First-principles calculation of thermoelectric properties

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Collaborator: **Yo Pierre Mizuta**

Outline

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I. Introduction
   I. Thermoelectric effect
   II. Anomalous thermoelectric effect
   III. Basic theory of thermoelectricity
II. Frist-principles calculations
III. Summary

Importance of Thermoelectricity

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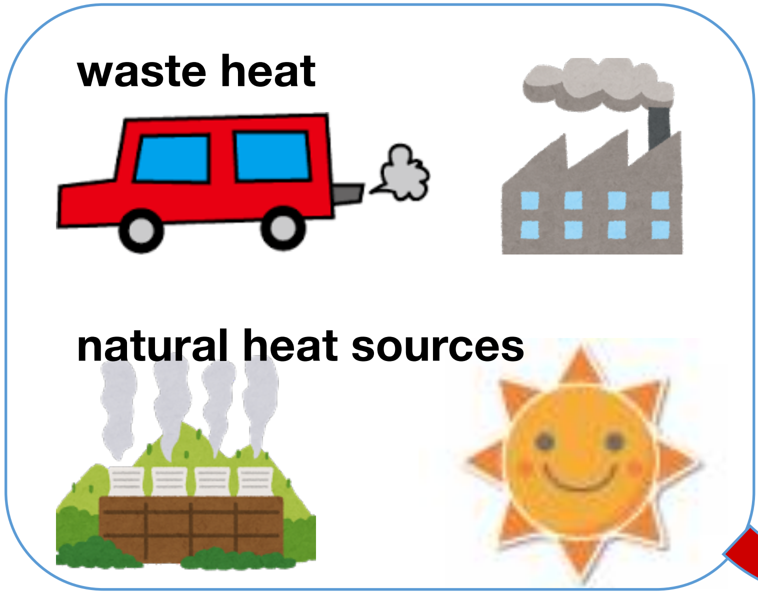
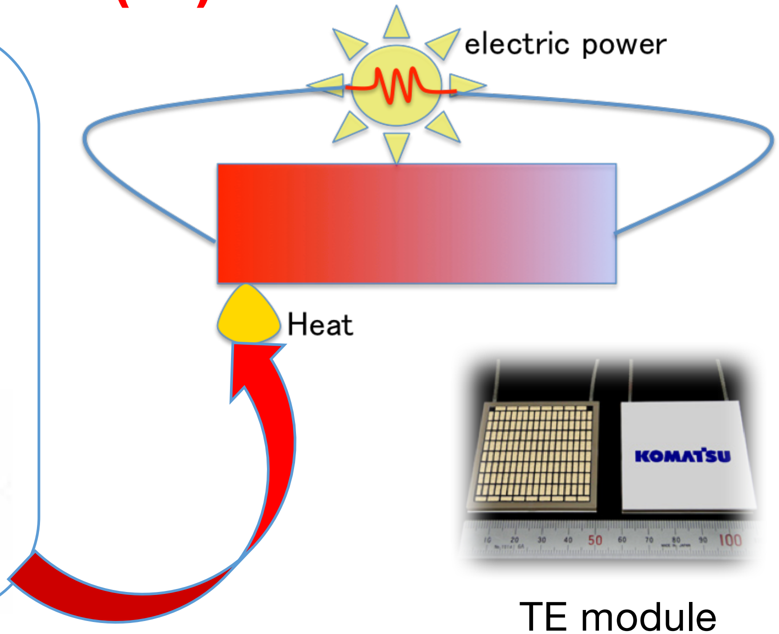
Energy / Environmental issues

- Need for eco-friendly energy sources
- Need for the reduction of CO_2 emission

One good aid: **Thermoelectric (TE) conversion**





TE module

Thermoelectric Conversion

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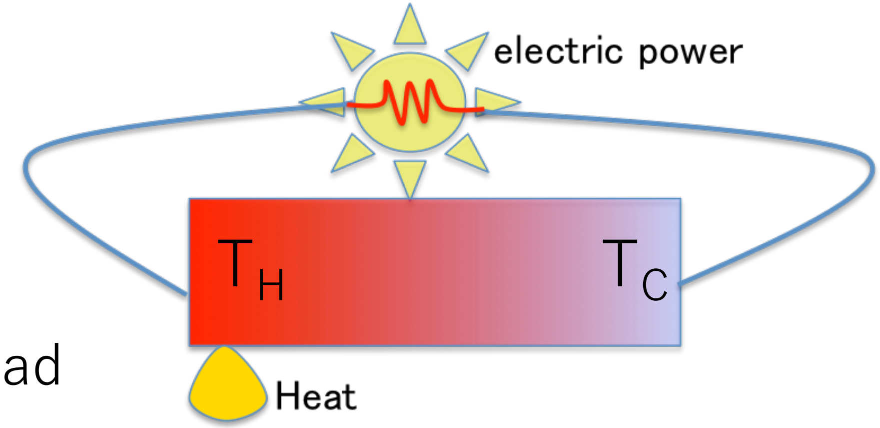
- **Seebeck Effect**

$$V_S = S(T_H - T_C)$$



promising in tackling environmental problems,
but still NOT efficient enough to become widespread

$$Z = \frac{\sigma S^2}{\kappa}$$

electrical conductivity

thermopower

Thermal conductivity

Here we focus on this!

Mechanism for Large Seebeck Coefficient Materials

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$$S_0 = -\frac{k_B}{e}\frac{\int d\varepsilon \boxed{\frac{\varepsilon-\mu}{k_B T}\frac{df(\varepsilon)}{d\varepsilon}}\sigma_{xx}(\varepsilon)}{\int d\varepsilon\,\sigma_{xx}(\varepsilon)\frac{df(\varepsilon)}{d\varepsilon}}$$

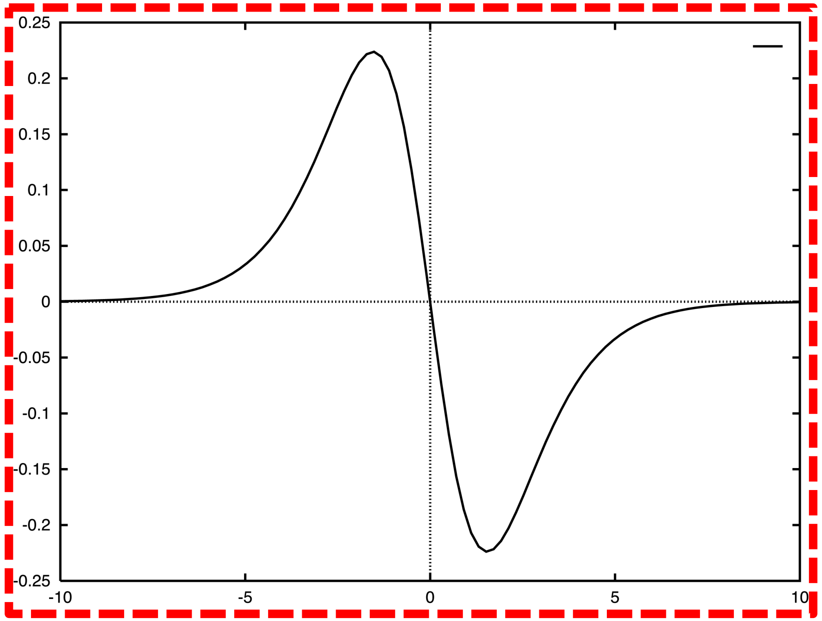
$$\sigma_{xx}(\varepsilon) = e^2 D(\varepsilon) v_x^2(\varepsilon)\tau$$

τ : constant approximaion

Asymmetry in $\sigma_{xx}(\varepsilon)$: D(ε), *$v_x(\varepsilon)$*,

is origin of large S

Narrow gap semiconductor, Semimetals



First-Principles Methods to Compute $\sigma_{xx}(\varepsilon)$

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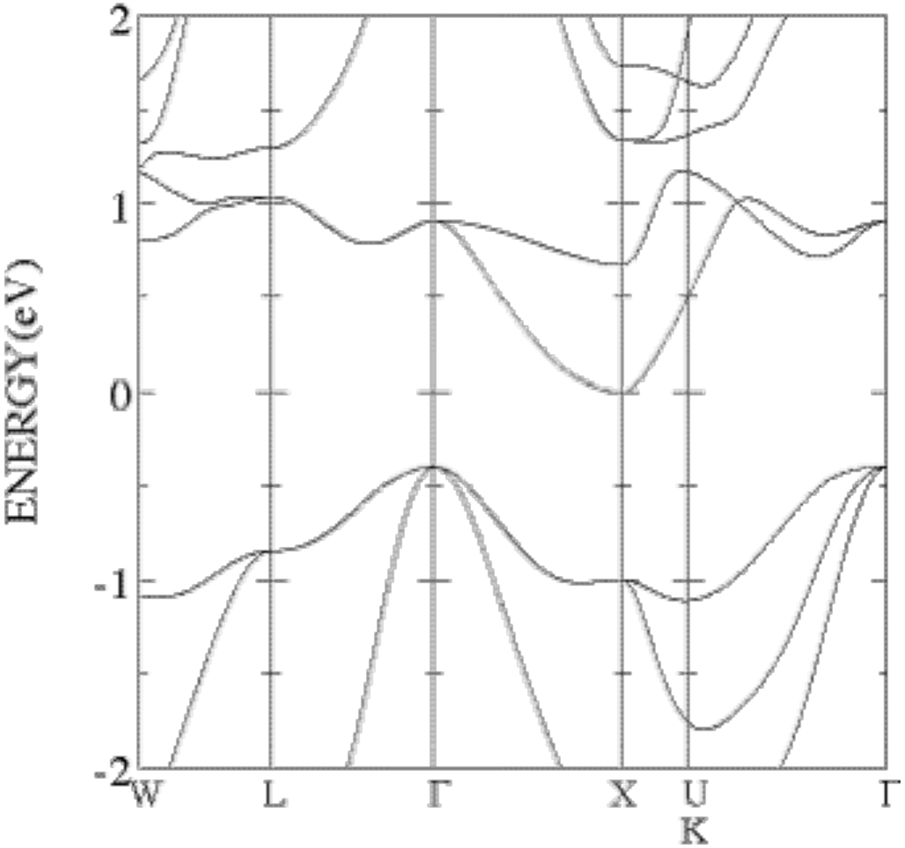
Band Structure $E_n^{\mathbf{k}}$



$$\sigma_{\alpha\alpha}(\epsilon) = \frac{2\Omega}{8\pi^3}\int \mathrm{d}\boldsymbol{k}\sum_n e^2\left(v_{n,\alpha}^{\boldsymbol{k}}\right)^2\tau\delta(\epsilon - E_n^{\boldsymbol{k}}) = e^2\tau D(\epsilon)v_\alpha^2(\epsilon)$$

$$D(\epsilon) = \frac{2\Omega}{8\pi^3}\int \mathrm{d}\boldsymbol{k}\sum_n \delta(\epsilon - E_n^{\boldsymbol{k}})$$

$$f^0(\epsilon) = \frac{1}{\exp\left(\dfrac{\epsilon-\mu}{k_\mathrm{B}T}\right)+1}$$

$$v_{n,\alpha}^{\boldsymbol{k}} = \frac{1}{\hbar}\frac{\partial E_n^{\boldsymbol{k}}}{\partial k_\alpha}$$

$$N = \int \mathrm{d}\epsilon\, D(\epsilon)f^0(\epsilon),$$

Seebeck Effect in Narrow Gap Semiconductor, Intermetallic Compounds (Kondo Insulator/Semimetals), F. Ishii, M. Onoue, T. Oguchi, Physica B, (2004)

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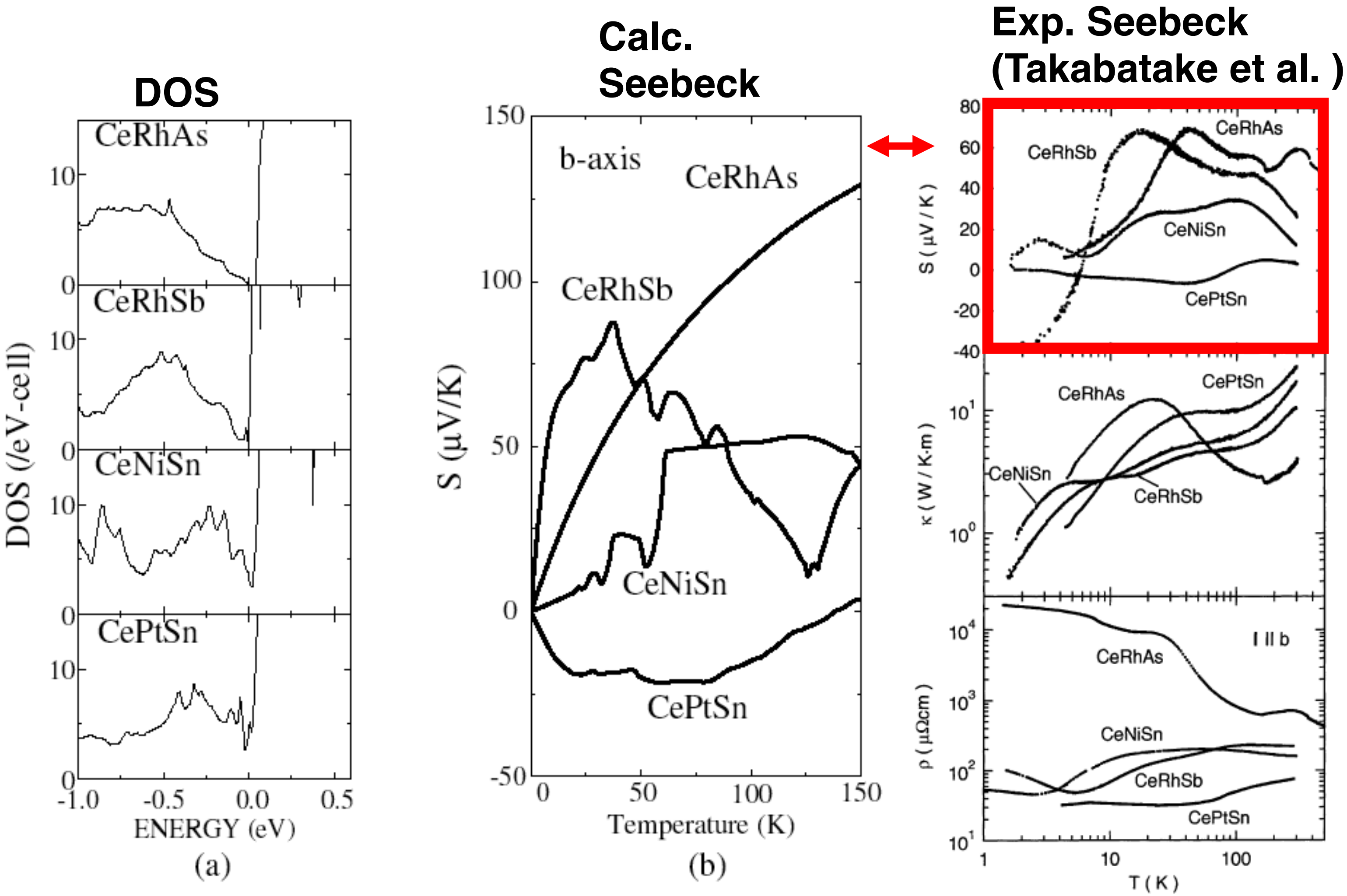

Seebeck Effect in Narrow Gap Semiconductor, Intermetallic Compounds $TiNiSn_{1-x}Sb_x$ F. Ishii, M. Onoue, T. Oguchi (2008)

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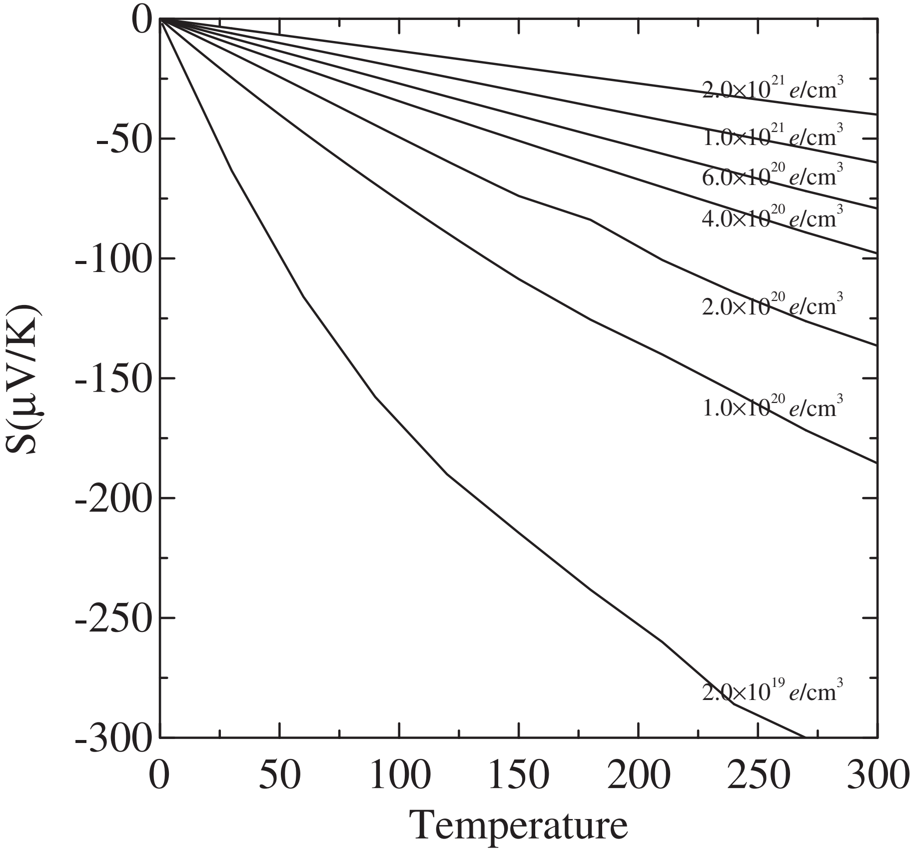
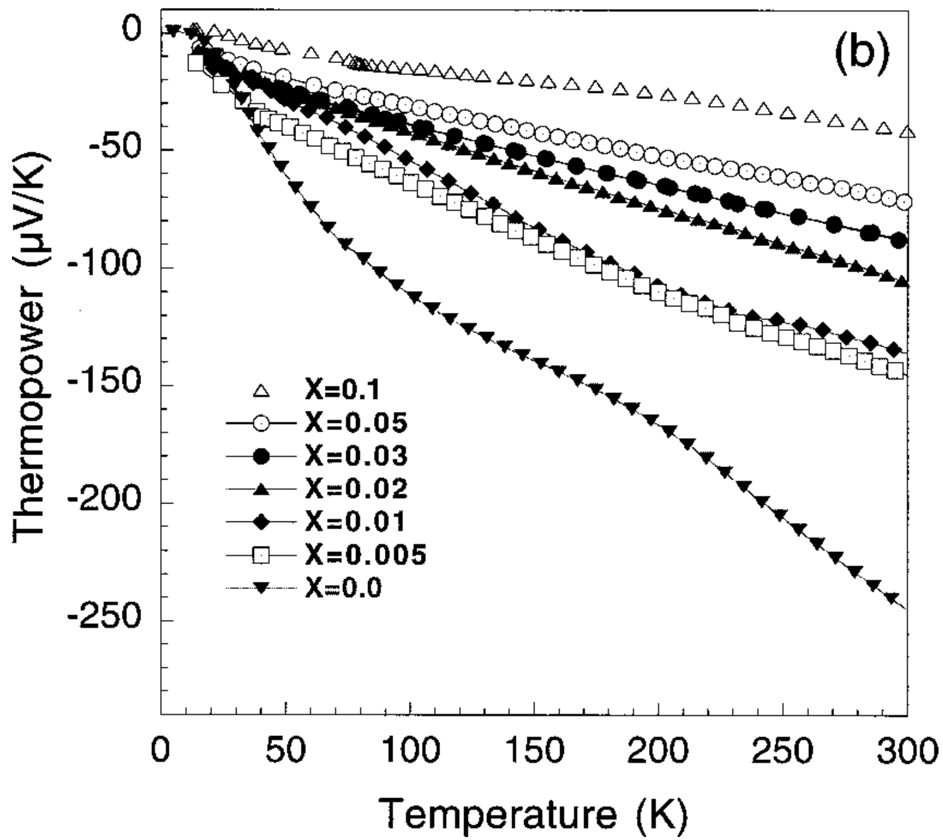
Calc.: M.Onoue, FI, T.Oguchi, JPSJ **77**, 054706 (2008)



Exp.: Bhattacharya et al. Appl. Phys. Lett. **77**, 2476 (2000)



Seebeck Effect in B20 Mono Silicide (Skyrmion Materials), A.Sakai , F. Ishii et al. JPSJ (2007)

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LETTERS

Thermoelectric Power in Transition-Metal Monosilicides

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We study, both experimentally and theoretically, temperature and electron-density (band-filling) dependence of Seebeck coefficient in B20-type transition-metal monosilicides to critically study the validity of the Boltzmann transport theory based on the band structure as a guiding principle for the materials design of metallic thermoelectric compounds. The global thermoelectric phase diagram for a wide range of materials (CrSi–MnSi–FeSi–CoSi–$Co_{0.85}Ni_{0.15}Si$ and their interpolating solid solutions) is obtained. Theoretical results derived from the calculated band structure can reproduce a global feature of experimental results except the higher temperature region of FeSi, providing the firm basis to understand the systematics of thermoelectricity in metallic compounds including the role of electron correlation and to develop the material design for larger thermoelectricity.

KEYWORDS: thermopower, B20, monosilicide, first-principle calculation, band filling, pseudogap
DOI: 10.1143/JPSJ.76.093601

Seebeck Effect in B20 Mono Silicide (Skyrmion Materials), A.Sakai , F. Ishii et al. JPSJ (2007)

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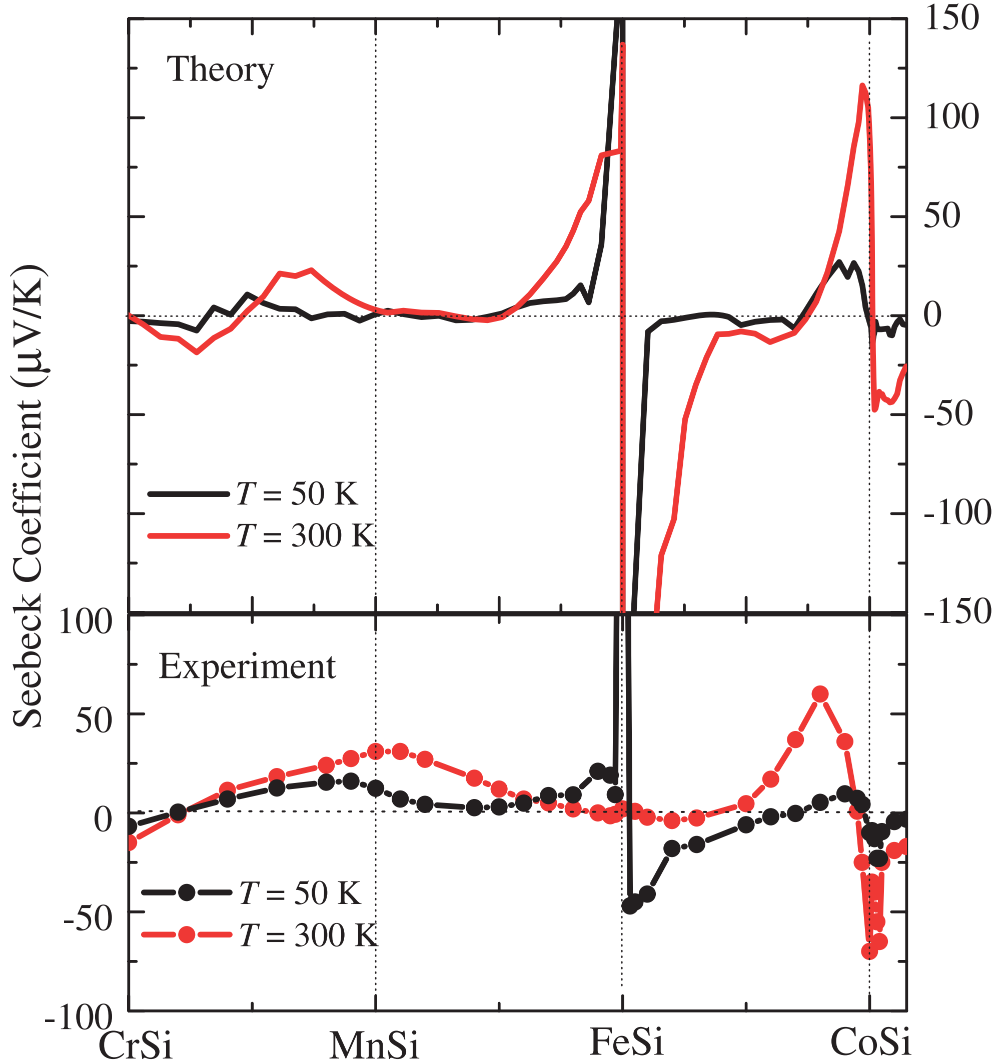

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Problem, Task & Strategy

Low efficiency : preventing the expansion of TE

Can the physics of electronic spin help improve it?

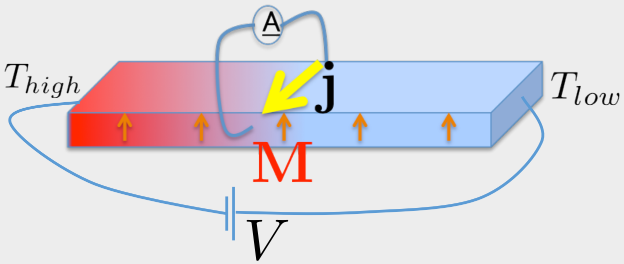
OUR STRATEGY

Spin-induced phenomena:

anomalous Hall effect (AHE) $\mathbf{j}_{AHE} \propto \mathbf{M} \times \mathbf{E}$

Nernst effect (ANE) $\mathbf{j}_{ANE} \propto \mathbf{M} \times (\nabla T)$

? **improved TE efficiency**



AHE & ANE :
observed in a wide range of materials

Thermoelectric Conversion

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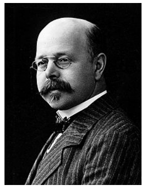
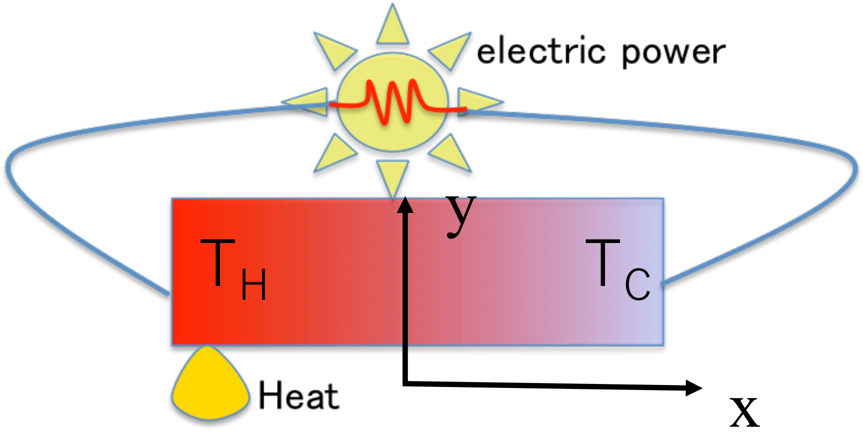
- **Seebeck Effect**

$$V_x = S_{xx}(T_H - T_C)_x$$



- **Nernst Effect**

$$V_y = S_{yx}(T_H - T_C)_x$$



Thermoelectric Conversion

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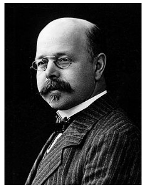
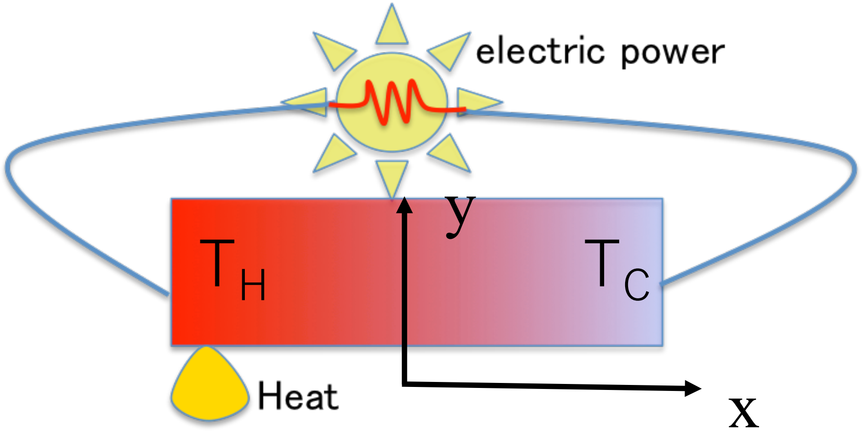
- **Seebeck Effect**

$$V_S = S(T_H - T_C)$$



- **Nernst Effect**

$$V_N = N(T_H - T_C)$$



electrical conductivity

Nernst Coefficient

$$Z = \frac{\sigma N^2}{\kappa}$$

Thermal conductivity

Here we focus on this!

Magnitude of AHE/ANE

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AHE

$$\sigma_{xy} = \mathcal{C}\frac{e^2}{h}$$

- **Experiments**

$$\mathcal{C}_{\max} \sim 1$$

- **Theory**

$$\mathcal{C}_{\max} > 10$$

[1]

ANE

$$E_x = N(\nabla T)_y$$

- **Experiments**

$|N| < 10\ \mu\mathrm{V/K}$, typically $\sim 1\ \mu\mathrm{V/K}$ [2]

c.f. good TE materials have Seebeck $|S| \sim 300\ \mu\mathrm{V/K}$[3]

- **Our calculation**

?

[1] H. Jiang, Z. Qiao, H. Liu, and Q. Niu, Phys. Rev. B **85**, 045445 (2012).
[2] Y. Sakuraba, Scripta Mater. (2015), http://dx.doi.org/10.1016/j.scriptamat.2015.04.034
[3] http://www.mrl.ucsb.edu:8080/datamine/thermoelectric.jsp

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Viewpoint Paper

Potential of thermoelectric power generation using anomalous Nernst effect in magnetic materials

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ABSTRACT

This article introduces the concept and advantage of thermoelectric power generation (TEG) using anomalous Nernst effect (ANE). The three-dimensionality of ANE can largely simplify a thermopile structure and realize TEG systems using heat sources with a non-flat surface. The improvement of *ZT* can be expected because of the orthogonal relationship between thermal and electric conductivities. The calculations of an achievable electric power predicted that an improvement of thermopower by one order of magnitude would open up a usage of practical applications.

If S_{ANE} reaches over 50 μV/K, their applications may be expanded widely.

What drives AHE and ANE? (See the review[1])

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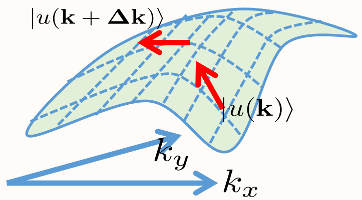
◆ Mechanism **1:** **spin-orbit coupling + ferromagnetism**

anomalous velocity generated by
Berry curvature

$$\Omega(\mathbf{k}) \equiv i\langle \partial_{\mathbf{k}} u_{\mathbf{k}} | \partial_{\mathbf{k}} u_{\mathbf{k}} \rangle$$

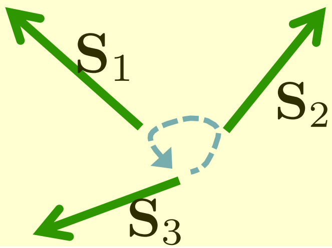
$$\psi_{\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$



in *momentum* space

◆ Mechanism **2:** **spin textures with finite chirality in real space**

Spin chirality $\mathbf{S}_1 \cdot (\mathbf{S}_2 \times \mathbf{S}_3)$
induces **Berry curvature**



[1] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys., **82**, 1539 (2010).

What drives AHE and ANE? (See the review[1])

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Intrinsic anomalous Hall conductivity (AHC)

Berry curv.

$$\sigma_{xy}^{AH} = \mathcal{C}\frac{e^2}{h} \quad \left(\mathcal{C} = \frac{1}{2\pi}\int_{E_{\mathbf{k}}<E_{\mathrm{F}}} d\mathbf{k}\Omega_z(\mathbf{k})\right)$$

For an isolated band in two dimensions,
C **is an integer called** ***Chern number.***

[1] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys., **82**, 1539 (2010).

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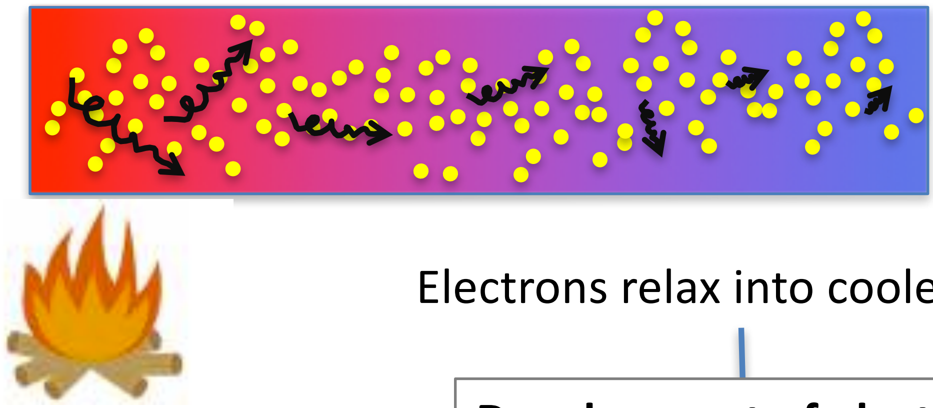
Basic theory of thermoelectricity

1. Semiclassical dynamics of electrons
2. Boltzmann transport + Linear response
3. Low temperature approximation

Thermoelectric Effect
- intuitive understanding -

$T + \Delta T$



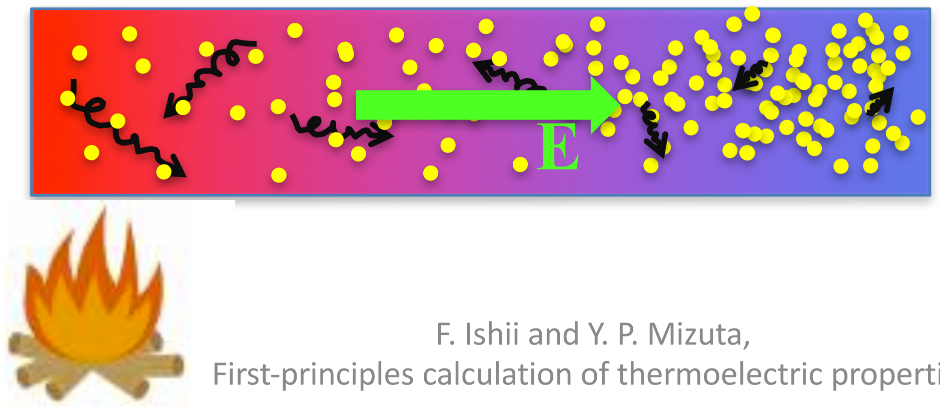
T

Electrons relax into cooler region.

Development of electric field
(Thermoelectric field)

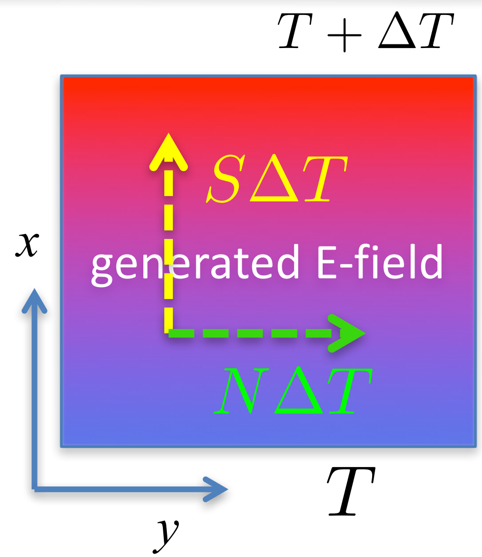
Electrons give up relaxing due to the pushing-back electrostatic force.

$T + \Delta T$



T

Thermoelectric coefficients

Without transverse transport	Including transverse (*xy*) transport
$\begin{cases} S_{xx} = S_0 \\ S_{yx} = 0 \end{cases}$	$\begin{cases} S_{xx} = \dfrac{S_0 + \theta_H N_0}{1+\theta_H^2} \\ S_{yx} = \dfrac{N_0 + \theta_H S_0}{1+\theta_H^2} \end{cases}$ 

conventional Seebeck $\boxed{S_0 = \dfrac{\alpha_{xx}}{\sigma_{xx}}}$

Hall angle $\boxed{\theta_H \equiv \dfrac{\sigma_{xy}}{\sigma_{xx}}}$

pure Nernst $\boxed{N_0 \equiv \dfrac{\alpha_{yx}}{\sigma_{xx}}}$

Conductivities are defined through the linear response relation of the charge current: $\mathbf{j} = \tilde{\sigma}\mathbf{E} + \tilde{\alpha}(-\nabla T)$

Semiclassical electron dynamics

A review including related topics:
D. Xiao, M-C. Chang, and Q. Niu, Rev. Mod. Phys. **82**, 1959 (2010).

Equation of motion of center coordinates $(\mathbf{r}, \mathbf{k})$ of wave-packet on band n [1] :

$$\dot{\mathbf{r}}_n = \frac{\partial \varepsilon_{n\mathbf{k}}}{\partial \mathbf{k}} - \dot{\mathbf{k}}_n \times \mathbf{\Omega}_{n\mathbf{k}}$$

$$\dot{\mathbf{k}}_n = q(\mathbf{E} + \dot{\mathbf{r}}_n \times \mathbf{B})$$

$\varepsilon_{n\mathbf{k}}$: band energy

$\mathbf{\Omega}_{n\mathbf{k}} = i\langle\partial_{\mathbf{k}} u_n| \times |\partial_{\mathbf{k}} u_n\rangle$: **Berry curvature** = **"magnetic field" in k-space**

[1] G. Sundaram and Q.Niu, Phys. Rev. B **59**, 14915 (1999).

Expression of charge current
- Brief review of Ref. [2] -

local current density

$$\mathbf{J} = q\sum_{n\mathbf{k}} \dot{\mathbf{r}}_{n\mathbf{k}} g_{n\mathbf{k}} + \nabla \times \sum_{n\mathbf{k}} f_{n\mathbf{k}} \mathbf{m}_{n\mathbf{k}}$$

orbital magnetic moment

classical particle contribution

quantum correction:
self-rotation of a wave-packet

transport current density (measured quantity)

orbital magnetization

$$\mathbf{j} = \mathbf{J} - \nabla \times \mathbf{M}(\mathbf{r})$$

$$= q\sum_{n\mathbf{k}} \left(\dot{\mathbf{r}}_{n\mathbf{k}} g_{n\mathbf{k}} + \nabla_{\mathbf{r}} \times \frac{1}{\beta(\mathbf{r})} \mathbf{\Omega}_{n\mathbf{k}} \log(1 + e^{-\beta(\mathbf{r})[\varepsilon_{n\mathbf{k}} - \mu(\mathbf{r})]}) \right)$$

[2] D. Xiao. Y. Yao, Z. Fang, and Q.Niu, Phys. Rev. Lett. **97**, 026603 (2006).

How to know the distribution $g_{n\mathbf{k}}$? - Boltzmann theory approach[3] -

Boltzmann equation :
(direct consequence of the Liouville's theorem = conservation of phase-space volume)

$$\mathrm{d}f = \partial_t f + \dot{\mathbf{k}} \cdot \partial_{\mathbf{k}} f + \dot{\mathbf{r}} \cdot \partial_{\mathbf{r}} f = \partial_t f_{n\mathbf{k}}|_{\mathrm{scatt.}}$$

Assumption:

- Small deviation from equilibrium state;
  $$f_{n\mathbf{k}} = f^0_{n\mathbf{k}} + g_{n\mathbf{k}}, \quad g \ll f^0$$
- local equilibrium; well-defined $T(\mathbf{r})$
- relaxation time approximation; $\partial_t f_{n\mathbf{k}}|_{\mathrm{scatt.}} \simeq -\dfrac{g_{n\mathbf{k}}}{\tau_{n\mathbf{k}}}$

When $\mathbf{B} = 0, \nabla\mu = 0$, keeping terms up to linear in $\mathbf{E}$ or ∇T,

$$g_{n\mathbf{k}} = \tau_{n\mathbf{k}} \dot{\mathbf{r}}_{n\mathbf{k}} \cdot \left[q\mathbf{E} + (\varepsilon_{n\mathbf{k}} - \mu) \left(-\frac{\nabla T}{T} \right) \right] \left(-\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}} \right)$$

[3] For example, see Chapter 7 of J.M. Ziman, *Principles of the theory of solids*, 2nd edition.

Details: From Boltz. eq. to $g_{n\mathbf{k}}$

(LHS) of Boltz.eq. with $\mathbf{B} = 0, \nabla\mu = 0$

$$= \partial_t g + (\mathbf{v}_0 + \mathbf{v}_a) \cdot (\partial_{\mathbf{r}} f^0 + \partial_{\mathbf{r}} g) + q\mathbf{E} \cdot (\partial_{\mathbf{k}} f^0 + \partial_{\mathbf{k}} g)$$

$$\simeq \partial_t g + \mathbf{v}_0 \cdot \left[(\varepsilon - \mu) \left(\frac{\nabla T}{T} \right) - q\mathbf{E} \right] \left(-\frac{\partial f^0}{\partial \varepsilon} \right),$$

where only the terms up to linear in $\mathbf{E}$ or ∇T were kept, based on the following:

- $\mathbf{v}_0 = \partial_{\mathbf{k}} \varepsilon \propto (\mathbf{E}^0,\ (\nabla T)^0)$ $\quad$ $\mathbf{v}_a = -q\mathbf{E} \times \mathbf{\Omega} \propto (\mathbf{E}^1,\ (\nabla T)^0)$
- $\partial_{\mathbf{r}} f^0 = (\varepsilon - \mu)\partial_{\mathbf{r}} \beta \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \left(-\frac{\partial \varepsilon}{\partial \xi} \right) = (\varepsilon - \mu) \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \left(\frac{\nabla T}{T} \right)$
- Since $g_{n\mathbf{k}}$ should be of the form $g = a(T)E_i + b(T)(\nabla T)_j$,

  $\partial_{\mathbf{r}} g = a'(T)E_i(\nabla T) + b'(T)(\nabla T)_j(\nabla T).$

Expression of conductivities

$$\mathbf{j} = q\sum_{n\mathbf{k}}\left(\dot{\mathbf{r}}_{n\mathbf{k}}(f^0_{n\mathbf{k}} + g_{n\mathbf{k}}) + \nabla_{\mathbf{r}} \times \frac{1}{\beta(\mathbf{r})}\boldsymbol{\Omega}_{n\mathbf{k}}\log(1 + e^{-\beta(\mathbf{r})[\varepsilon_{n\mathbf{k}}-\mu(\mathbf{r})]})\right)$$

$$g_{n\mathbf{k}} = \tau_{n\mathbf{k}}\dot{\mathbf{r}}_{n\mathbf{k}} \cdot \left[q\mathbf{E} + (\varepsilon_{n\mathbf{k}} - \mu)\left(-\frac{\nabla T}{T}\right)\right]\left(-\frac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}\right)$$

$$\dot{\mathbf{r}}_n = \frac{\partial \varepsilon_{n\mathbf{k}}}{\partial \mathbf{k}} - q\mathbf{E} \times \boldsymbol{\Omega}_{n\mathbf{k}}$$

Comparing term-by-term with the definition: $\mathbf{j} = \tilde{\sigma}\mathbf{E} + \tilde{\sigma}(-\nabla T)$,
the form of $\tilde{\sigma} = [\sigma^{\mathrm{vv}}_{ij} + \sigma^{\Omega}_{ij}]$ and $\tilde{\alpha} = [\alpha^{\mathrm{vv}}_{ij} + \alpha^{\Omega}_{ij}]$ is found as,

$$\begin{cases} \sigma^{\mathrm{vv}}_{ij} = \dfrac{q^2}{V}\displaystyle\sum_{n\mathbf{k}} \tau_{n\mathbf{k}} v^{n\mathbf{k}}_i v^{n\mathbf{k}}_j \left(-\dfrac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}\right), \\ \sigma^{\Omega}_{ij} = -\dfrac{q^2}{V}\displaystyle\sum_{n\mathbf{k}} \Omega^{n\mathbf{k}}_{ij} f^0_{n\mathbf{k}} \end{cases}$$

anomalous Hall effect (AHE)

$$\begin{cases} \alpha^{\mathrm{vv}}_{ij} = \dfrac{qk_{\mathrm{B}}}{V}\displaystyle\sum_{n\mathbf{k}} \tau_{n\mathbf{k}} v^{n\mathbf{k}}_i v^{n\mathbf{k}}_j \left(\dfrac{\varepsilon_{n\mathbf{k}} - \mu}{k_{\mathrm{B}}T}\right)\left(-\dfrac{\partial f^0_{n\mathbf{k}}}{\partial \varepsilon_{n\mathbf{k}}}\right), \\ \alpha^{\Omega}_{ij} = -\dfrac{qk_{\mathrm{B}}}{V}\displaystyle\sum_{n\mathbf{k}} \Omega^{n\mathbf{k}}_{ij}\left[\left(\dfrac{\varepsilon_{n\mathbf{k}} - \mu}{k_{\mathrm{B}}T}\right) f^0_{n\mathbf{k}} + \log(1 + e^{-\beta(\varepsilon_{n\mathbf{k}}-\mu)})\right] \end{cases}$$

anomalous Nernst effect (ANE)

F. Ishii and Y. P. Mizuta,
First-principles calculation of thermoelectric properties

Relation between $\tilde{\sigma}$ & $\tilde{\alpha}$

They can be rewritten as

$$\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(T,\mu) = \int d\varepsilon \left[\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(\varepsilon)\right]_{T=0,\mu=\varepsilon} \left(-\frac{\partial f^0(T,\mu)}{\partial \varepsilon}\right),$$

$$\alpha_{ij}^{(\mathrm{vv},\ \Omega)}(T,\mu) = \frac{k_\mathrm{B}}{q} \int d\varepsilon \left[\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(\varepsilon)\right]_{T=0,\mu=\varepsilon} \left(\frac{\varepsilon-\mu}{k_\mathrm{B}T}\right) \left(-\frac{\partial f^0(T,\mu)}{\partial \varepsilon}\right)$$

Therefore, the only system-characteristic information needed to calculate these

is the Fermi-energy dependence $\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(\varepsilon_\mathrm{F})$.

Low temperature approximation

Making use of the Sommerfeld expansion (valid when $k_\mathrm{B}T \ll \varepsilon_F$):

$$\int_0^\infty d\varepsilon H(\varepsilon)\left(-\frac{\partial f^0}{\partial \varepsilon}\right) = H(\varepsilon_F) + (\mu - \varepsilon_F)H'(\varepsilon_F) + \frac{\pi^2}{6}H''(\varepsilon_F)(k_\mathrm{B}T)^2 + \mathcal{O}((k_\mathrm{B}T)^4),$$

conductivities are approximated up to T-linear terms as,

$$H(\varepsilon) \equiv \left[\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(\varepsilon)\right]_{T=0,\mu=\varepsilon} \Rightarrow \sigma_{ij}^{(\mathrm{vv},\ \Omega)}(T,\mu) \simeq \sigma_{ij}^{(\mathrm{vv},\ \Omega)}(0,\varepsilon_F)$$

$$H(\varepsilon) \equiv \left[\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(\varepsilon)\right]_{T=0,\mu=\varepsilon}\left(\frac{\varepsilon-\mu}{k_\mathrm{B}T}\right) \Rightarrow \alpha_{ij}^{(\mathrm{vv},\ \Omega)}(T,\mu) = \frac{\pi^2 k_\mathrm{B}^2}{3q}\frac{d\sigma_{ij}^{(\mathrm{vv},\ \Omega)}(0,\varepsilon_F)}{d\varepsilon_F}T$$

Mott rule

and likewise approximated thermoelectric coefficients are

$$S_{xx} = \frac{\pi^2 k_\mathrm{B}^2}{3q}\frac{1}{1+\theta_H^2}\frac{\sigma' + \theta_H \sigma'_{xy}}{\sigma}T, \qquad S_{yx} = \frac{\pi^2 k_\mathrm{B}^2}{3q}\frac{1}{1+\theta_H^2}\frac{\sigma'_{yx} + \theta_H \sigma'}{\sigma}T$$

with all quantities on the RHS being evaluated at T=0, and $\sigma_{xx} = \sigma_{yy} \equiv \sigma$ was assumed for simplicity.

F. Ishii and Y. P. Mizuta,
First-principles calculation of thermoelectric properties

Outline

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I. Introduction
   I. Thermoelectric effect
   II. Anomalous Thermoelectric effect
   III. Basic theory of thermoelectricity
II. Frist-principles calculations
III. Summary

Method and Procedures

Spin texture in real-space

First-principles calculation

with ***OpenMX*** [1]

spin constraining method

Self-consistent electronic states

: almost fully spin-polarized in the desired texture

Wannier90 [2]

Maximally localized Wannier functions

Wannier90

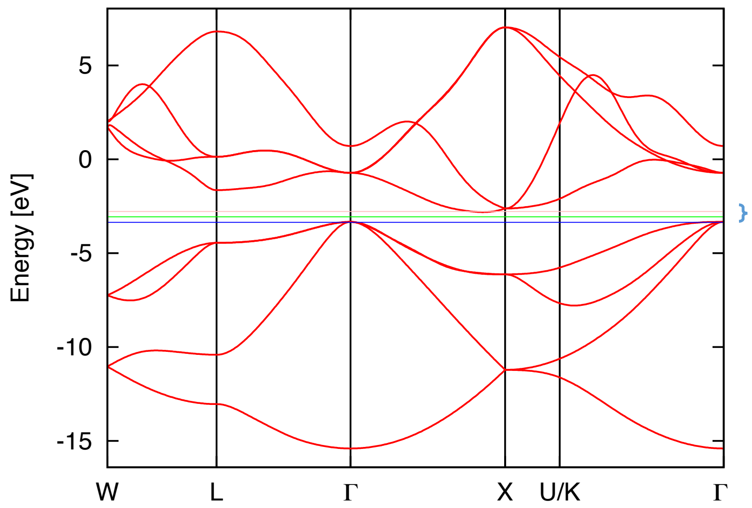
Transport coefficients

Semiclassical Boltzmann theory with constant relaxation time τ for σ_{xx} and S_0

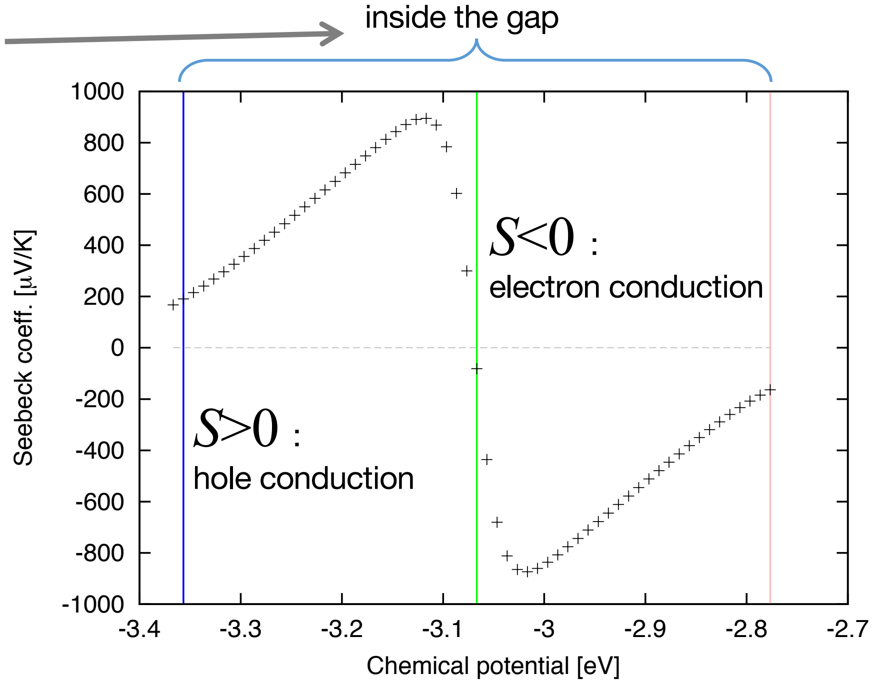
[1] www.openmx-squatre.org [2] www.wannier.org

Seebeck coefficient of silicon

An approach with ***OpenMX*** + ***Wannier90***



◀ 8 Wannier bands
constructed from *OpenMX* solutions
via *Wannier90*



▶ Seebeck coefficient at T=300K
estimated from the 8 Wannier bands

First-principles calculations of thermoelectric properties including AHE/ANE

Examples: AHE by mechanism 1

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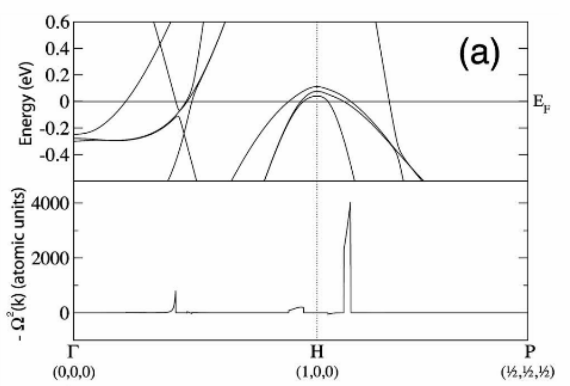
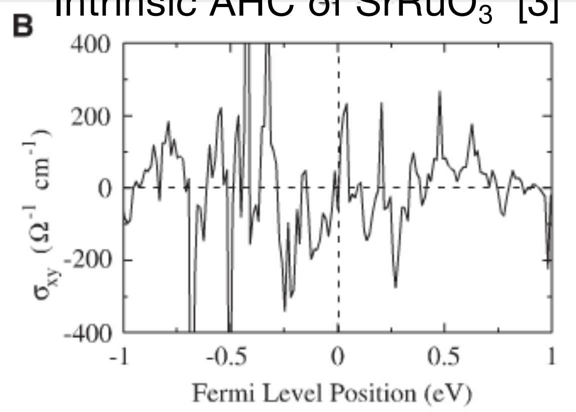
spin-orbit coupling + ferromagnetism

Berry curvature (lower panel) of bcc Fe [2]



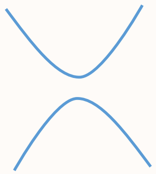
Intrinsic AHC of $SrRuO_3$ [3]



Our previous study [Y. P. Mizuta and F. Ishii, JPS Conf. Proc. **5**, 011023 (2015)]

Dirac electron with Zeeman splitting (DZ model)

simplest model of magnetic topological surfaces/interfaces



dispersion of DZmodel

Rather large effect of AHE/ANE on TE found!

[2] X.Wang *et al.*, Phys. Rev. B **74**, 195118 (2006).

[3] Z. Fang *et al.*, Science **302**, 92 (2003).

An example: AHE by mechanism 2

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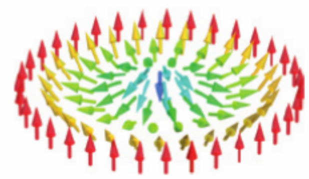
spin textures with finite chirality in real space

Previous study as a background of this study:

PHYSICAL REVIEW B **92**, 115417 (2015)

Quantized topological Hall effect in skyrmion crystal

Keita Hamamoto,[1] Motohiko Ezawa,[1] and Naoto Nagaosa[1,2]
[1]*Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[2]*RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan*
(Received 22 April 2015; published 11 September 2015)



single skyrmion

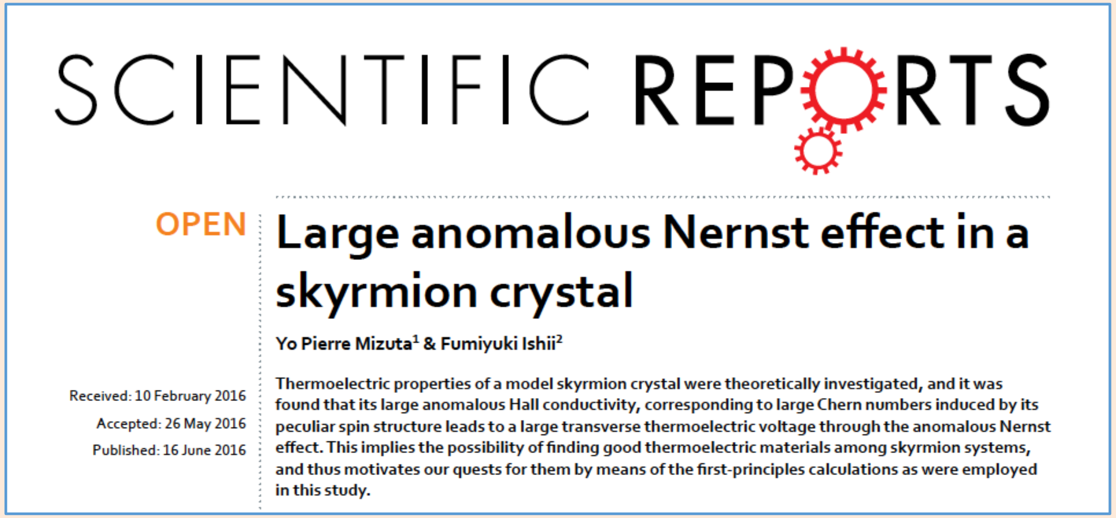
"Skyrmion crystal (SkX) ---> large AHC"

Aim of this study

good TE properties??

- s-orbital SkX model –
(Hydrogen Atom with OpenMX)

Y. P. Mizuta and F. Ishii, *Scientific Reports* **6,** 28076 (2016)


SCIENTIFIC REPORTS

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Large anomalous Nernst effect in a skyrmion crystal

Yo Pierre Mizuta[1] & Fumiyuki Ishii[2]

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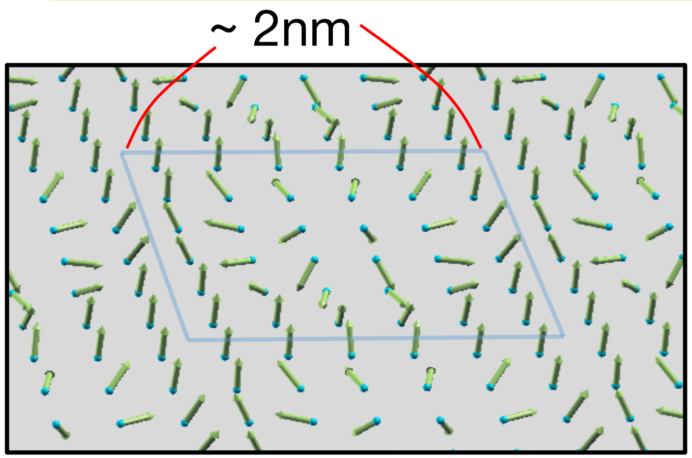
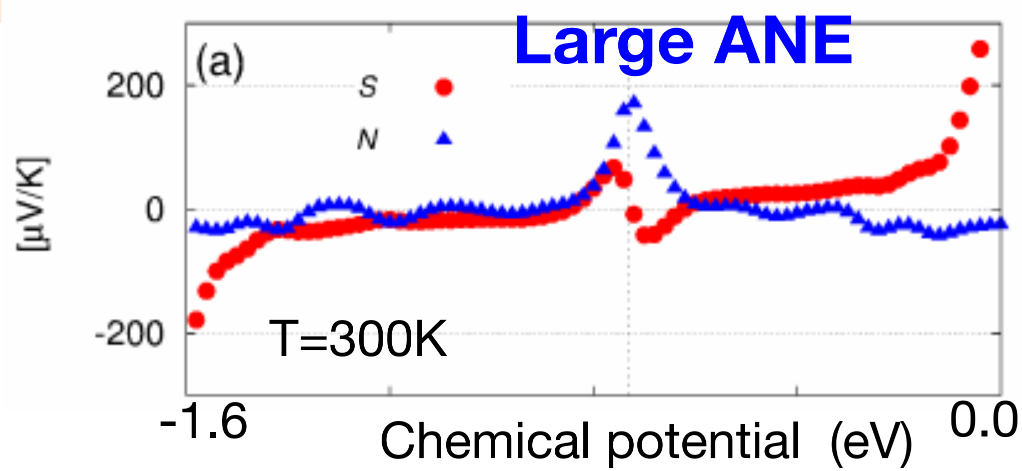
Accepted: 26 May 2016
Published: 16 June 2016

Thermoelectric properties of a model skyrmion crystal were theoretically investigated, and it was found that its large anomalous Hall conductivity, corresponding to large Chern numbers induced by its peculiar spin structure leads to a large transverse thermoelectric voltage through the anomalous Nernst effect. This implies the possibility of finding good thermoelectric materials among skyrmion systems, and thus motivates our quests for them by means of the first-principles calculations as were employed in this study.

http://dx.doi.org/10.1038/srep28076





Model SkX

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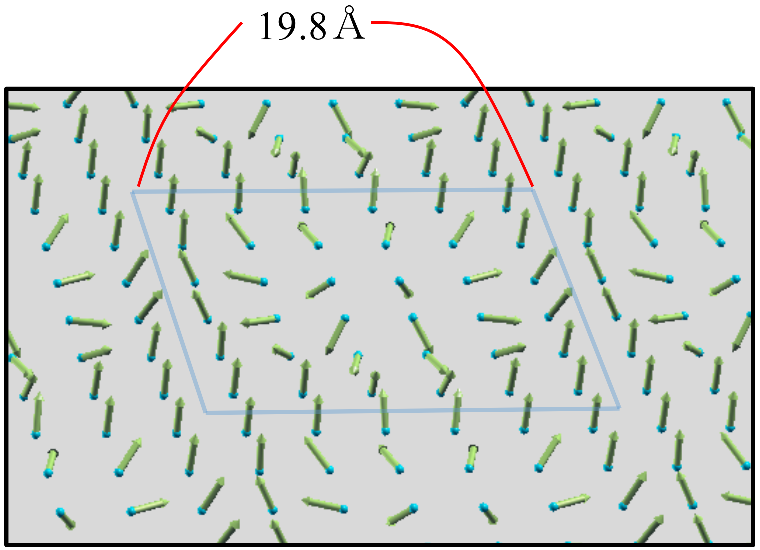


◀ system of n=6

- Skyrmions on a square lattice
- Spin-1/2 of Hydrogen atom
- Unitcell containing $n \times n$ sites (n=6, 8, 10, 12)
- ***Constraint Density Functional Theory***

Large anomalous Nernst effect in a Skyrmion crystal
Y. P. Mizuta and F. Ishii, *Scientific Reports* **6,** 28076 (2016)

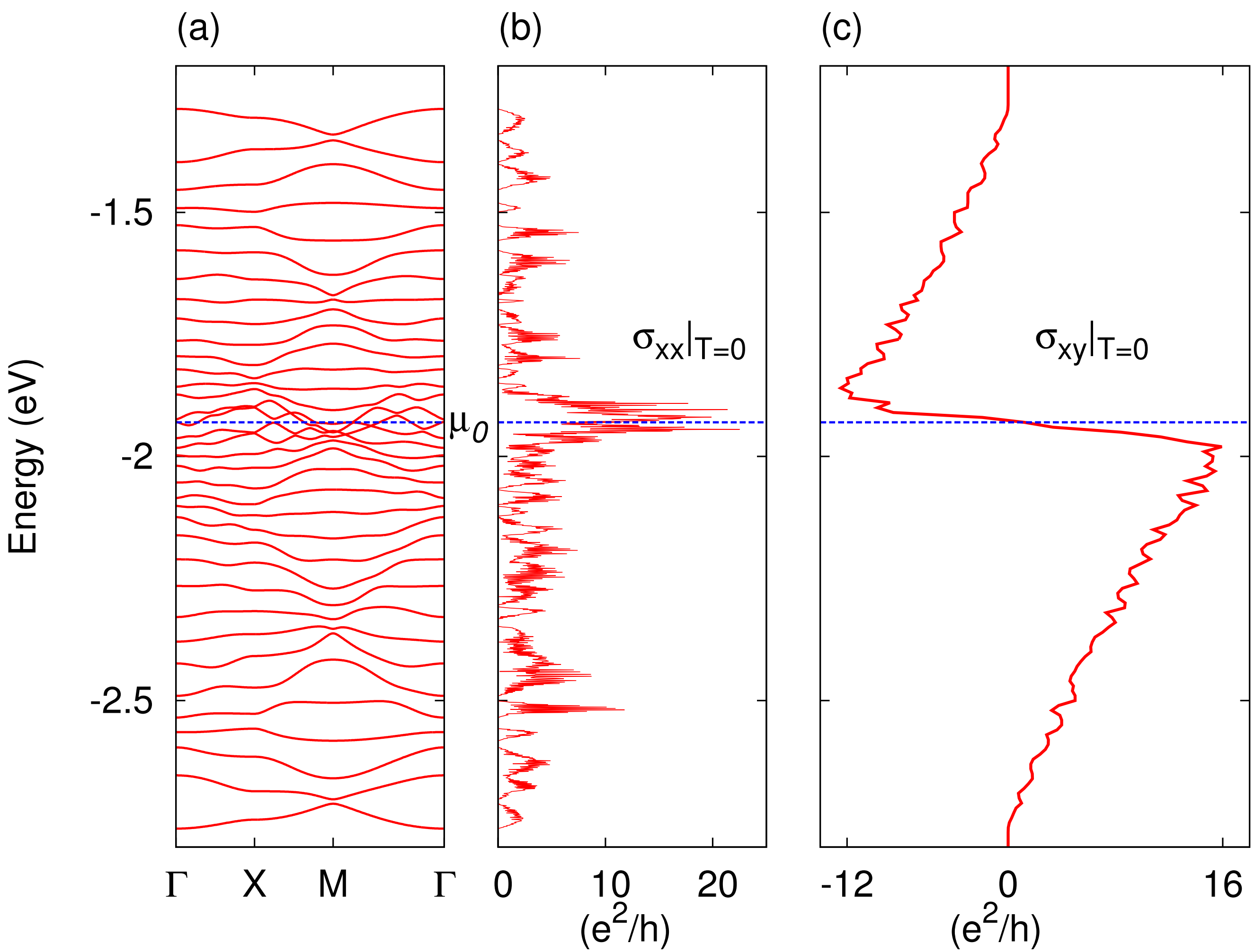
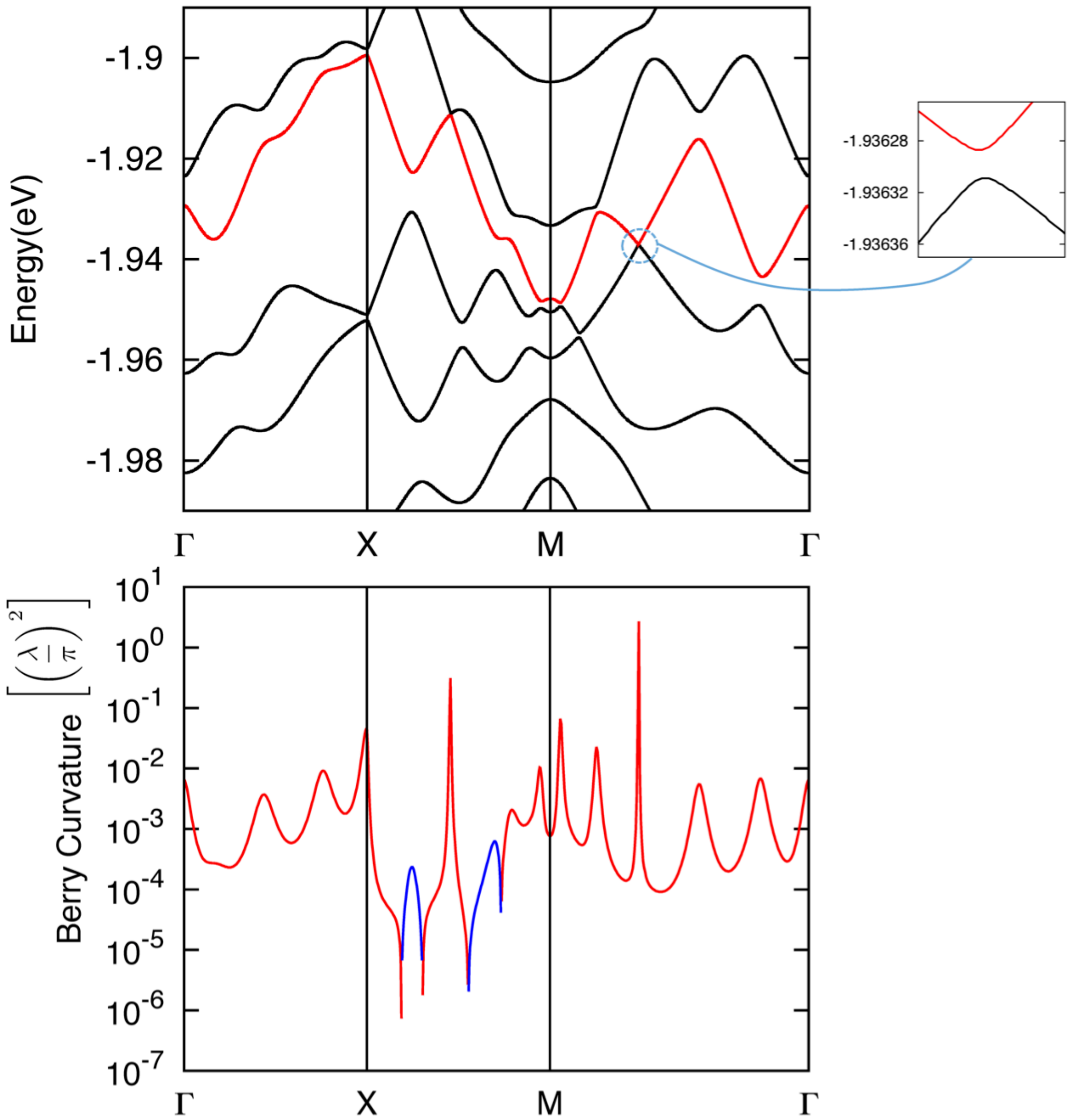


Figure 2. (**a**) Band structure and Fermi energy dependence of (**b**) longitudinal and (**c**) anomalous Hall conductivity of 6×6 SkX. The blue dashed line indicates the μ_0 mentioned in the main text.



(Top) Band dispersion of central bands and (Bottom) Berry curvature on 21th (from the lowest) band (red line in the top panel) along the path Γ-X-M-Γ. The latter is in logarithmic scale and the red (blue) part indicates its positive (negative) value. The Berry curvature is in unit of $(\lambda/\pi)^2$, where λ is half the value of the lattice constant.

Variation with size n=6, 8, 10, 12

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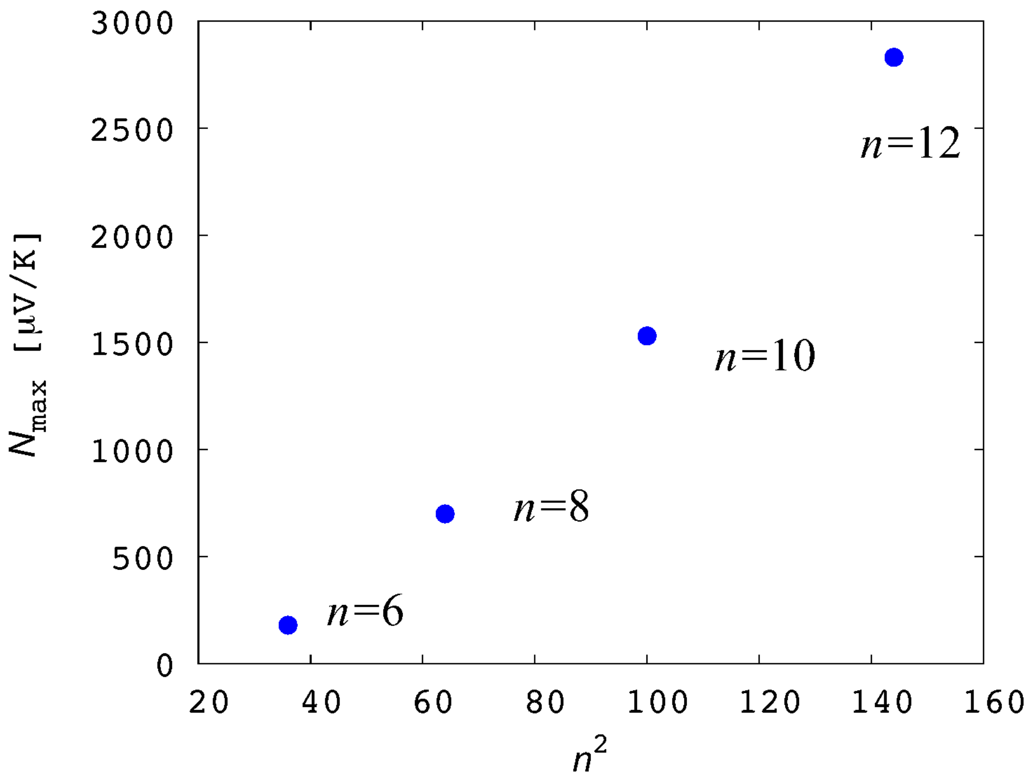

Variation of the maximum N in the space of μ as the skyrmion size (n^2) grows.

Larger SkX gives stronger TE voltage

Summary

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- Basic theory to calculate thermoelectricity based on Boltzmann transport equation
- Contribution of Berry curvature (AHE) to thermoelectricity (Seebeck, ANE)
- First-principles calculations of Seebeck and anomalous Nernst coefficient