# Application of interface to Wannier90
# : anomalous Nernst effect

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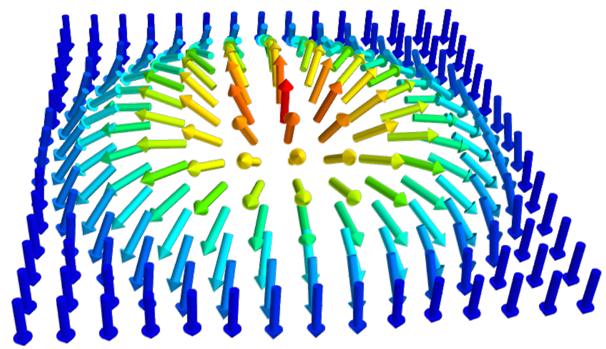

스키루미온

# Outline

1. Interface to Wannier90
2. Anomalous Nernst effect

# Wannier90 http://www.wannier.org

WANNIER90

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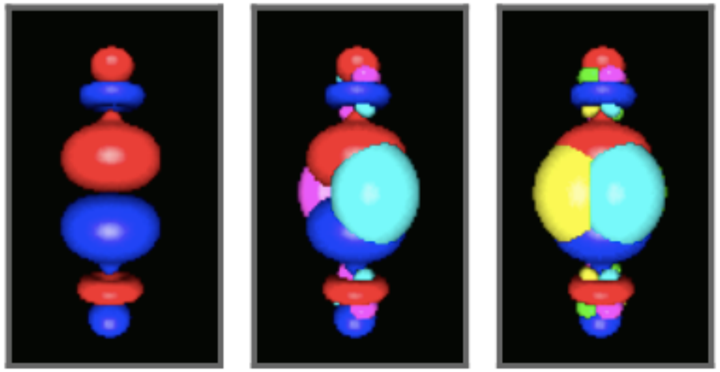
## Welcome!

This is the home of maximally-localised Wannier functions (MLWFs) and Wannier90, the computer program that calculates them. Wannier90 is released under the GNU General Public License.



## Latest News

**2 APRIL 2015**

Wannier90 (v2.0.1) is now available for download here.

See here for our news archive.

# Capabilities of Wannier90

- Boltzmann transport (Seebeck etc.)
- Quantum transport
- Anomalous Hall effect
- Optical conductivity
- Orbital magnetization

# Interface with Wannier90

## Calculations with OpenMX

**(1) SCF calculation with OpenMX**

**Input**: Keywords in the input file of OpenMX

| | |
|---|---|
| Wannier.Func.Calc | on |
| Wannier90.fileout | on |

**(2) Calculation of overlap and projection matrices with OpenMX**

**Output**: Generated files being input files for Wannier90

| | |
|---|---|
| System.Name.mmn | $M_{mn}^{(\mathbf{k},\mathbf{b})} = \langle u_{m\mathbf{k}} \vert u_{n,\mathbf{k}+\mathbf{b}} \rangle$ |
| System.Name.amn | $A_{mn} = \langle \psi_{m\mathbf{k}} \vert g_n \rangle$ |
| System.Name.eig | $\varepsilon_{n,\mathbf{k}}$ |
| System.Name.win | Input of wannier90 |

## Calculations with Wannier90

**(3) Calculation of maximally localized Wannier functions with Wannier90**

**Input**: for wannier90.x in Wannier90

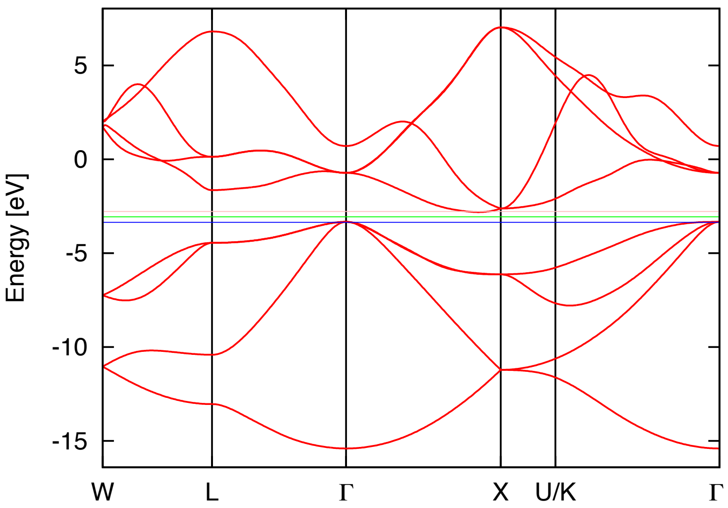
| | |
|---|---|
| System.Name.mmn | $M_{mn}^{(\mathbf{k},\mathbf{b})} = \langle u_{m\mathbf{k}} \vert u_{n,\mathbf{k}+\mathbf{b}} \rangle$ |
| System.Name.amn | $A_{mn} = \langle \psi_{m\mathbf{k}} \vert g_n \rangle$ |
| System.Name.eig | $\varepsilon_{n,\mathbf{k}}$ |
| System.Name.win | Input of wannier90 |

**Using postw90.x**

**(4) Calculation of physical properties such as optical conductivity**

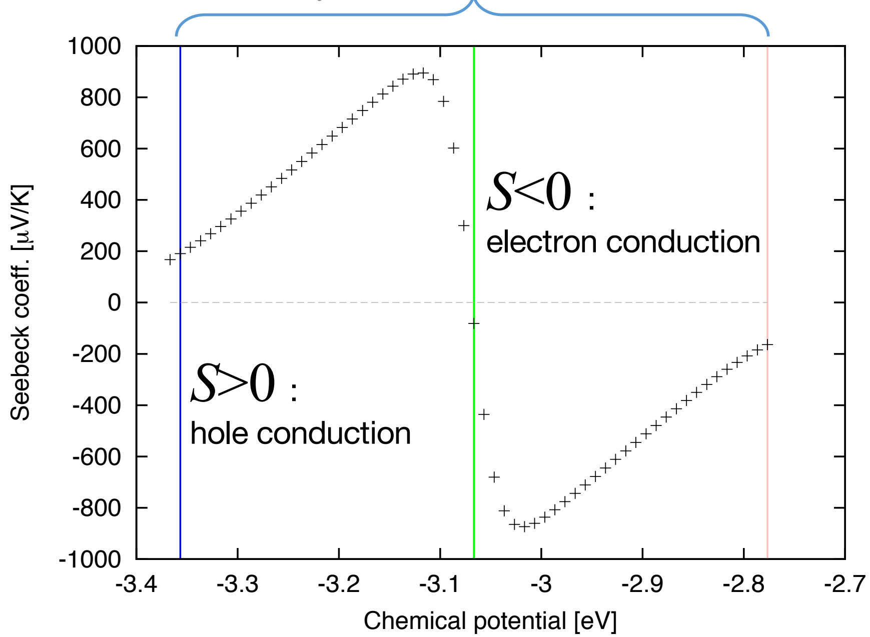
# Seebeck coefficient of silicon

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



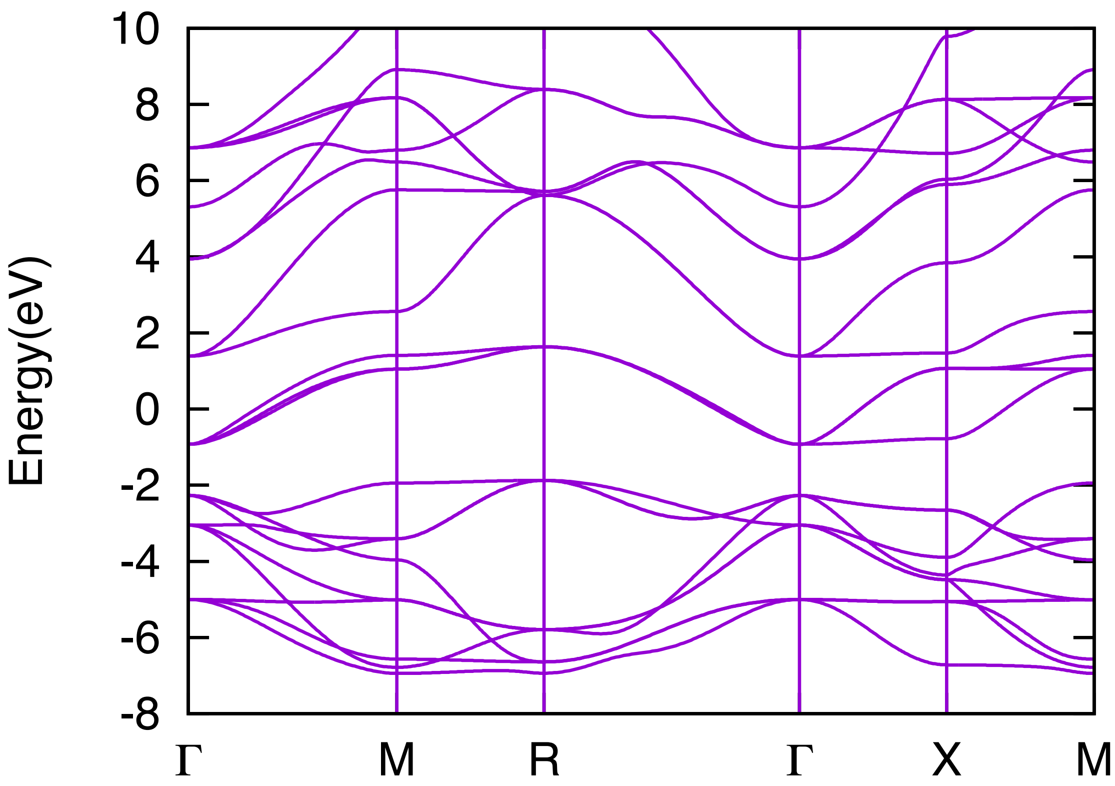

- 8 Wannier bands constructed from *OpenMX* solutions via *Wannier90*

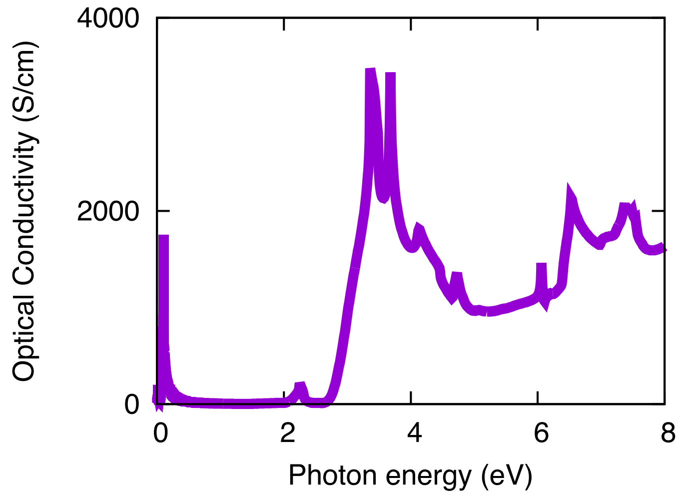
inside the gap



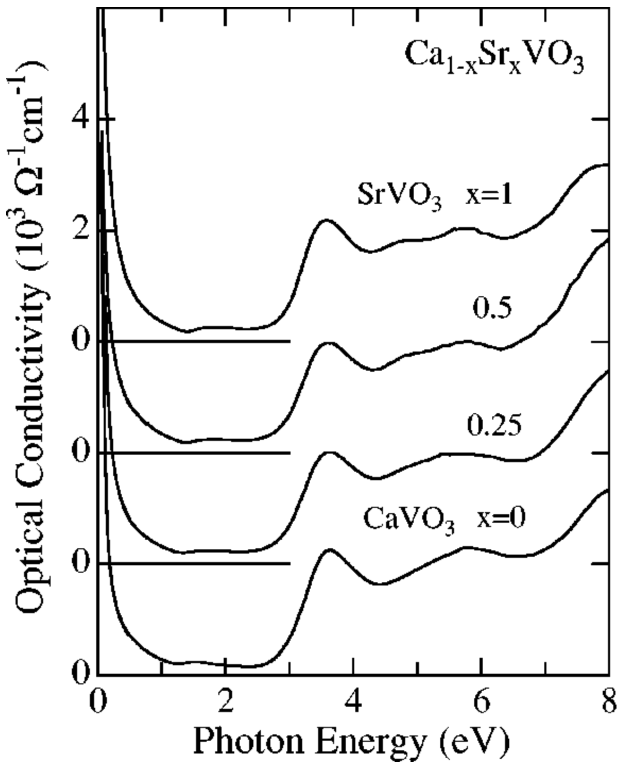

- Seebeck coefficient at $T$=300K estimated from the 8 Wannier bands

# Optical conductivity of $SrVO_3$




Experiment:
Makino et al., PRB 58 4384(1998)



# Thermoelectric coefficients

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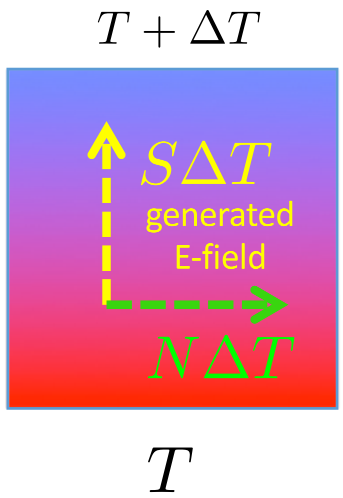
Y. P. Mizuta, & F. I, JPS Conf. Proc. **3**, 017035(2014), ibid. **5**, 011023 (2015).
Sci. Rep. **6**, 2876(2016)

Seebeck coeff. $$S = \frac{S_0 + \theta_H N_0}{1+\theta_H^2}$$

Nernst coeff. $$N = \frac{N_0 - \theta_H S_0}{1+\theta_H^2}$$




$$\sigma_{xx} = e^2\tau \sum_n \int d\mathbf{k}\, v_x^n(\mathbf{k})^2 \left(-\frac{\partial f}{\partial \varepsilon_{n\mathbf{k}}}\right),$$

$$\sigma_{xy} = -\frac{e^2}{\hbar}\sum_n \int d\mathbf{k}\, \Omega_z^n(\mathbf{k}) f(\varepsilon_{n\mathbf{k}}) = -\sigma_{yx},$$

$$\alpha_{ij} = \frac{1}{e}\int d\varepsilon \sigma_{ij}(\varepsilon)|_{T=0} \frac{\varepsilon-\mu}{T}\left(-\frac{\partial f}{\partial \varepsilon}\right)$$
$$\text{for} \quad i = x \text{ or } y, \quad j = x \text{ or } y,$$

pure (conventional) Seebeck coeff. $$S_0 \equiv \frac{\alpha_{xx}}{\sigma_{xx}}$$

Hall angle $$\theta_H \equiv \frac{\sigma_{xy}}{\sigma_{xx}}$$

pure Nernst coeff. $$N_0 \equiv \frac{\alpha_{xy}}{\sigma_{xx}}$$

linear response conductivities in
$$\mathbf{j} = \tilde{\sigma}\mathbf{E} + \tilde{\alpha}(-\nabla T)$$

# Mechanism for Large Seebeck Coefficient

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

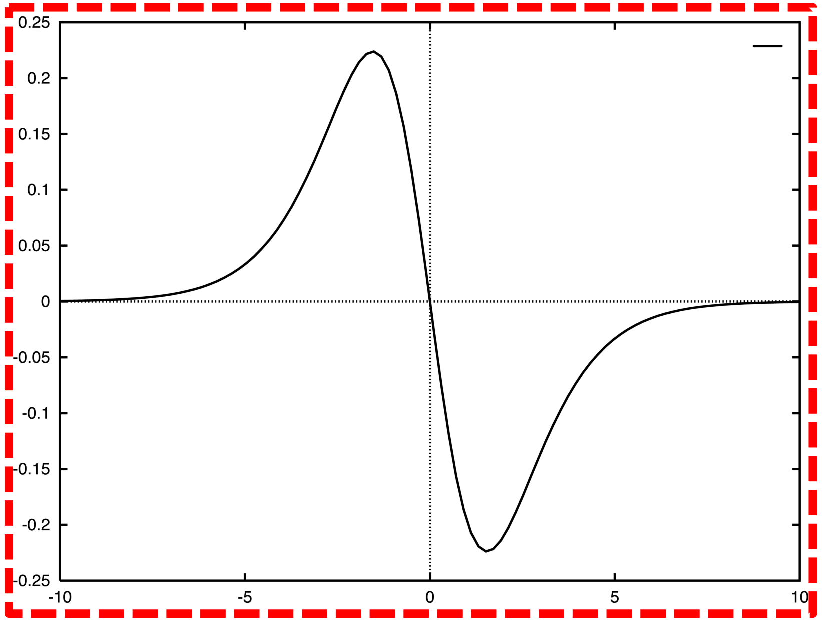
$$\sigma_{xx}(\varepsilon) = e^2 D(\varepsilon) v_x^2(\varepsilon)\tau$$

$\tau$ : constant approximaion

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

**is origin of large S**

**Narrow gap semiconductor, Semimetals**



# Mechanism for Large Nernst Coefficient

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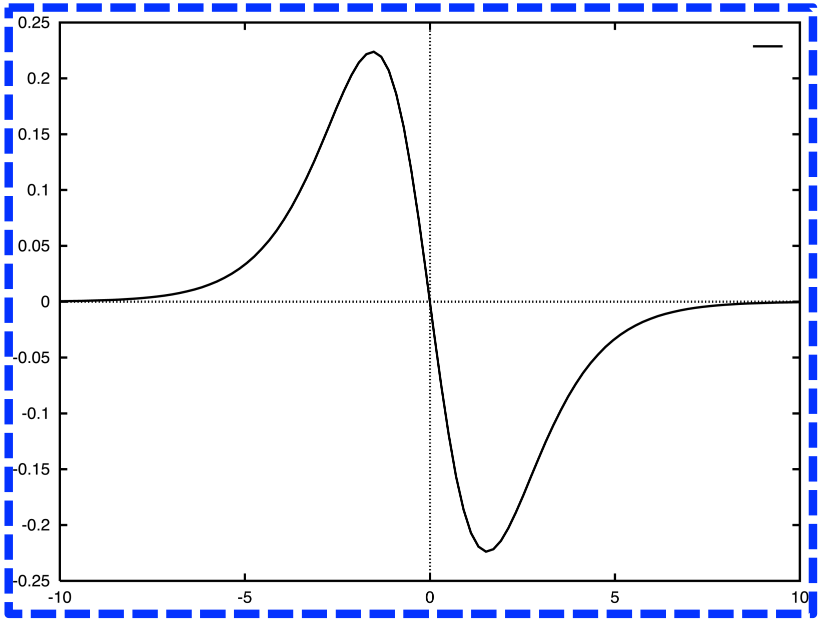
$$N_0 = -\frac{k_B}{e} \frac{\int d\varepsilon \frac{\varepsilon - \mu}{k_B T} \frac{df(\varepsilon)}{d\varepsilon} \sigma_{xy}(\varepsilon)}{\int d\varepsilon \frac{df(\varepsilon)}{d\varepsilon} \sigma_{xx}(\varepsilon)}$$

$$\sigma_{xy}(\varepsilon) = \frac{e^2}{h} D(\varepsilon)\Omega(\varepsilon)$$

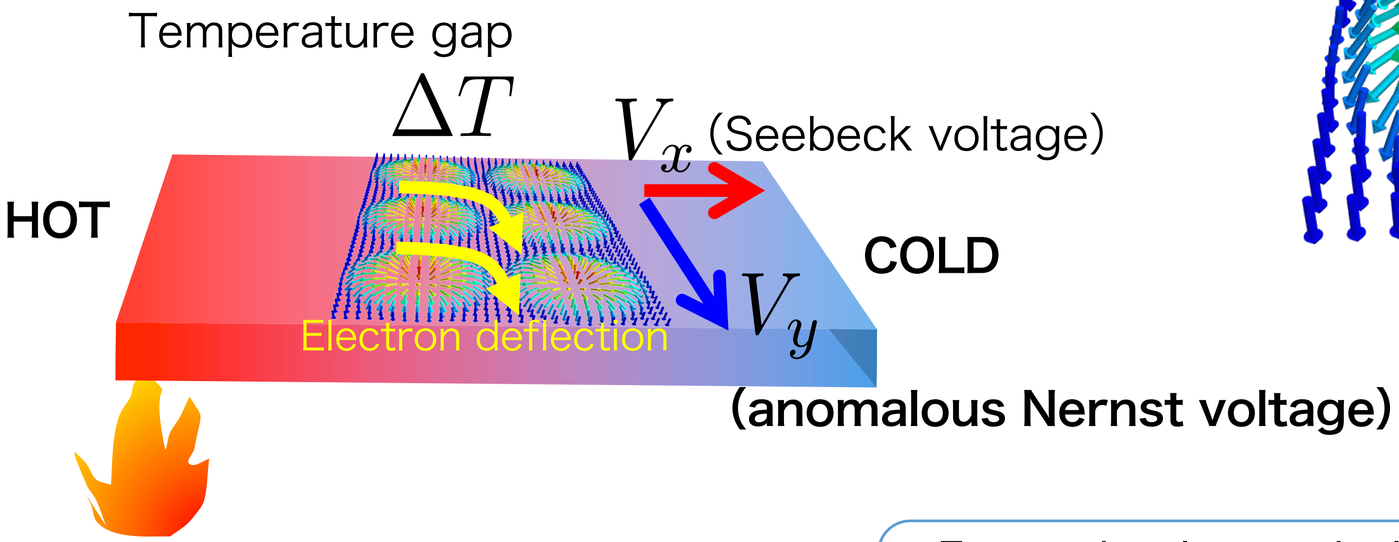


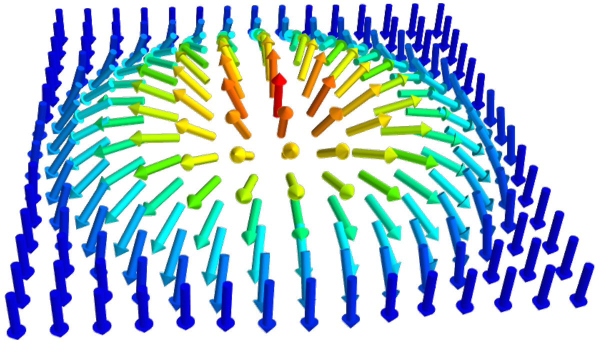

**Asymmetry in $\sigma_{xy}(\varepsilon)$ : $\Omega(\varepsilon)$, $D(\varepsilon)$,**

**is origin of large $N_0$**

**Candidate Material ?**

# Anomalous Nernst Effect (ANE) in Skyrmion Crystal



non-trivial spin texture (SkX etc.)

→ emergent "magnetic field"

→ Berry curvature in k-space: $\Omega_z(\mathbf{k})$

→ anomalous Hall conductivity (AHC)

anomalous Nernst conductivity (ANC)

※ For any insulator or isolated band,

$$\sigma^A_{xy} = \mathcal{C}\frac{e^2}{h}$$ $\mathcal{C}$: Chern number

$$\sigma^A_{xy} = -\frac{e^2}{\hbar}\sum_n \int d\mathbf{k}\ [\boldsymbol{\Omega}_n(\mathbf{k})]_z f(\varepsilon_{n\mathbf{k}})$$

$$\alpha^A_{xy} = \frac{1}{e}\int d\varepsilon [\sigma^A_{xy}(\varepsilon)]_{T=0}\frac{\varepsilon-\mu}{T}\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

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

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

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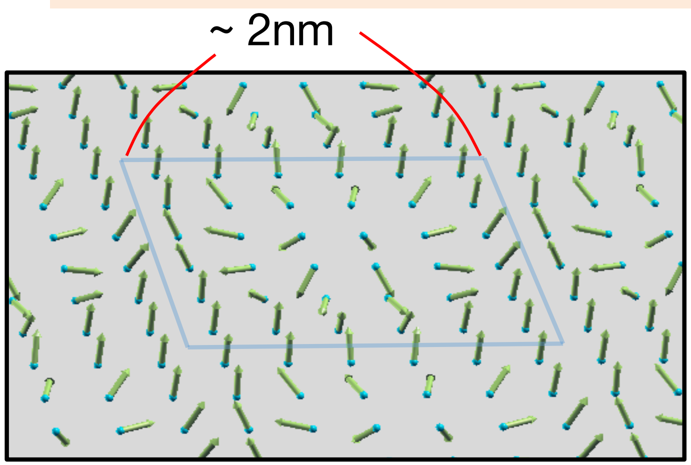
## Large anomalous Nernst effect in a skyrmion crystal

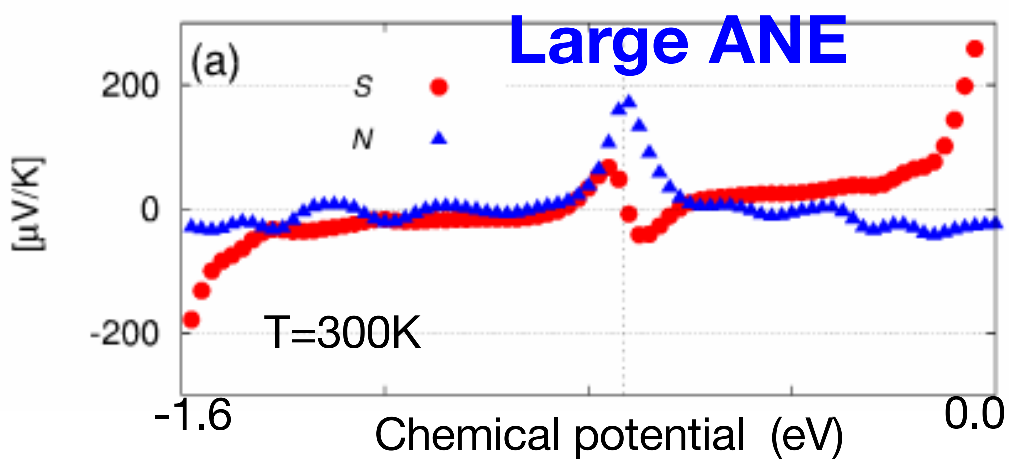
Yo Pierre Mizuta[1] & Fumiyuki Ishii[2]

Received: 10 February 2016
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



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

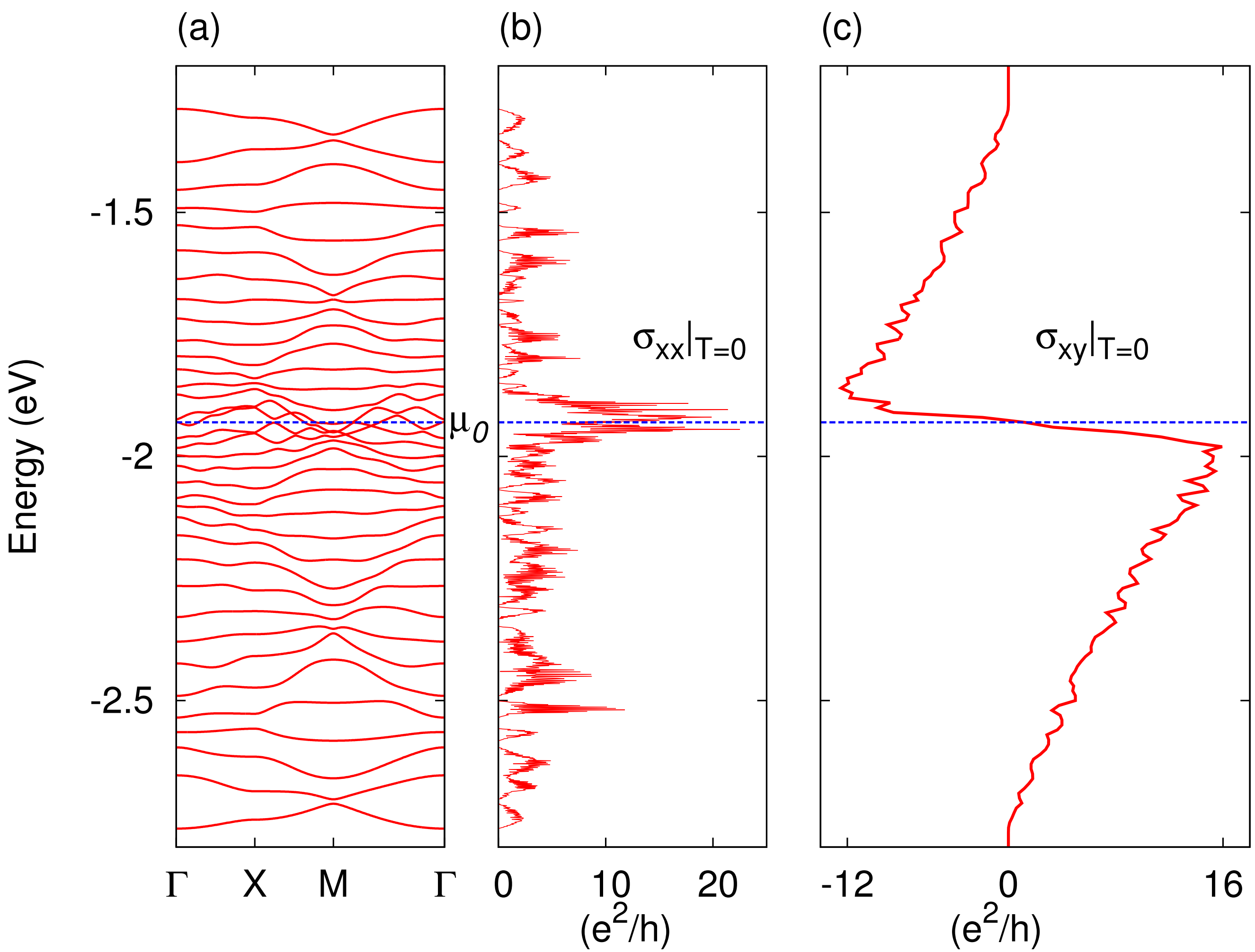



**Figure 2.** (**a**) Band structure and Fermi energy dependence of (**b**) longitudinal and (**c**) anomalous Hall conductivity of $6 \times 6$ SkX. The blue dashed line indicates the $\mu_0$ mentioned in the main text.

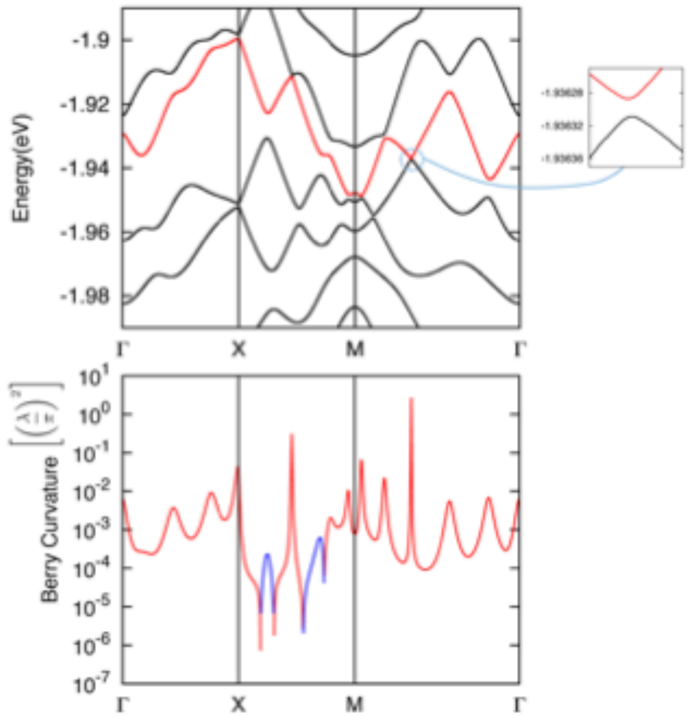



**Figure 2.** (Top) Band dispersion of central bands and (Bottom) Berry curvature on 21th (from the lowest) band (red line in the top panel) along the path Γ-X-M-Γ. The latter is in logarithmic scale and the red (blue) part indicates its positive (negative) value. The Berry curvature is in unit of $(\lambda/\pi)^2$,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

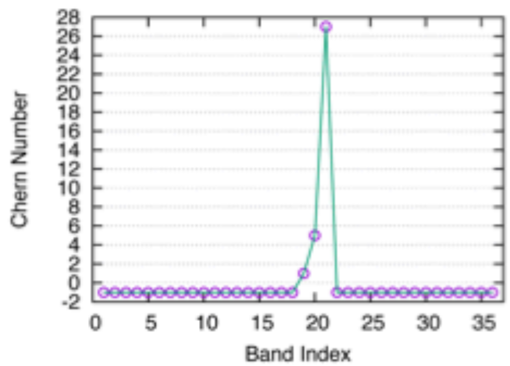
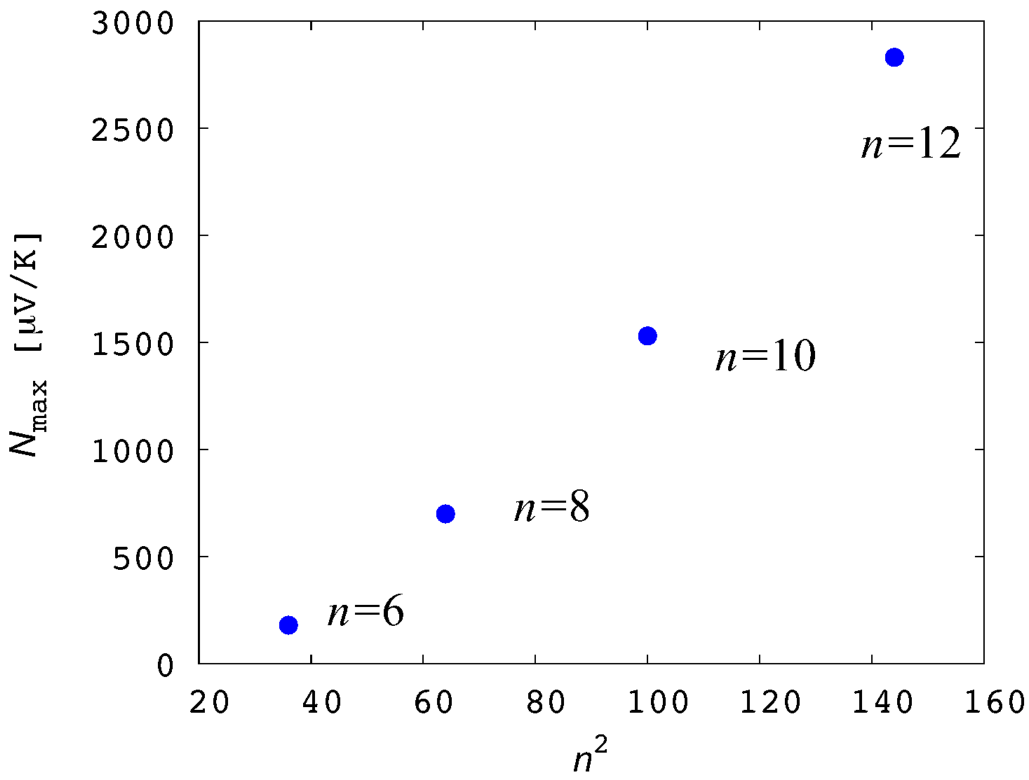



**Figure 3.** The band index dependence of Chern number.

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






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

**Larger SkX gives stronger TE voltage**