Invariant Theory and Symmetry Analysis of Magnetism and Spin-Orbitronics

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Outline

Lecture 1: A primer on spin-orbitronics
Spin-orbit coupling in crystals, Dzyaloshinskii-Moriya interaction, spin-orbit torques

Lecture 2: Representation Theory applied to crystals
Group of symmetries, reducible and irreducible representations, orthogonality theorem, characters

Lecture 3: Character tables of crystal point groups
Salient features of the character table, invariant functions, decomposition theorem, product group

Lecture 4: Application to the C_{3v} point group
Hamiltonian, conductivity tensor, DMI and SOT

Lecture 5: Your turn, with the C_{4v} point group
Surprise me ☺

Physical properties and product of groups

When considering the physical properties of a system, we often encounter effects that combine functions that belong to different representations. An instructive example is given by the electronic transitions enabled by an electromagnetic field

The Hamiltonian reads

$$\begin{cases} \mathcal{H}_0 = \dfrac{p^2}{2m} + V(\boldsymbol{r}) & \text{Scalar, belongs to E (highest symmetry)} \\ \mathcal{H}'_{\text{em}} = -\dfrac{e}{mc}\boldsymbol{p}\cdot\boldsymbol{A} & \text{Polar vector, reduces the symmetry} \end{cases}$$

We look for the states that are allowed by this stimulus

$$\psi_j^{(\Gamma_i)} \longrightarrow \mathcal{H}'\psi_j^{(\Gamma_i)}$$

Product of groups

We now define the *direct product of two groups*. Let $G_A = E, A_2, \ldots, A_{h_a}$ and $G_B = E, B_2, \ldots, B_{h_b}$ be two groups such that all operators A_R commute with all operators B_S. Then the direct product group is

$$G_A \otimes G_B = E, A_2, \ldots, A_{h_a}, B_2, A_2 B_2, \ldots, A_{h_a} B_2, \ldots, A_{h_a} B_{h_b}$$

Theorem. *The direct product of the representations of the groups A and B forms a representation of the direct product group.*

All irreducible representations of the direct product group can be generated from the irreducible representations of the original groups before they are joined.

Product of groups

Theorem. *The simplest imaginable formulas are assumed by the characters in direct product groups or in taking the direct product of two representations:*

(a) If the direct product occurs between two groups, then the characters for the irreducible representations in the direct product group are obtained by multiplication of the characters of the irreducible representations of the original groups according to

$$\chi^{(a\otimes b)}(A_k B_\ell) = \chi^{(a)}(A_k)\,\chi^{(b)}(B_\ell)\,. \tag{6.23}$$

(b) If the direct product is taken between two representations of the same group, then the character for the direct product representation is written as

$$\chi^{(\ell_1\otimes\ell_2)}(R) = \chi^{(\ell_1)}(R)\,\chi^{(\ell_2)}(R)\,. \tag{6.24}$$

Product of groups

In general, if we take the direct product between two irreducible representations of a group, then the resulting direct product representation will be reducible. If it is reducible, the character for the direct product can then be written as a linear combination of the characters for irreducible representations of the group

$$\chi^{(\lambda)}(R)\chi^{(\mu)}(R) = \sum_{\nu} a_{\lambda\mu\nu}\chi^{(\nu)}(R)$$

$$a_{\lambda\mu\nu} = \frac{1}{h}\sum_{\mathcal{C}_\alpha} N_{\mathcal{C}_\alpha}\chi^{(\nu)}(\mathcal{C}_\alpha)^* \left[\chi^{(\lambda)}(\mathcal{C}_\alpha)\chi^{(\mu)}(\mathcal{C}_\alpha)\right]$$

Product of groups

	$C_{4h} \equiv C_4 \otimes i$				$(4/m)$				
	E	C_2	C_4	C_4^3	i	iC_2	iC_4	iC_4^3	
A_g	1	1	1	1	1	1	1	1	
B_g	1	1	−1	−1	1	1	−1	−1	even under
E_g	1	−1	i	$-i$	1	−1	i	$-i$	inversion (g)
	1	−1	$-i$	i	1	−1	$-i$	i	
A_u	1	1	1	1	−1	−1	−1	−1	
B_u	1	1	−1	−1	−1	−1	1	1	odd under
E_u	1	−1	i	$-i$	−1	1	$-i$	i	inversion (u)
	1	−1	$-i$	i	−1	1	i	$-i$	

$\mathcal{H}'_{\mathrm{em}} = -\frac{e}{mc}\boldsymbol{p}\cdot\boldsymbol{A}$ transforms as T_{1u} and assume we intend to excite $\psi_{T_{2g}}$

repr.	basis functions	E	$3C_4^2$	$6C_4$	$6C_2'$	$8C_3$	i	$3iC_4^2$	$6iC_4$	$6iC_2'$	$8iC_3$
A_{1g}	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	$\begin{cases} x^4(y^2-z^2)+ \\ y^4(z^2-x^2)+ \\ z^4(x^2-y^2) \end{cases}$	1	1	−1	−1	1	1	1	−1	−1	1
E_g	$\begin{cases} x^2-y^2 \\ 2z^2-x^2-y^2 \end{cases}$	2	2	0	0	−1	2	2	0	0	−1
T_{1u} (Perturbation)	x, y, z	3	−1	1	−1	0	−3	1	−1	1	0
T_{2u}	$z(x^2-y^2)\ldots$	3	−1	−1	1	0	−3	1	1	−1	0
A_{1u}	$\begin{cases} xyz[x^4(y^2-z^2)+ \\ y^4(z^2-x^2)+ \\ z^4(x^2-y^2)] \end{cases}$	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	xyz	1	1	−1	−1	1	−1	−1	1	1	−1
E_u	$xyz(x^2-y^2)\ldots$	2	2	0	0	−1	−2	−2	0	0	1
T_{1g}	$xy(x^2-y^2)\ldots$	3	−1	1	−1	0	3	−1	1	−1	0
T_{2g} (Initial state)	xy, yz, zx	3	−1	−1	1	0	3	−1	−1	1	0

Perturbation → T_{1u}

Initial state → T_{2g}

	E	$3C_4^2$	$6C_4$	$6C_2'$	$8C_3$	i	$3iC_4^2$	$6iC_4$	$6iC_2'$	$8iC_3$
T_{1u}	3	-1	1	-1	0	-3	1	-1	1	0
T_{2g}	3	-1	-1	1	0	3	-1	-1	1	0
$T_{1u} \otimes T_{2g}$	9	1	-1	-1	0	-9	-1	1	1	0

$$T_{1u} \otimes T_{2g} = \sum_i \alpha_i \Gamma^i = \alpha_{A_{2u}} A_{2u} + \alpha_{E_u} E_u + \alpha_{T_{1u}} T_{1u} + \alpha_{T_{2u}} T_{2u}$$

$$\alpha_{A_{2u}} = \frac{1}{h} \sum_k N_k \chi^{T_{1u}}(C_k) \chi^{T_{2g}}(C_k) \chi^{A_{2u}}(C_k) = \frac{1}{48}(1 \times 3 \times 3 \times 1 + \cdots) = 1$$

$$T_{1u} \otimes T_{2g} = A_{2u} + E_u + T_{1u} + T_{2u}$$

Get back to our Hamiltonian for D_3

	E	$2C_3$	$3C_2$	Linear	Quadratic
A_1	1	1	1		x^2+y^2, z^2
A_2	1	1	-1	z, R_z	
E	2	-1	0	$(x,y), (R_x, R_y)$	$(xz, yz), (x^2-y^2, xy)$
$E\otimes E$	4	1	0		

$$E\otimes E = \frac{1}{h}\sum_i \alpha_i \Gamma^i = \alpha_{A_1}A_1 + \alpha_{A_2}A_2 + \alpha_E E$$

$$\alpha_{A_1} = \frac{1}{6}(1\times 1\times 4 + 3\times 1\times 0 + 2\times 1\times 1) = 1$$

$$\alpha_{A_2} = \frac{1}{6}(1\times 1\times 4 + 3\times -1\times 0 + 2\times 1\times 1) = 1$$

$$\alpha_E = \frac{1}{6}(1\times 4\times 2 + 3\times 0\times 0 + 2\times -1\times 1) = 1$$

$$\begin{matrix} R_x x + R_y y \\ R_x y - R_y x \\ \begin{cases} R_x x - R_y y \\ R_x y + R_y x \end{cases} \end{matrix} \rightarrow \begin{matrix} A_1 \\ A_2 \\ E \end{matrix}$$

$$H = \frac{p_z^2}{2m_z} + \frac{p_x^2 + p_y^2}{2m_{||}} + \alpha_z p_z \sigma_z + \alpha_{||}(\sigma_x p_x + \sigma_x p_x)$$

Now, let's practice!

Linear conductivity tensor

The current vector is a *polar* vector

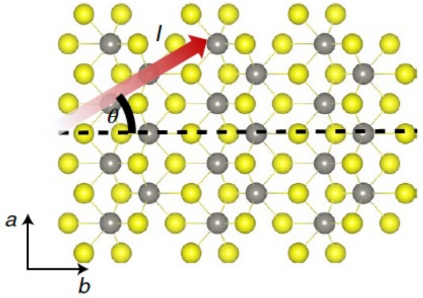
$$j_\alpha = \sigma_{\alpha\beta} E_\beta + \sigma^{i}_{\alpha\beta} m_i E_\beta + \sigma^{ij}_{\alpha\beta} m_i m_j E_\beta \ldots$$

polar vector (E_β)   *axial* vector (m_i)

Nonlinear conductivity tensor

$$j^{n}_\alpha = \sigma_{\alpha\beta\gamma} E_\beta E_\gamma + \sigma_{\alpha\beta\gamma\delta} E_\beta E_\gamma E_\delta \ldots$$

Same idea…but the possibility for nonlinear Hall effect in nonmagnetic materials!

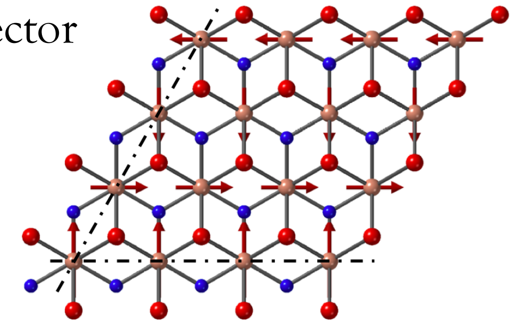


Dzyaloshinskii-Moriya interaction

The magnetic energy is a *scalar*, even in magnetization

$$W_{DM} = m_i \partial_j m_k + m_i \partial_j \partial_k m_l + \cdots$$

polar vector (∂_j)

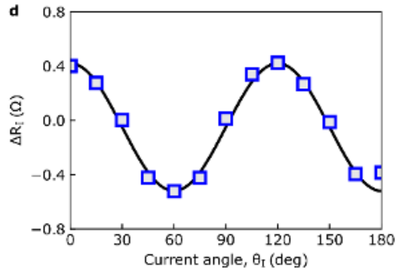


Spin-orbit torque

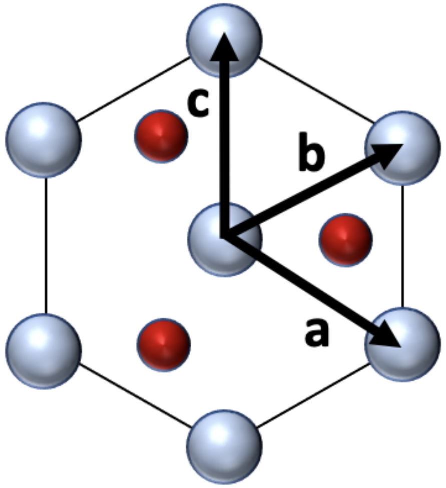
The spin-orbit field is an *axial* vector

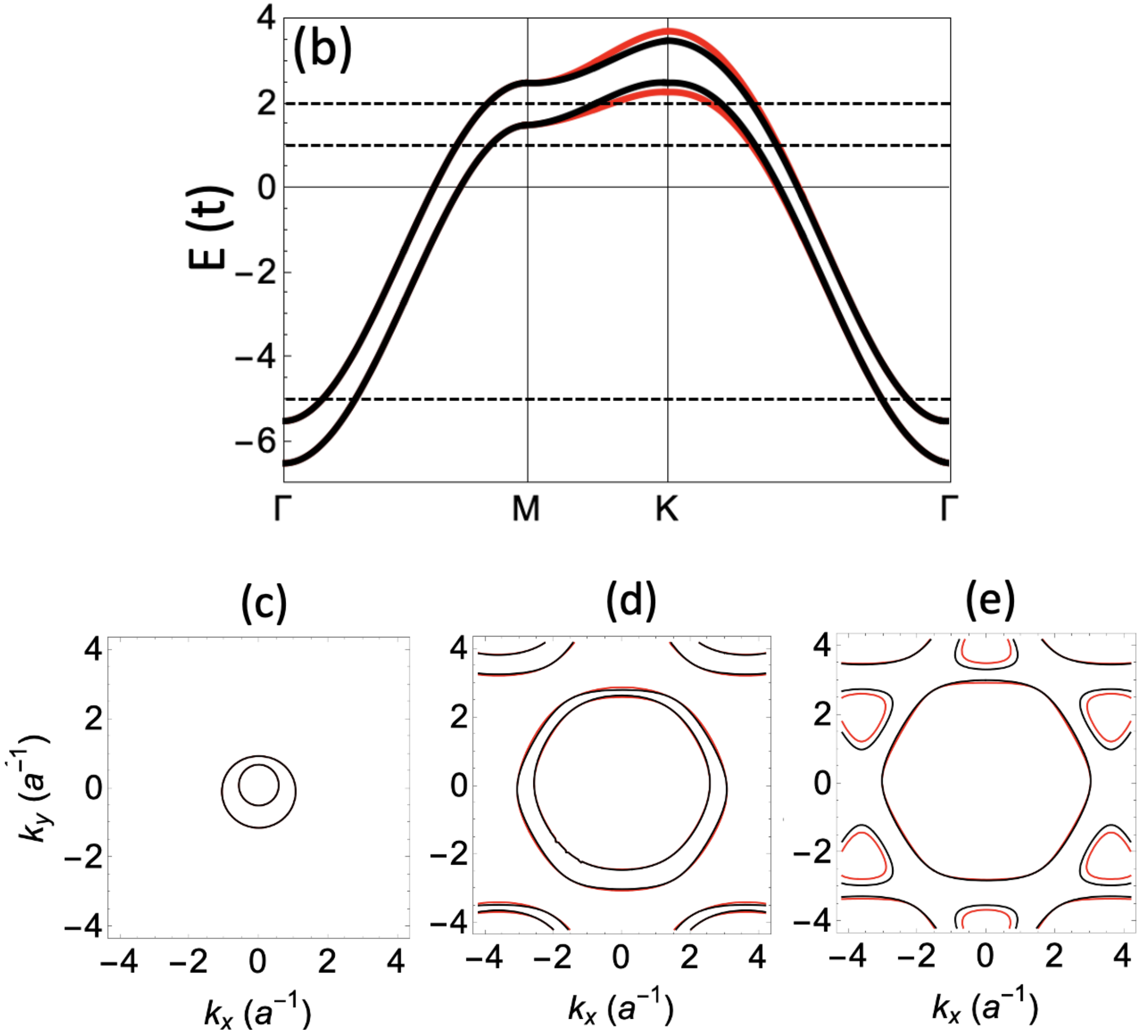
$$h_\alpha = \tau_{\alpha\beta} E_\beta + \tau^{i}_{\alpha\beta} m_i E_\beta + \tau^{ij}_{\alpha\beta} m_i m_j E_\beta$$

$$h^{n}_\alpha = \tau_{\alpha\beta\gamma} E_\beta E_\gamma + \tau^{i}_{\alpha\beta\gamma} m_i E_\beta E_\gamma \ldots$$



A C_{3v} minimal model: Rashba + warping





$$\mathcal{H}_0 = \varepsilon_{\boldsymbol{k}} + \Delta\boldsymbol{\sigma}\cdot\boldsymbol{m} + \alpha_R \boldsymbol{k}\cdot(\boldsymbol{z}\times\boldsymbol{\sigma}) + \beta_{3R} k_y\left(k_y^2 - 3k_x^2\right)\sigma_z$$

Linear + Cubic Rashba

See, e.g., Fu PRL 103, 266801 (2009)
Garcia-Ovalle et al., arXiv:2301.01133 (2022)

Looking for the microscopic origin of the 3m torque

Character table of C_{3v}

	E	$2C_3$	$3\sigma_v$	Linear	Quadratic	Cubic
A_1	1	1	1	z	$x^2+y^2,\ z^2$ $m_x^2+m_y^2,\ m_z^2$	$z^3,\ z(x^2+y^2),\ x(x^2-3y^2)$ $m_y(3m_x^2-m_y^2)$
A_2	1	1	-1	m_z	-	$y(3x^2-y^2)$ $m_x(m_x^2-3m_y^2)$
E	2	-1	0	(x,y) (m_x,m_y)	$(x^2-y^2,xy),\ (xz,yz)$ $(m_x^2-m_y^2,m_xm_y)$ (m_xm_z,m_ym_z)	$(z(x^2-y^2),xyz),\ (xz^2,yz^2),\ (x(x^2+y^2),y(x^2+y^2))$ $(m_z(m_x^2-m_y^2),m_xm_ym_z),\ (m_xm_z^2,m_ym_z^2)$ $(m_x(m_x^2+m_y^2),m_y(m_x^2+m_y^2))$

Combine the invariants into new terms fulfilling A_1+E (polar vector)

Current vector first order in *E* and second order in *m*

$$\boldsymbol{J} \sim \left[1+m_y(3m_y^2-m_x^2)\right]\boldsymbol{E} + \left[m_z+m_x(m_x^2-3m_y^2)\right]\boldsymbol{z}\times\boldsymbol{E}$$

$$+\begin{pmatrix} 2m_xm_yE_y+(m_x^2-m_y^2)E_x \\ 2m_xm_yE_x-(m_x^2-m_y^2)E_y \\ 0 \end{pmatrix} + \begin{pmatrix} m_xE_y+m_yE_x \\ m_xE_x-m_yE_y \\ 0 \end{pmatrix} + m_z\boldsymbol{z}\times\begin{pmatrix} m_xE_y+m_yE_x \\ m_xE_x-m_yE_y \\ 0 \end{pmatrix}$$

AMR+PHE — In-plane Hall effect — Chiral Hall effect

Looking for the microscopic origin of the 3m torque

Character table of C_{3v}

	E	$2C_3$	$3\sigma_v$	Linear	Quadratic	Cubic
A_1	1	1	1	z	$x^2+y^2,\ z^2$ $m_x^2+m_y^2,\ m_z^2$	$z^3,\ z(x^2+y^2),\ x(x^2-3y^2)$ $m_y(3m_x^2-m_y^2)$
A_2	1	1	-1	m_z	-	$y(3x^2-y^2)$ $m_x(m_x^2-3m_y^2)$
E	2	-1	0	(x,y) (m_x,m_y)	$(x^2-y^2,xy),\ (xz,yz)$ $(m_x^2-m_y^2,m_xm_y)$ (m_xm_z,m_ym_z)	$(z(x^2-y^2),xyz),\ (xz^2,yz^2),\ (x(x^2+y^2),y(x^2+y^2))$ $(m_z(m_x^2-m_y^2),m_xm_ym_z),\ (m_xm_z^2,m_ym_z^2)$ $(m_x(m_x^2+m_y^2),m_y(m_x^2+m_y^2))$

Combine the invariants into new terms fulfilling A_1 (scalar)

Magnetic energy at the second order in *m* and up the third order in spatial gradient

$$E_0 = m_z \boldsymbol{\nabla}\cdot\boldsymbol{m}$$
$$E_1 = D\left[\nabla_x\left(m_x^2-m_y^2\right)-2\nabla_y\left(m_xm_y\right)\right]$$
$$E_2 = Dm_x\left(m_x^2-3m_y^2\right)\boldsymbol{\nabla}\cdot\boldsymbol{m}$$
$$E_3 = D\nabla_x\left(\nabla_x^2-3\nabla_y^2\right)m_z^2$$

Looking for the microscopic origin of the 3m torque

Character table of C_{3v}

	E	$2C_3$	$3\sigma_v$	Linear	Quadratic	Cubic
A_1	1	1	1	z	$x^2+y^2,\ z^2$ $m_x^2+m_y^2,\ m_z^2$	$z^3,\ z(x^2+y^2),\ x(x^2-3y^2)$ $m_y(3m_x^2-m_y^2)$
A_2	1	1	-1	m_z	-	$y(3x^2-y^2)$ $m_x(m_x^2-3m_y^2)$
E	2	-1	0	(x,y) (m_x,m_y)	$(x^2-y^2,xy),\ (xz,yz)$ $(m_x^2-m_y^2,m_xm_y)$ (m_xm_z,m_ym_z)	$(z(x^2-y^2),xyz),\ (xz^2,yz^2),\ (x(x^2+y^2),y(x^2+y^2))$ $(m_z(m_x^2-m_y^2),m_xm_ym_z),\ (m_xm_z^2,m_ym_z^2)$ $(m_x(m_x^2+m_y^2),m_y(m_x^2+m_y^2))$

Combine the invariants into new terms fulfilling A_2+E (axial vector)

Spin-orbit torques

$$\boldsymbol{h}_{\parallel} = h_{\mathrm{FL}}(1+\eta_{\mathrm{FL}}m_z^2+\delta_{\mathrm{FL}}m_y(3m_x^2-m_y^2))\mathbf{z}\times\mathbf{E}$$
Field-like torque

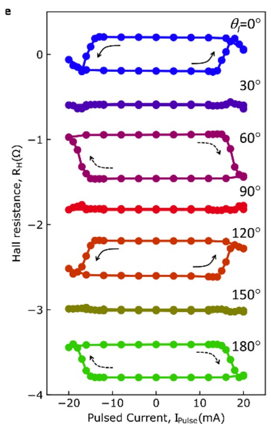
$$+h_{\mathrm{DL}}((1+\eta_{\mathrm{DL}}m_z^2)m_z+\delta_{\mathrm{DL}}m_x(m_x^2-3m_y^2))\mathbf{E}$$
Damping-like torque

$$+h_{3m}(1+\eta_{3m}m_z^2)[(m_xE_x-m_yE_y)\mathbf{x}-(m_yE_x+m_xE_y)\mathbf{y}]$$
3m torque

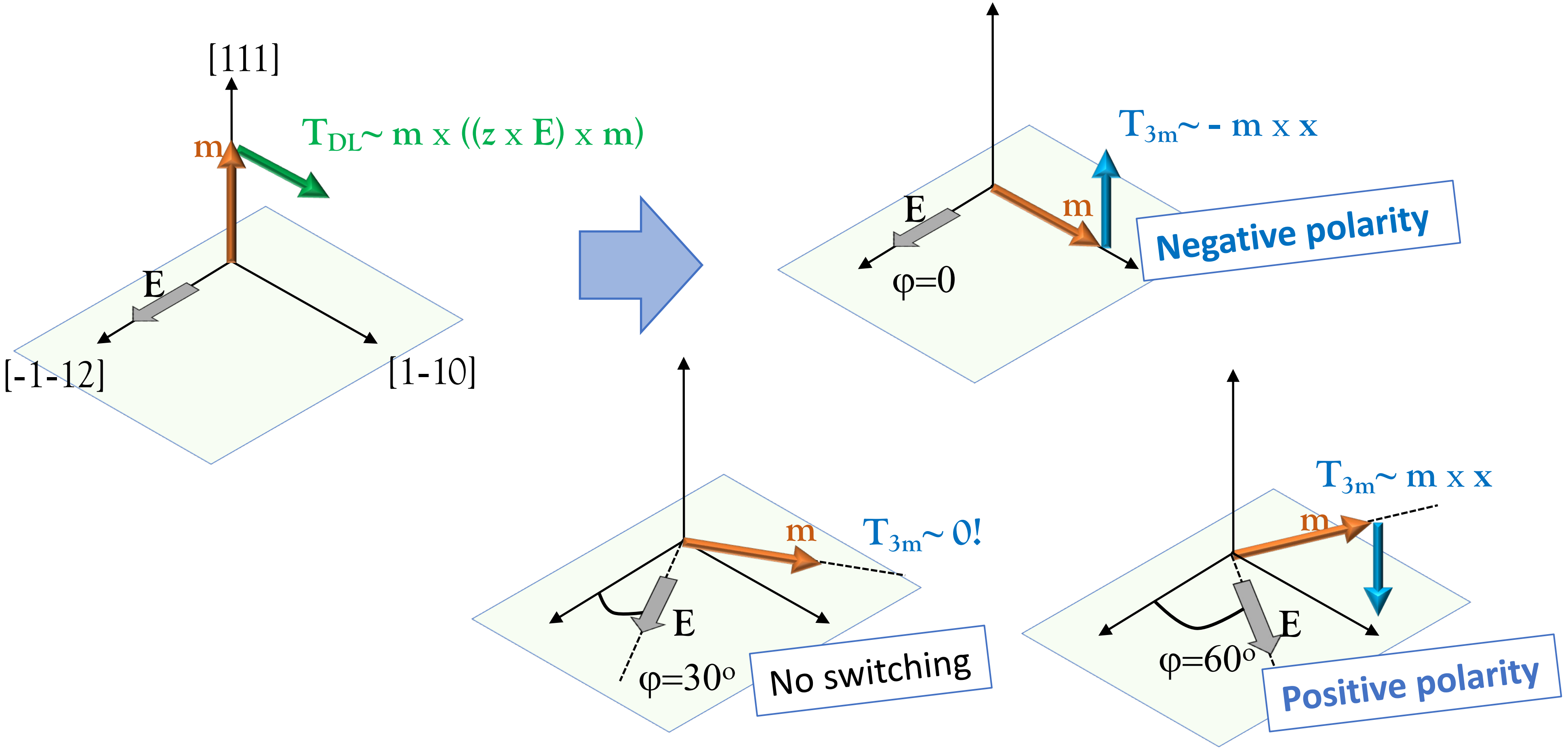
Planar Hall torque
$$+h_{\mathrm{PH}}[((m_x^2-m_y^2)E_y-2m_xm_yE_x)\mathbf{x}+((m_x^2-m_y^2)E_x+2m_xm_yE_y)\mathbf{y}]$$

Chiral torque
$$+h_{\chi}m_z[((m_x^2-m_y^2)E_x+2m_xm_yE_y)\mathbf{x}-((m_x^2-m_y^2)E_y-2m_xm_yE_x)\mathbf{y}]$$

Field-free switching with 3-fold symmetry



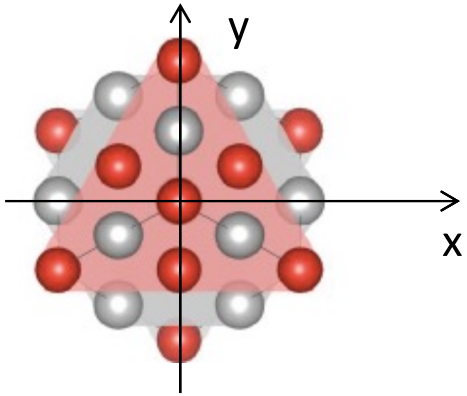
$$\boldsymbol{\tau} = \tau_{\perp}\mathbf{m}\times(\mathbf{z}\times\mathbf{E}) + \tau_{\parallel}\mathbf{m}\times[(\mathbf{z}\times\mathbf{E})\times\mathbf{m}] + \tau_{3m}\mathbf{m}\times[(m_yE_x + m_xE_y)\mathbf{x} + (m_xE_x - m_yE_y)\mathbf{y}]$$

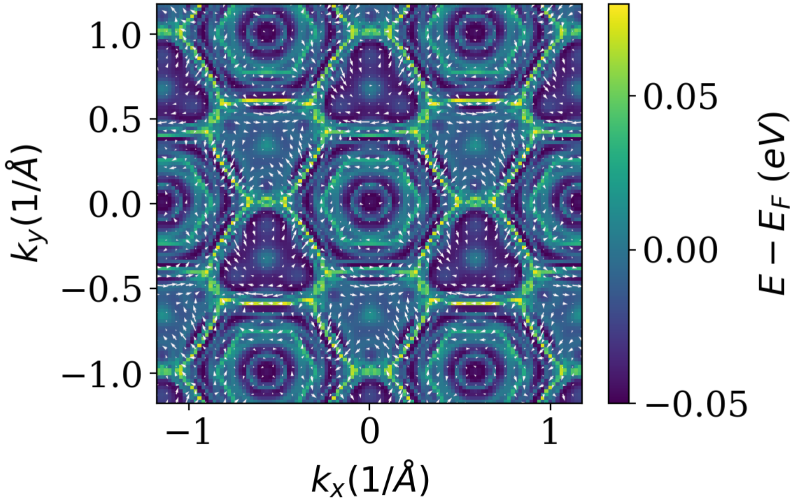


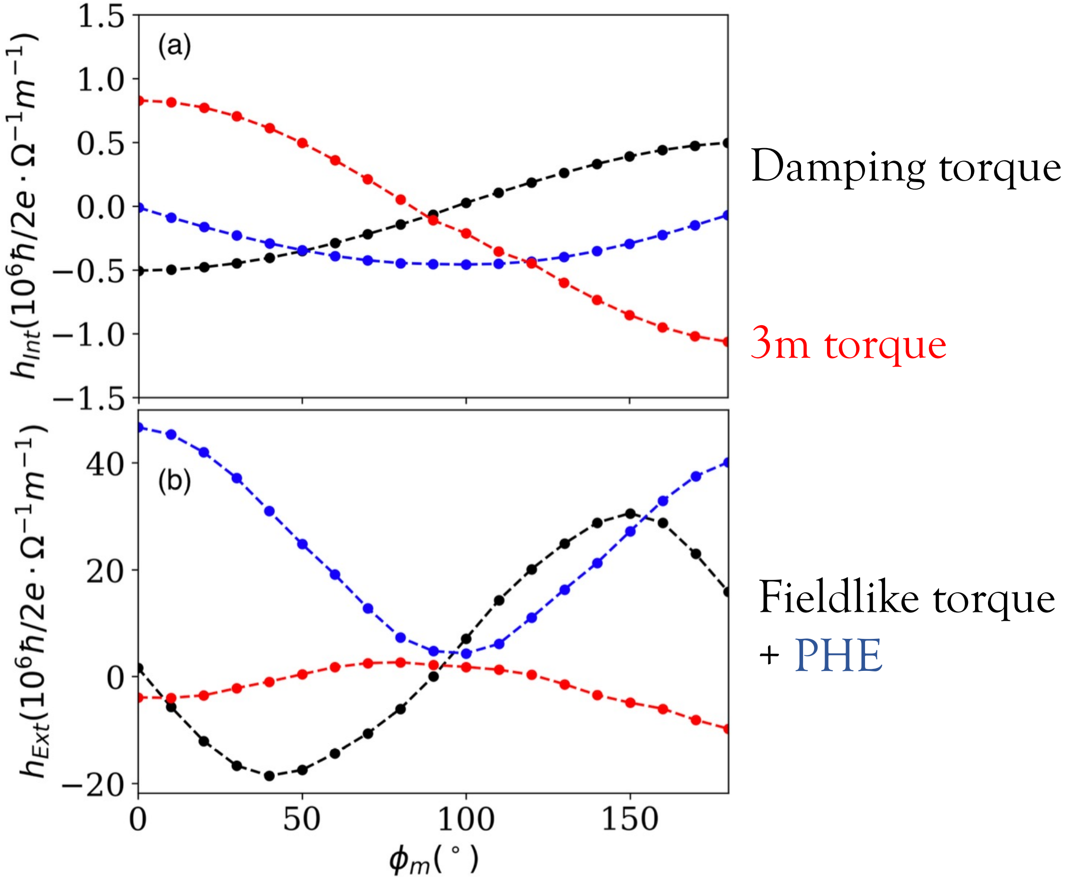
Liu et al. Nature Nanotechnology 16, 277 (2021)

Searching for the "magic" torque

$$\boldsymbol{\tau} = \tau_{\perp}\mathbf{m} \times (\mathbf{z} \times \mathbf{E}) + \tau_{\parallel}\mathbf{m} \times [(\mathbf{z} \times \mathbf{E}) \times \mathbf{m}] + \tau_{3m}\mathbf{m} \times [(m_y E_x + m_x E_y)\mathbf{x} + (m_x E_x - m_y E_y)\mathbf{y}]$$

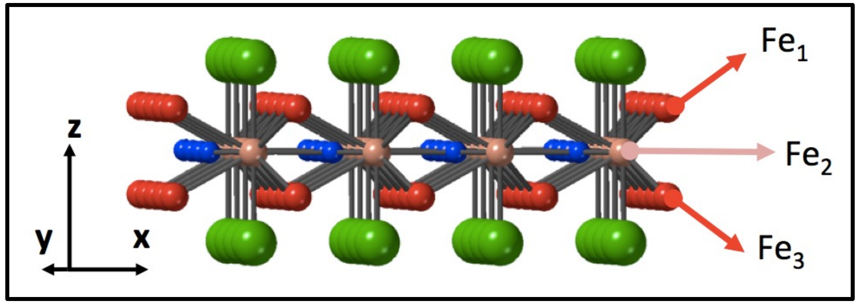






Ovalle et al., PRB 107, 194422 (2023)

Spin-orbit torque in 2D magnets: Fe_3GeTe_2



Current Control of Magnetism in Two-Dimensional Fe_3GeTe_2

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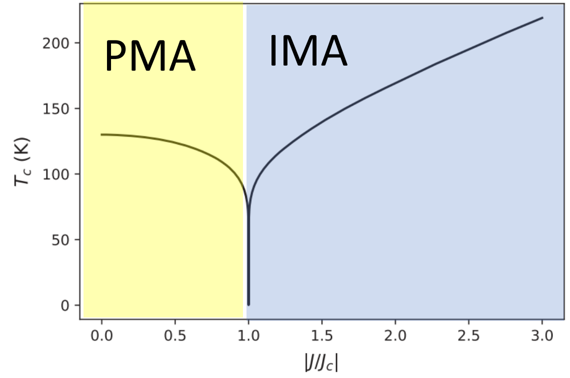
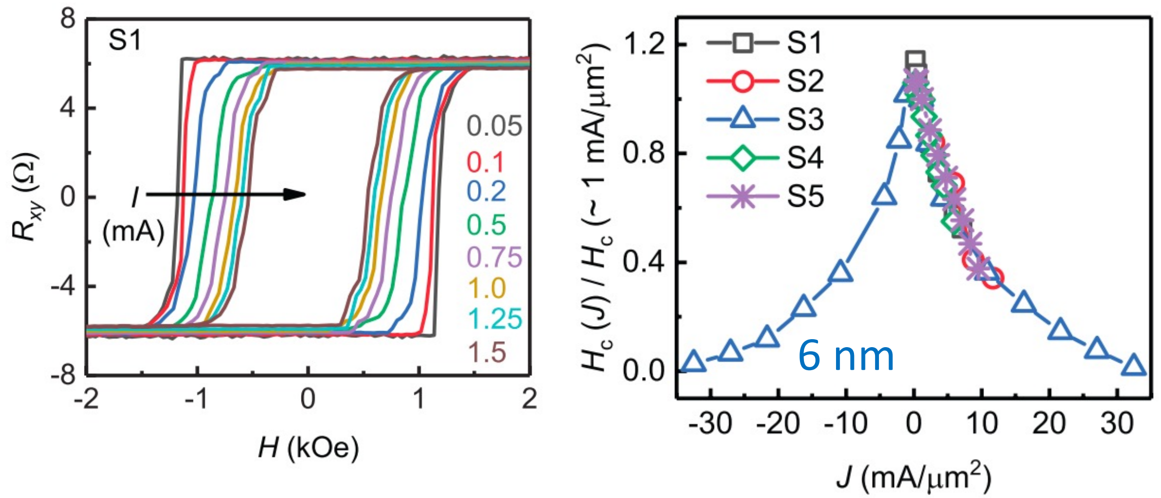
$$\boldsymbol{H}_{\mathrm{SOT}} = \Gamma_0[(m_x J_x - m_y J_y)\boldsymbol{e}_x - (m_y J_x + m_x J_y)\boldsymbol{e}_y]$$

$$f_{\mathrm{SOT}}[\boldsymbol{m}] = M_s \Gamma_0 \left[J_y m_x m_y - \frac{1}{2} J_x (m_x^2 - m_y^2) \right]$$

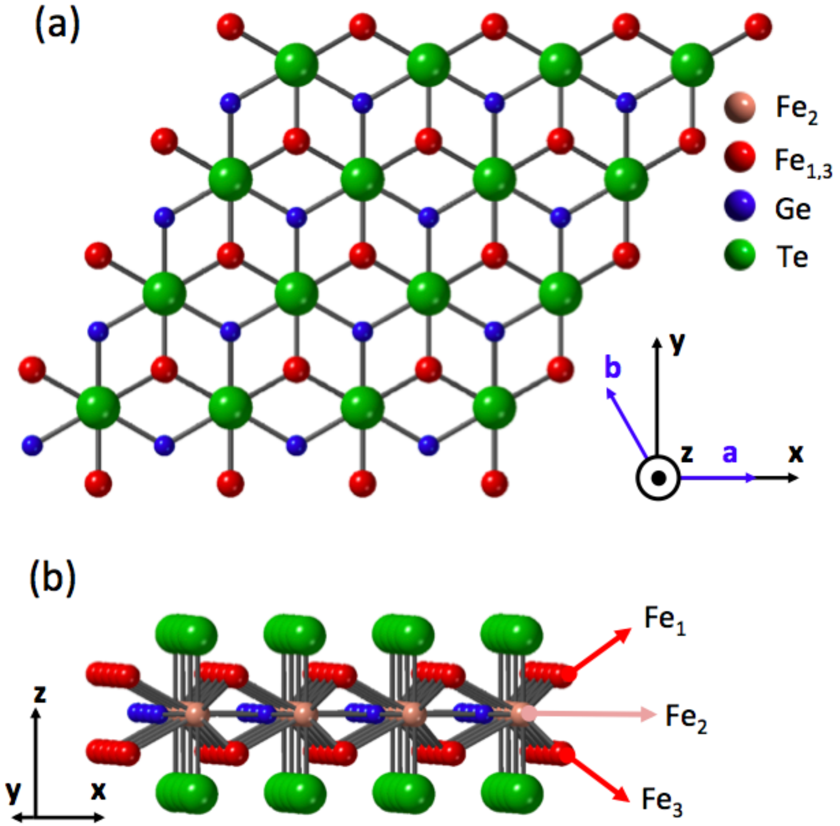


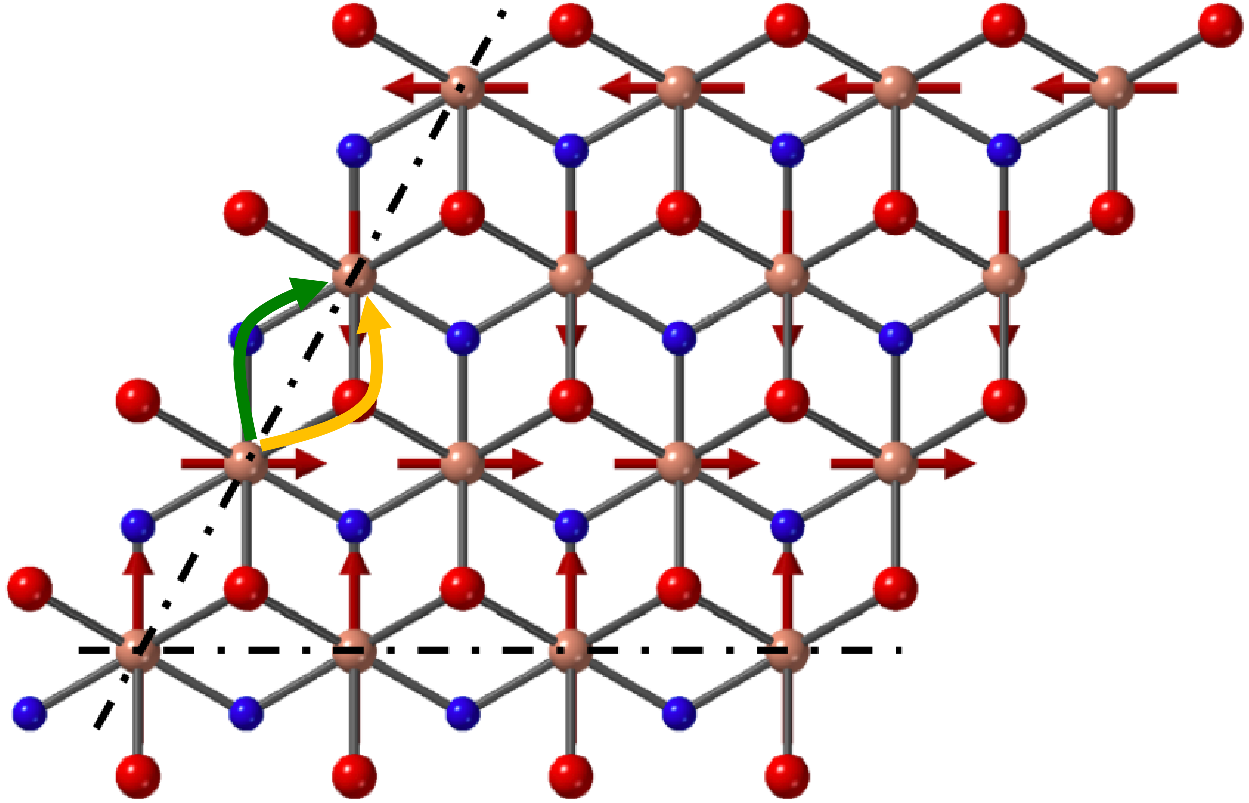
Gigantic Current Control of Coercive Field and Magnetic Memory Based on Nanometer-Thin Ferromagnetic van der Waals Fe_3GeTe_2

Kaixuan Zhang, Seungyun Han, Youjin Lee, Matthew J. Coak, Junghyun Kim, Inho Hwang, Suhan Son, Jeacheol Shin, Mijin Lim, Daegeun Jo, Kyoo Kim, Dohun Kim, Hyun-Woo Lee,* and Je-Geun Park**



What about Dzyaloshinskii-Moriya interaction?





S. Laref et al., Physical Review B 102, 060402(R) (2020)

PhD and postdoc position available

PhD Fellowships

Theory of laser-induced high-harmonic generation in topological materials

Topological spin textures and excitations in van der Waals magnets

Postdoctoral Fellowships

Spin-charge interconversion in ferroelectric Rashba gas

Band structure engineering of graphene by supramolecular network