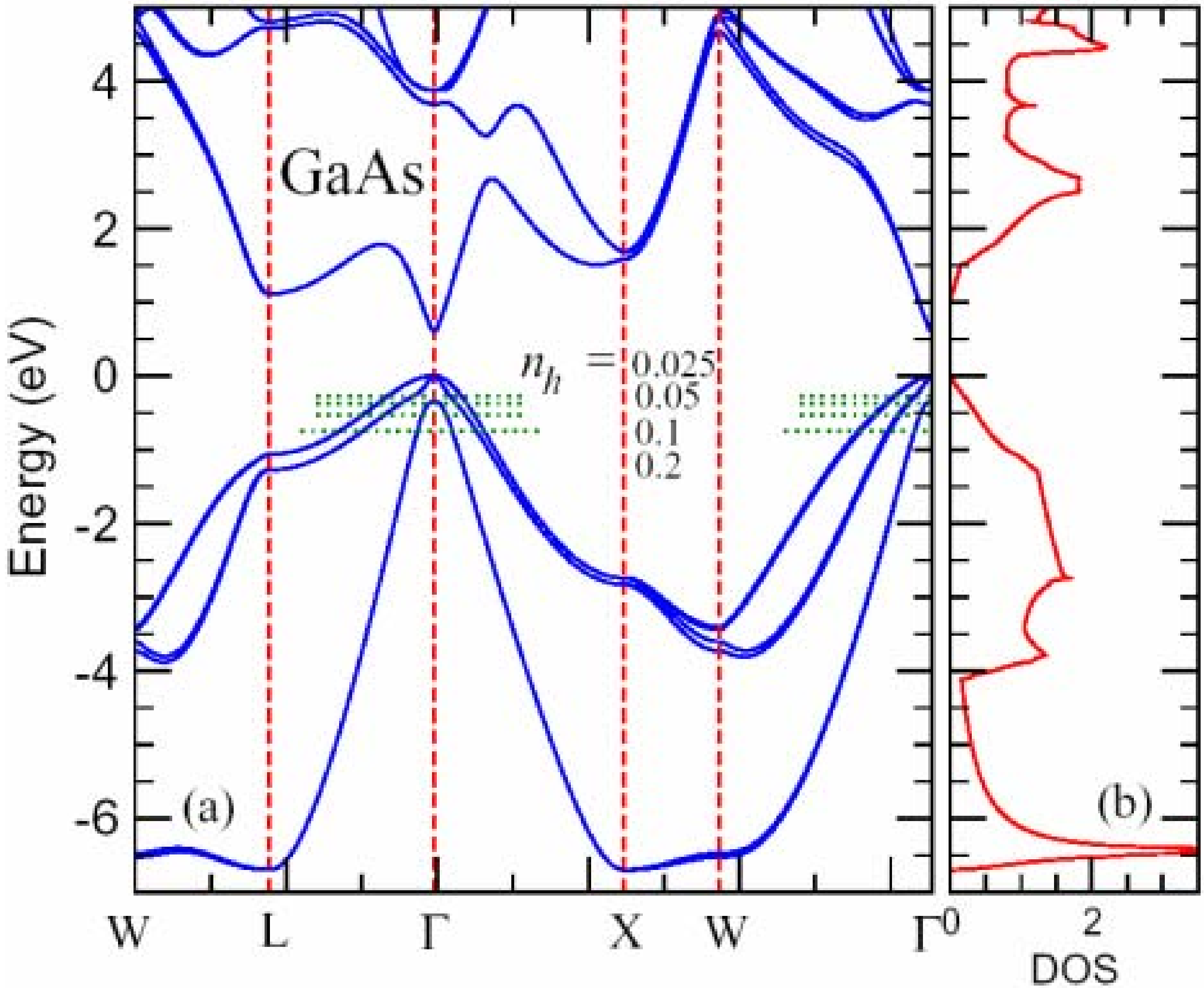
III. Calculated intrinsic spin and orbital-angular-momentum Hall effects

1. *dc* Hall conductivity

TABLE II: Calculated dc spin Hall (σ_{xy}^{sH}) and orbital-angular-momentum Hall (σ_{xy}^{oH}) conductivity of the hole-doped [n_h = 0.1 (e/f.u.)] and undoped [n_h = 0.0 (e/f.u.)] semiconductors.

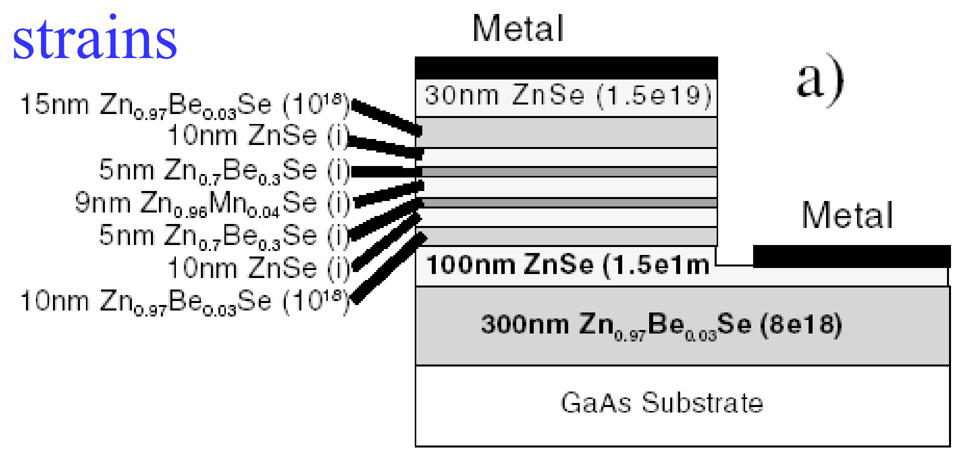
	σ_{xy}^{sH} ($\hbar$/eΩcm)		σ_{xy}^{oH} ($\hbar$/eΩcm)	
	n_h = 0.0	0.1 (e/f.u.)	n_h = 0.0	0.1 (e/f.u.)
Si	0.4	-6.9	0.0	-0.2
Ge	9.0	63.1	0.0	4.7
GaAs	10.6	117.1	0.0	1.4
AlAs	2.5	111.5	0.0	0.5

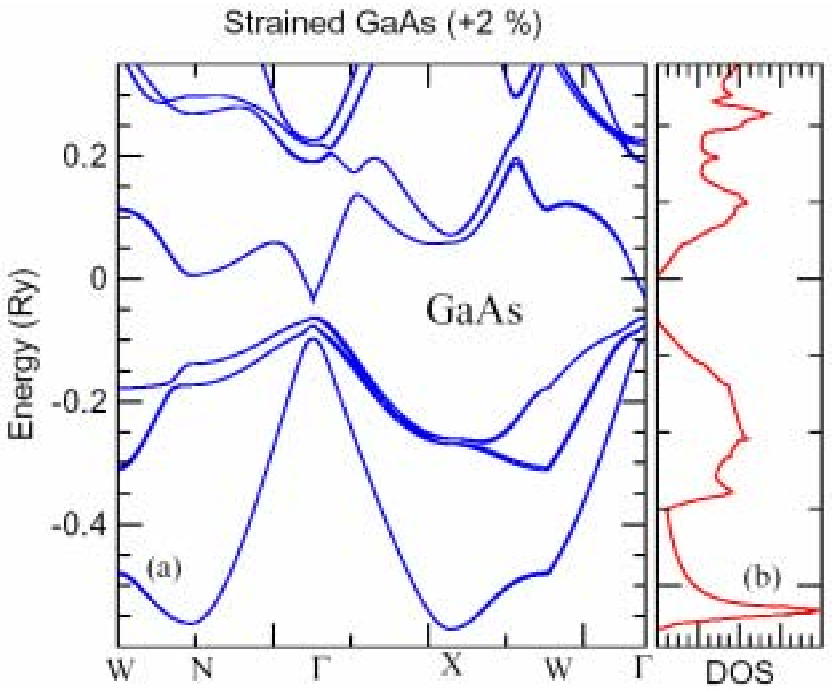


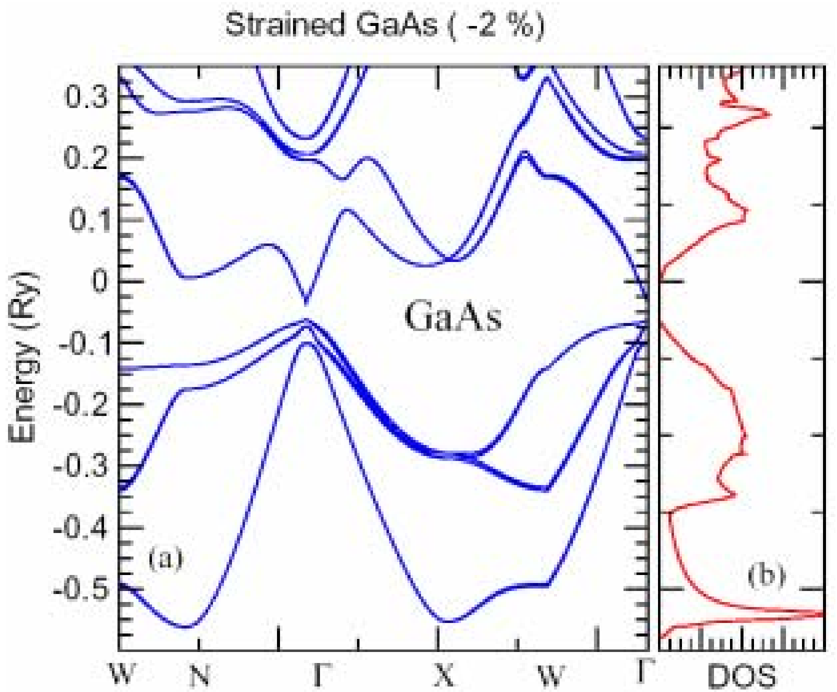


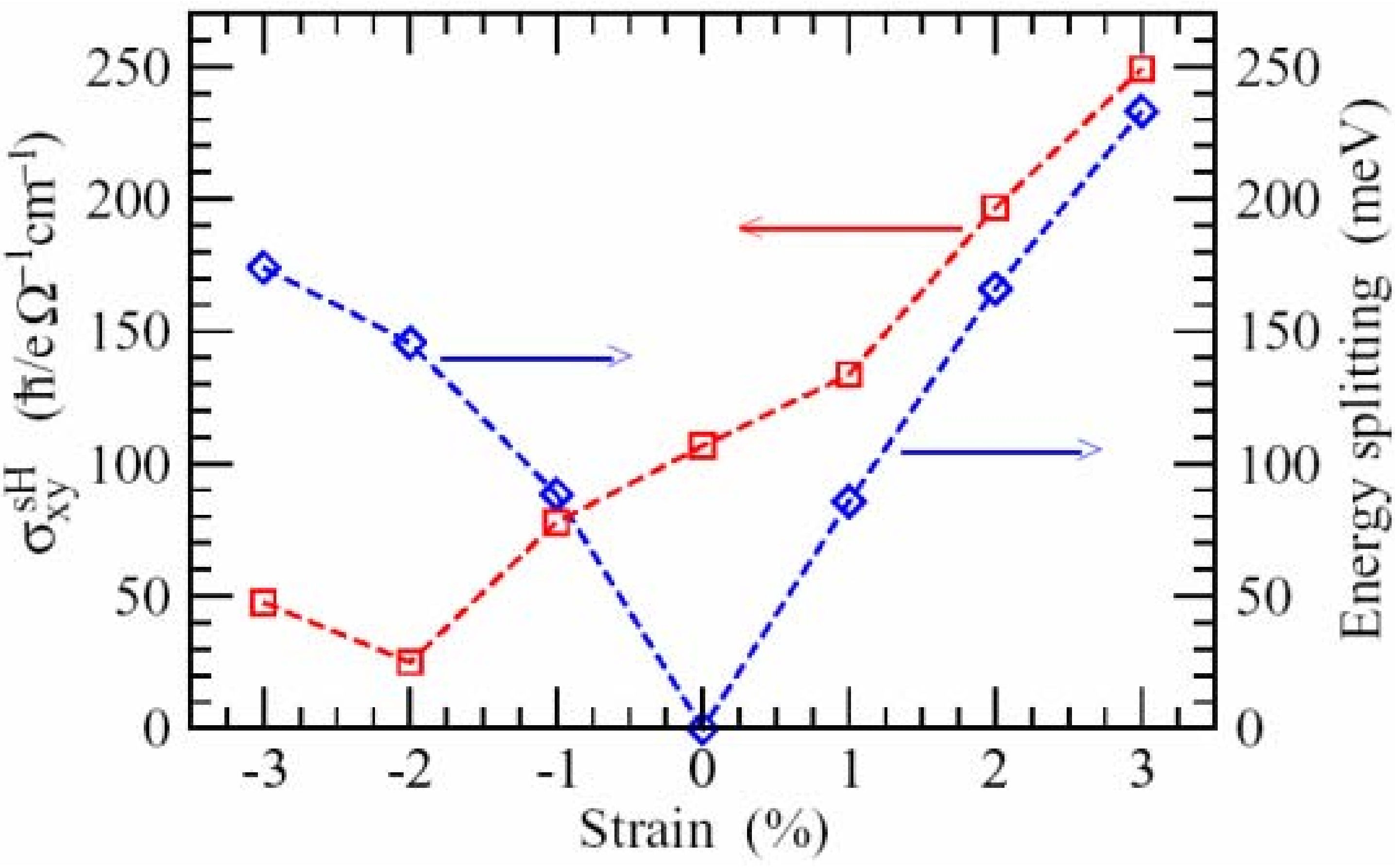
GaAs
Energy (eV)
n_h = 0.025
0.05
0.1
0.2
(a)
(b)
W
L
Γ
X
W
Γ
DOS
4
2
0
-2
-4
-6
0
2

2. Effects of lattice mismatch strains



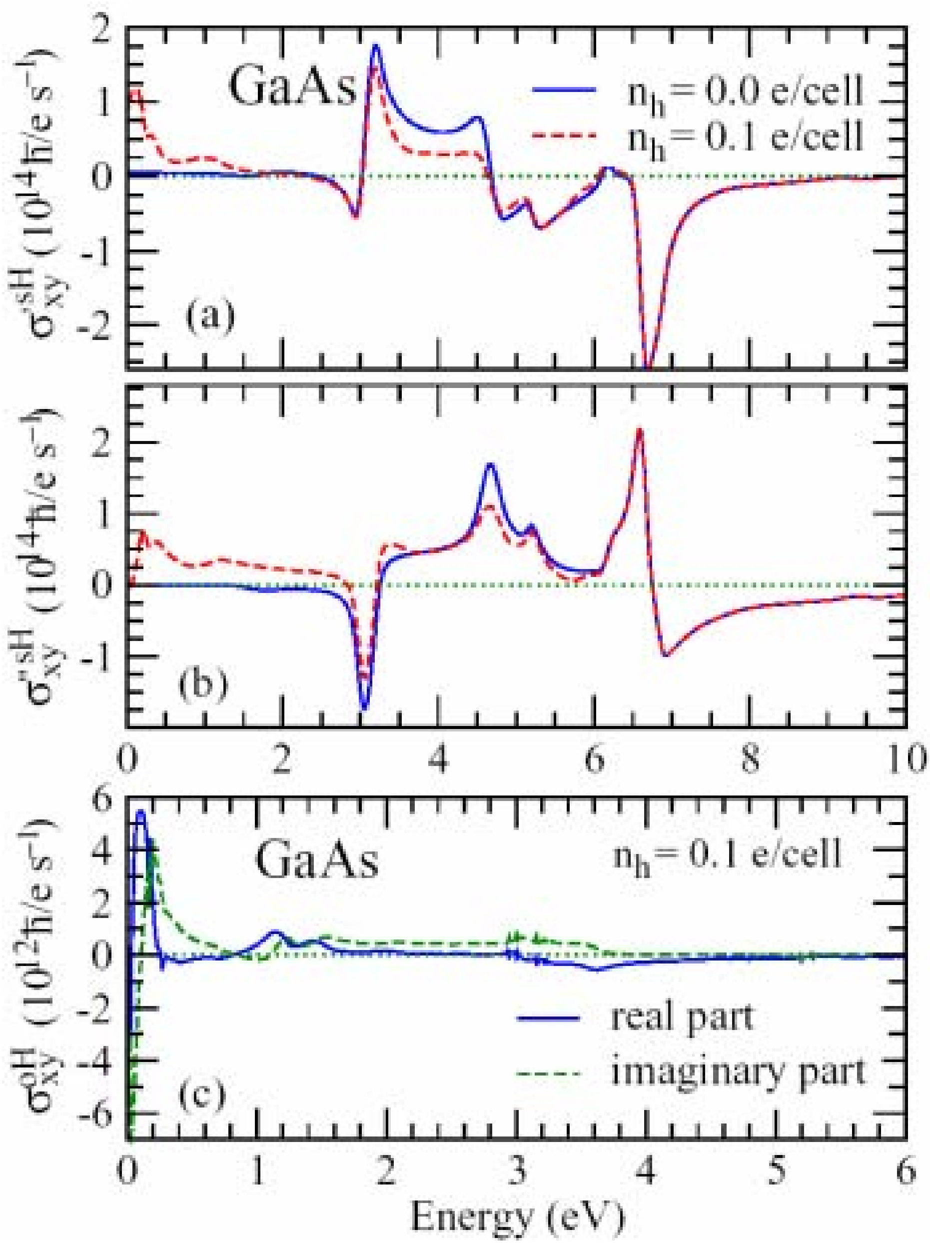






250
200
150
100
50
0
-3
-2
-1
0
1
2
3
Strain (%)
σ_{xy}^{sH} ($\hbar$/eΩ^{-1}cm^{-1})
Energy splitting (meV)

3. *ac* Hall conductivity



IV. Conclusions

1. Relativistic band theoretical calculations reveal that intrinsic spin Hall conductivity in hole-doped semiconductors Ge, GaAs and AlAs is large, showing the possibility of spin Hall effect beyond the Luttinger Hamiltonian.
2. The calculated orbital Hall conductivity is one order of magnitude smaller, indicating no cancellation between the spin and orbital Hall effects in bulk semiconductors.
3. The spin Hall effect can be strongly manipulated by strains.
4. The *ac* spin Hall conductivity is also large in pure as well as doped semiconductors.
5. The spin Hall effects in semiconductors have just been observed [Kato *et al.* (2004), Wunderlich *et al.* (2004)], another milestone in spintronics research, though the intrinsic or extrinsic nature needs to be established.

[Kato *et al.*, Science 306, 1910 (2004)]

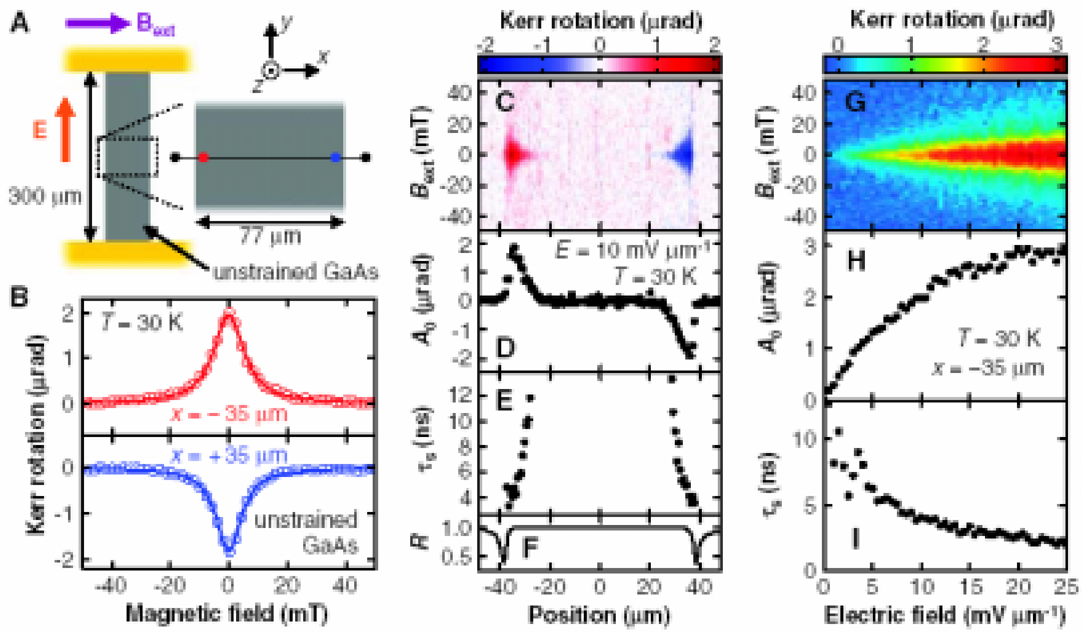


Fig. 1. The spin Hall effect in unstrained GaAs. Data are taken at T = 30 K; a linear background has been subtracted from each B_{ext} scan. (A) Schematic of the unstrained GaAs sample and the experimental geometry. (B) Typical measurement of KR as a function of B_{ext} for x = −35 μm (red circles) and x = +35 μm (blue circles) for E = 10 mV μm^{-1}. Solid lines are fits as explained in text. (C) KR as a function of x and B_{ext} for E = 10 mV μm^{-1}. (D and E) Spatial dependence of peak KR A_0 and spin lifetime τ_s across the channel, respectively, obtained from fits to data in (C). (F) Reflectivity R as a function of x. R is normalized to the value on the GaAs channel. The two dips indicate the position of the edges and the width of the dips gives an approximate spatial resolution. (G) KR as a function of E and B_{ext} at x = −35 μm. (H and I) E dependence of A_0 and τ_s, respectively, obtained from fits to data in (G).

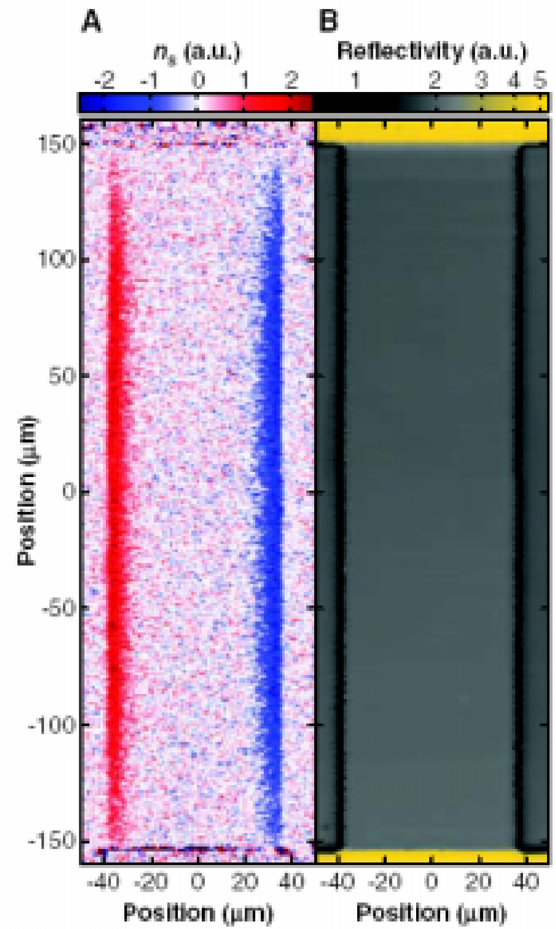


Fig. 2. (A and B) Two-dimensional images of spin density n_s and reflectivity R, respectively, for the unstrained GaAs sample measured at T = 30 K and E = 10 mV μm^{-1}.

Part II: Magnetic Nanostructures

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Outline of this second part of the talk

I. Free standing transition metal atomic chains

II. Metal atomic chains in/on, and wetted layers on BN nanotubes

III. Bulk, thin films, nanowires and nanopartices of FePt