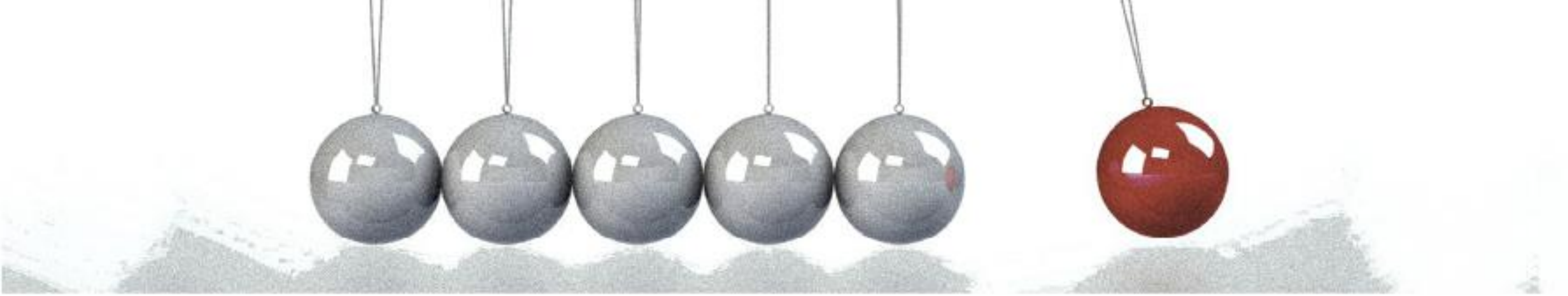

UiO : Department of Physics
University of Oslo

Thermoelectric Phenomena
and
Bulk and Interface Transport

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Outline:

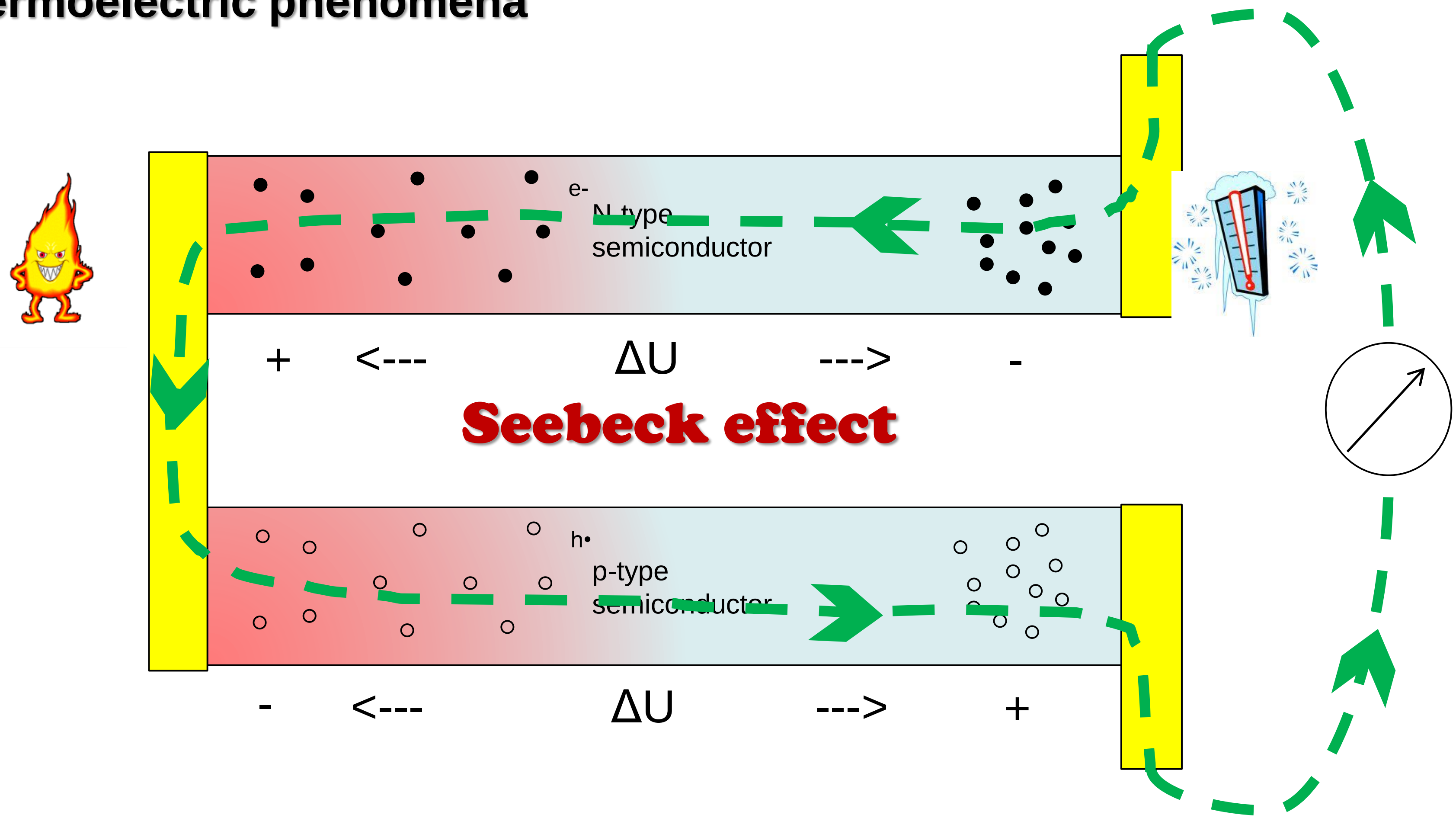
- **Bulk transport** – two approaches

  Laudauer approach – illustrative for phenomena

  BTE – describtive for correlations in transport

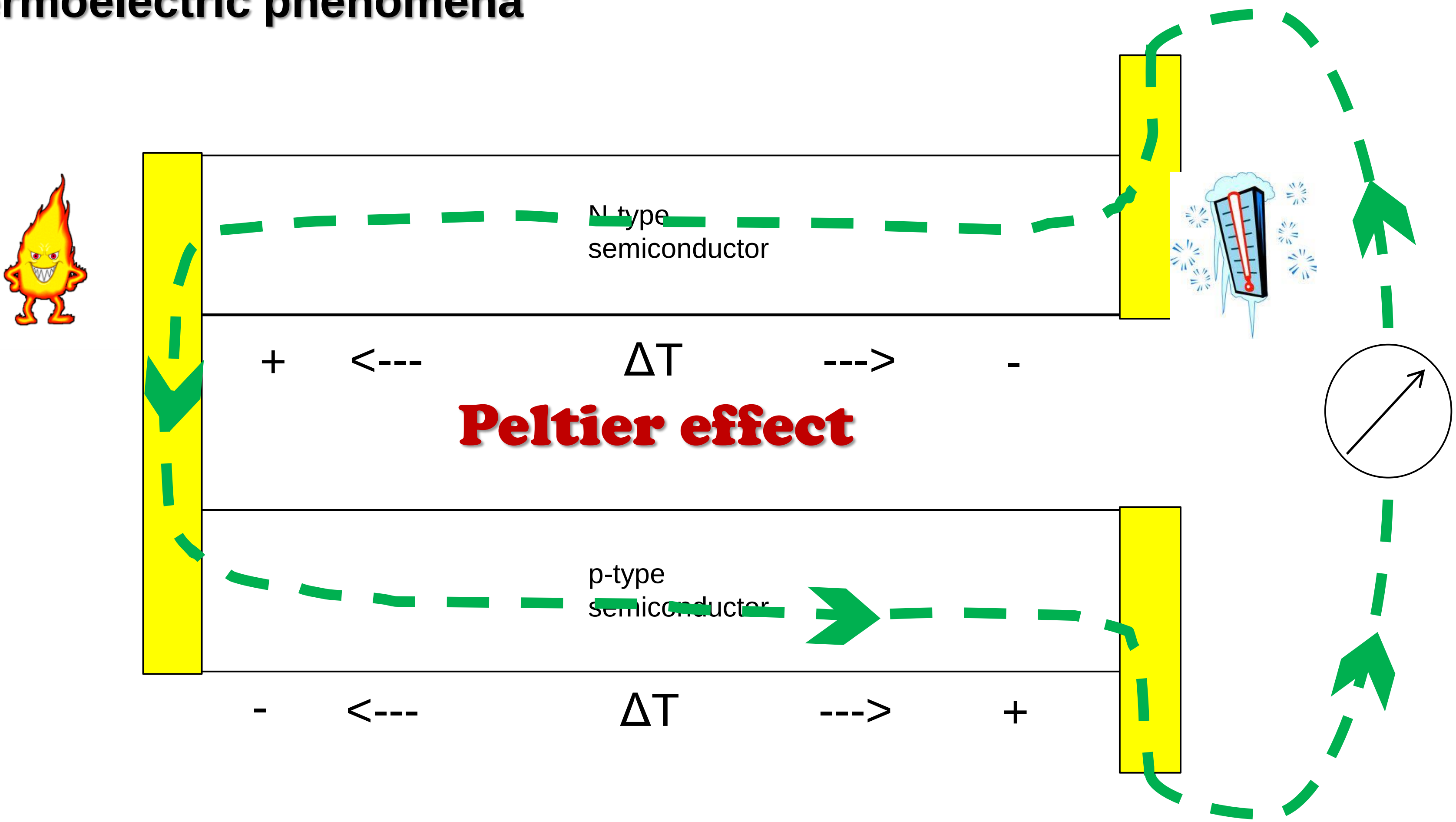
- **Transport at interface**

Thermoelectric phenomena



Thermoelectric circuit

Thermoelectric phenomena

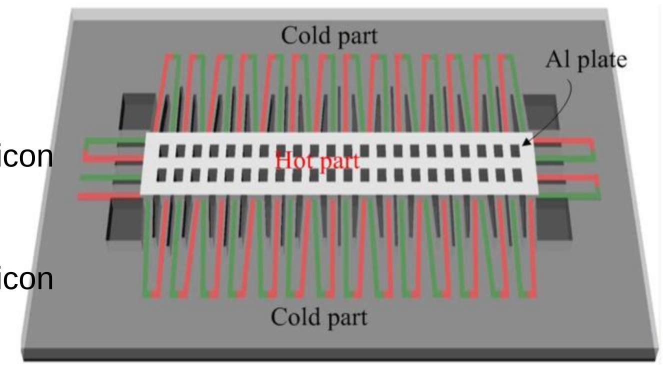


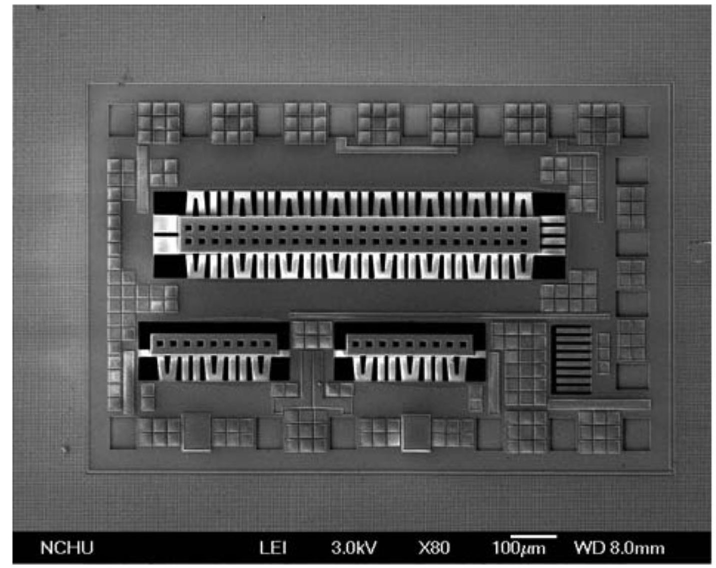
Thermoelectric circuit

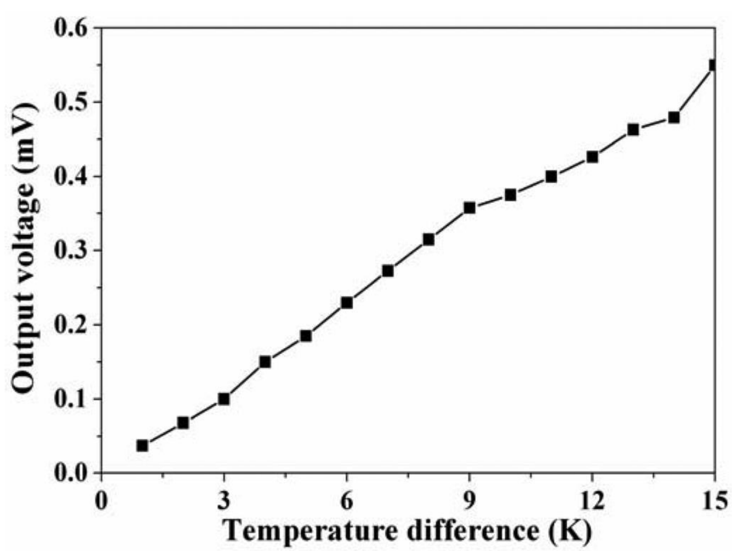
MEMS thermoelectric generator

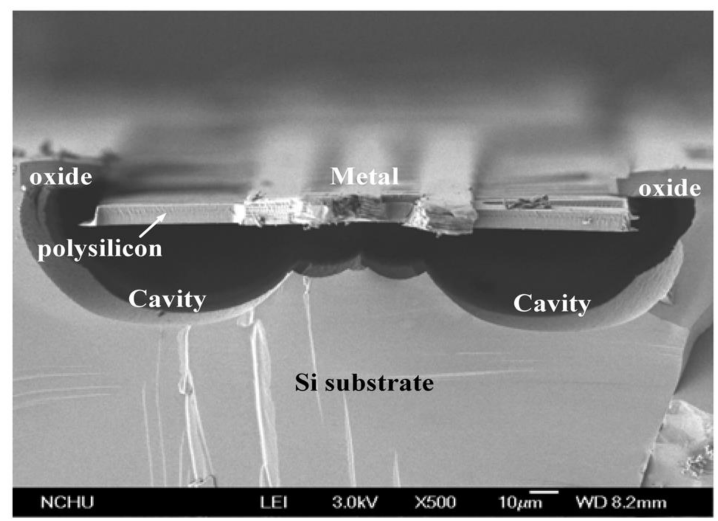
p-type polysilicon

n-type polysilicon



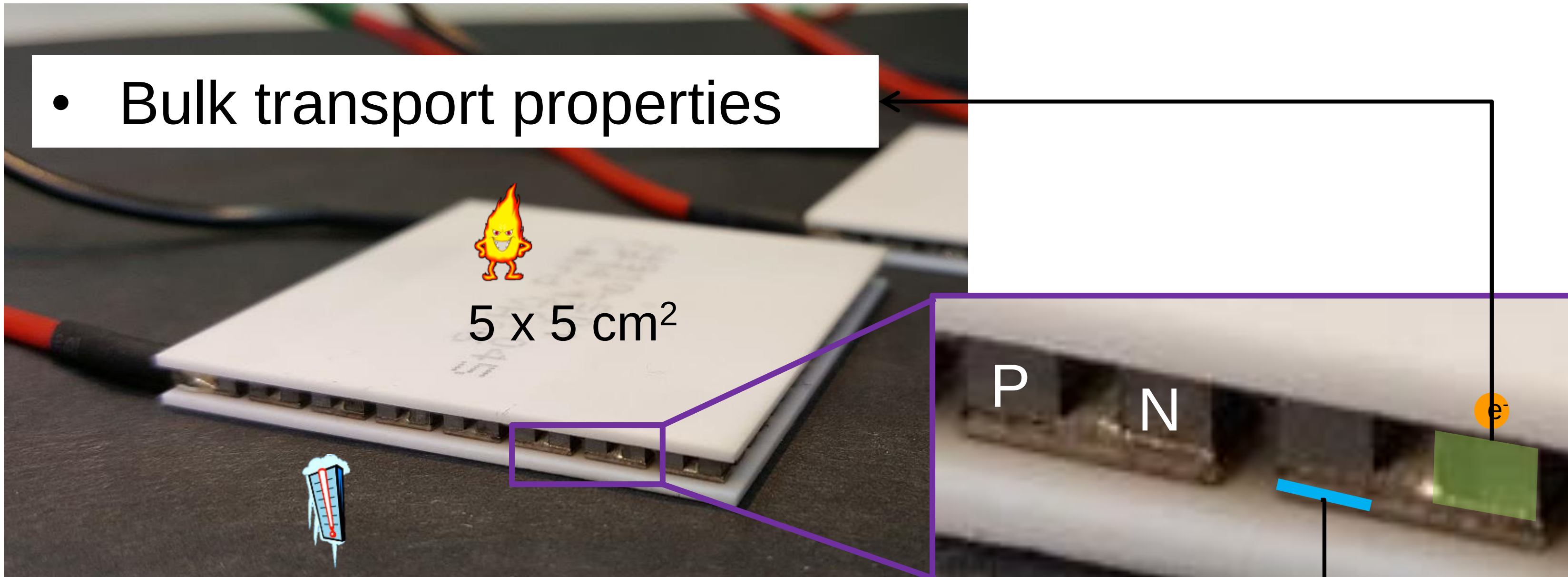






Yang et al. (2013), *Sensors*, *13*(2), 2359-2367

- Bulk transport properties



- Interface transport properties

- Bulk transport properties

  - **Landauer approach – Thermoelectric phenomena**

    Ballistic transport;

    Approximate but illustrative.

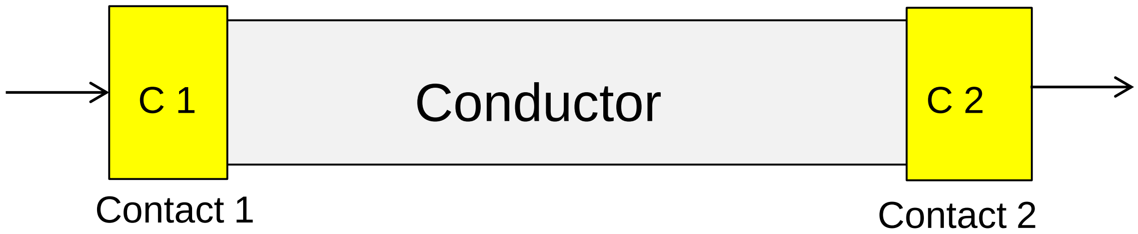
  - **Boltzmann transport equations – transport coefficients**

    Diffusive transport;

    Statistical behaviour, relatively closer to reality, but **realitively**;

    Correlation of transport coefficients.

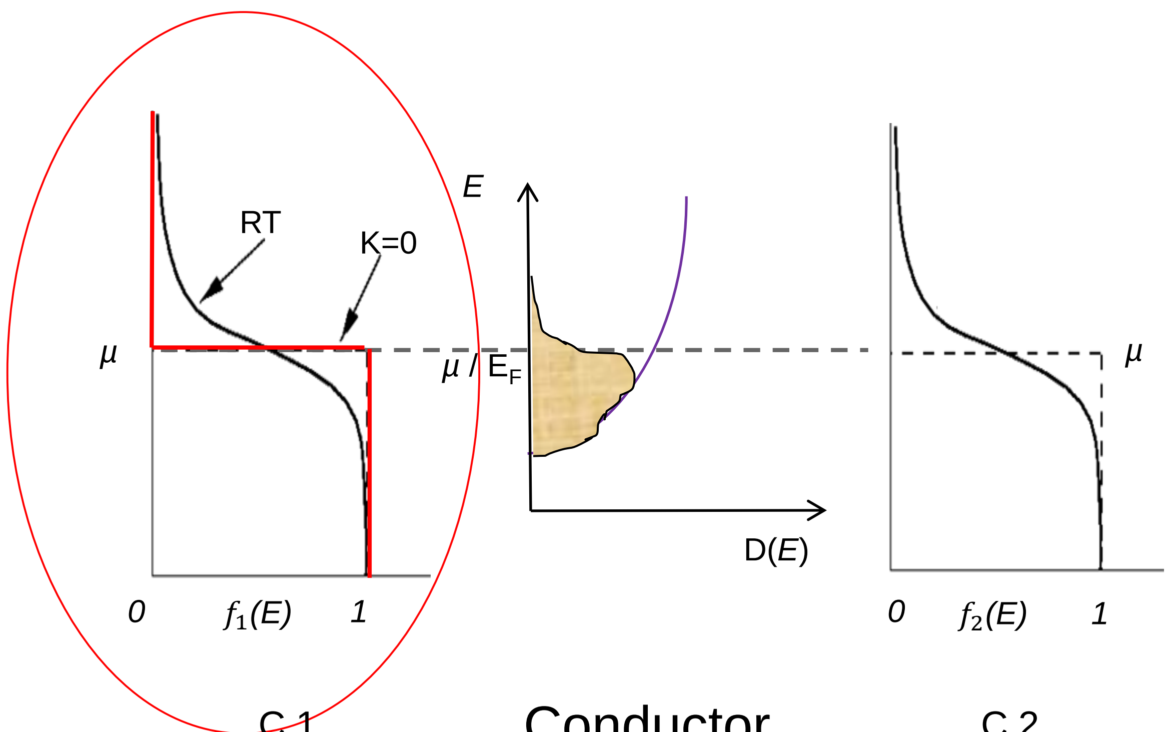
Thermoelectric phenomena - Landauer



- Equilibrium, no external force

$$I = G\Delta V + G_s\Delta T$$

Ohmic current — Seebeck current



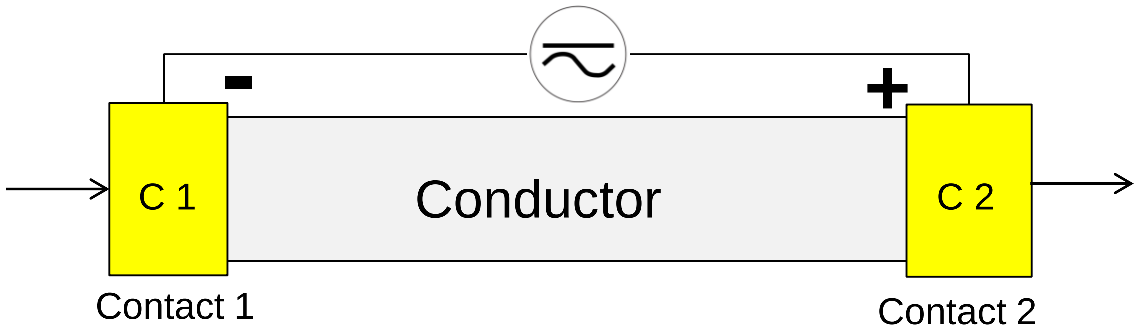
Fermi Distribution

$$\left.\begin{matrix} G \\ G_s \end{matrix}\right\} \propto A \int D(E)(f_1 - f_2)$$

$$\propto \int D(E)\left(-\frac{\partial f_0}{\partial E}\right)$$

No net current

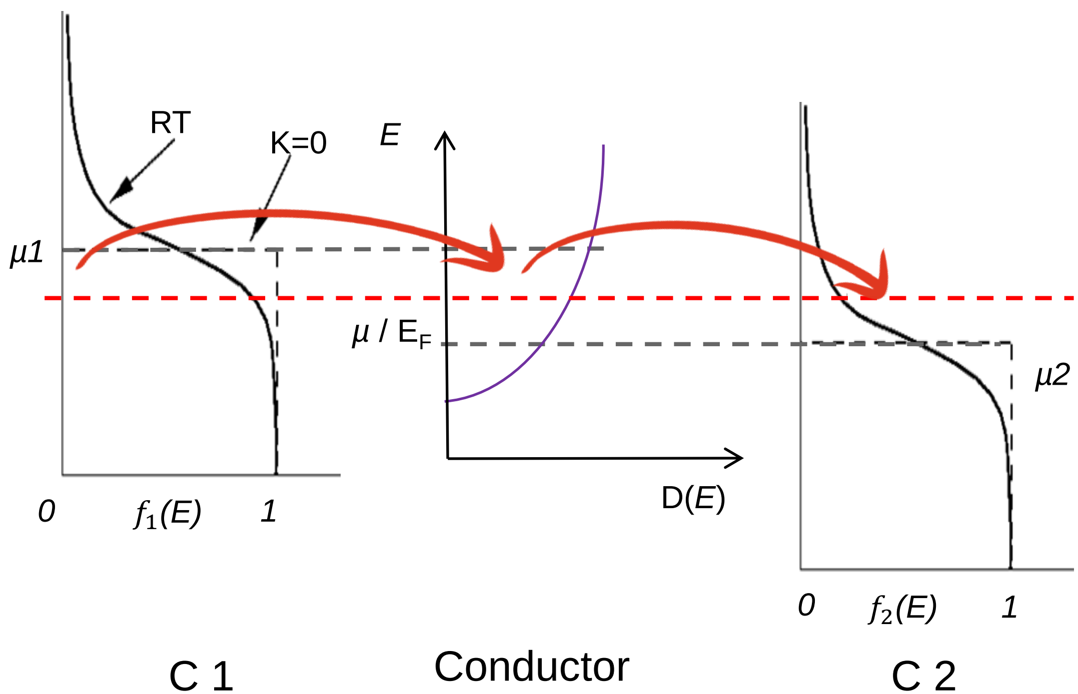
Thermoelectric phenomena - Landauer

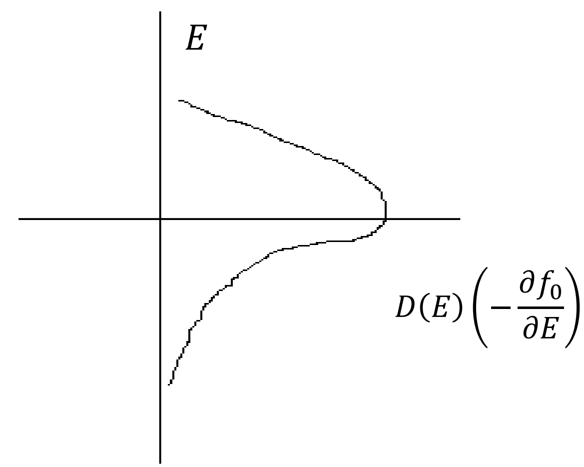


$$I = G\Delta V + \ldots\Delta T$$

Ohmic current | Seebeck current

- When apply electric force



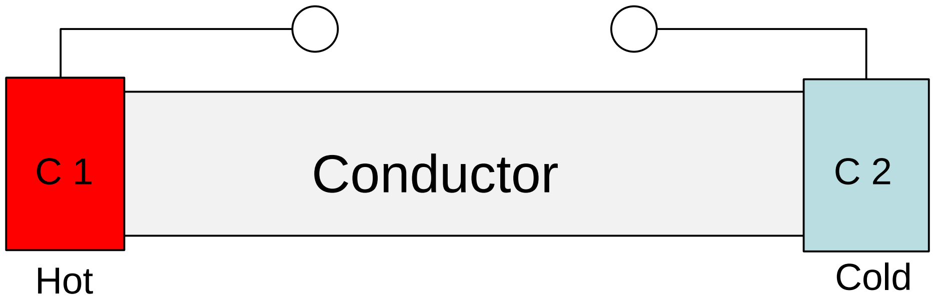


$$\left.\begin{matrix} G \\ G_S \end{matrix}\right\} \propto A \int D(E)(f_1 - f_2)$$

$$\propto \int D(E)\left(-\frac{\partial f_0}{\partial E}\right)$$

External force changes the chemical potential

Thermoelectric phenomena

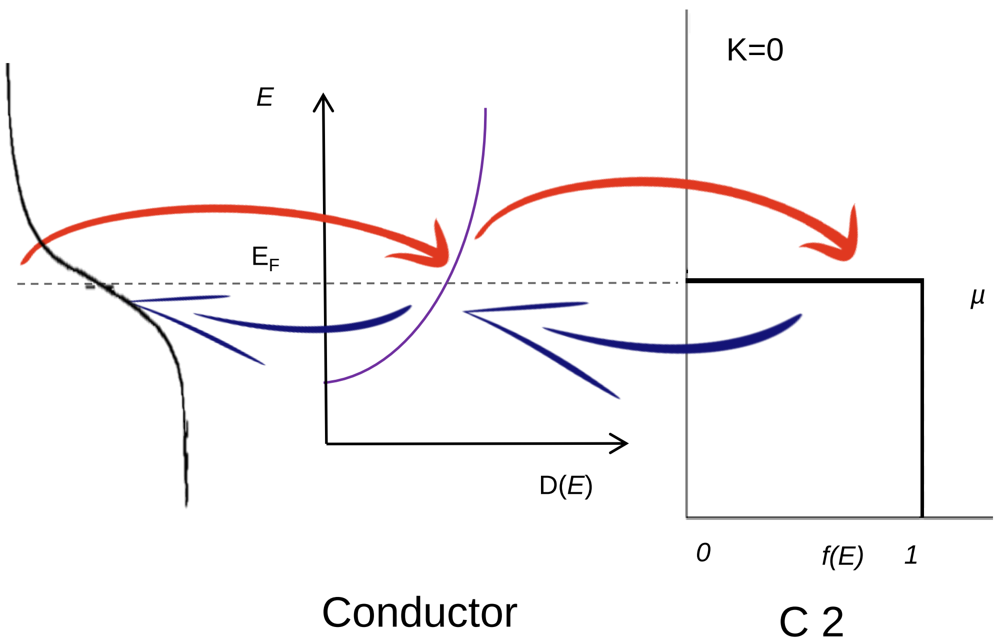


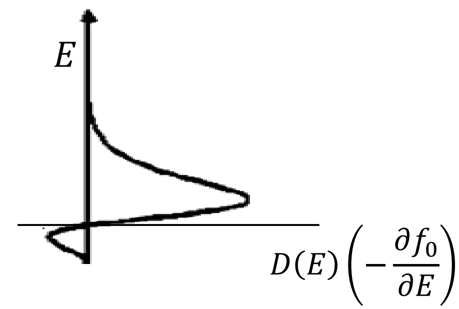
$$I = G\Delta V + G_s\Delta T$$

$$\Delta V = \frac{I}{G} + \frac{G_s}{G}\Delta T$$

Seebeck coefficient

- When apply temperature difference on an open circuit





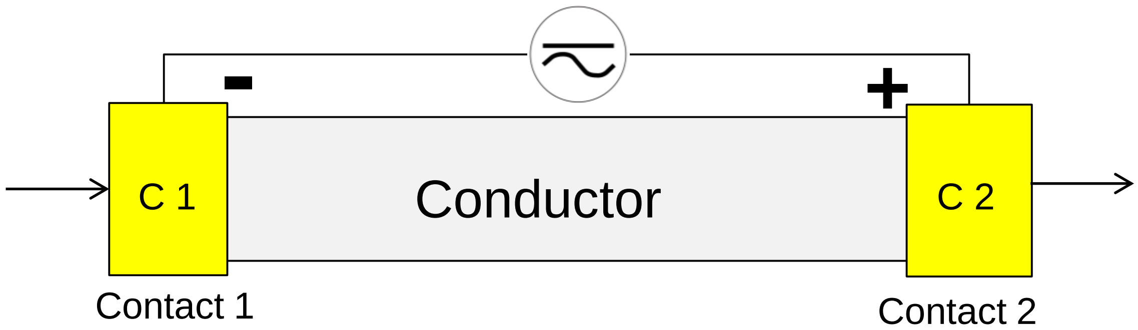
$$\left.\begin{matrix} G \\ G_s \end{matrix}\right\} \propto A \int D(E)(f_1 - f_2)$$

$$\propto \int D(E)\left(-\frac{\partial f_0}{\partial E}\right)$$

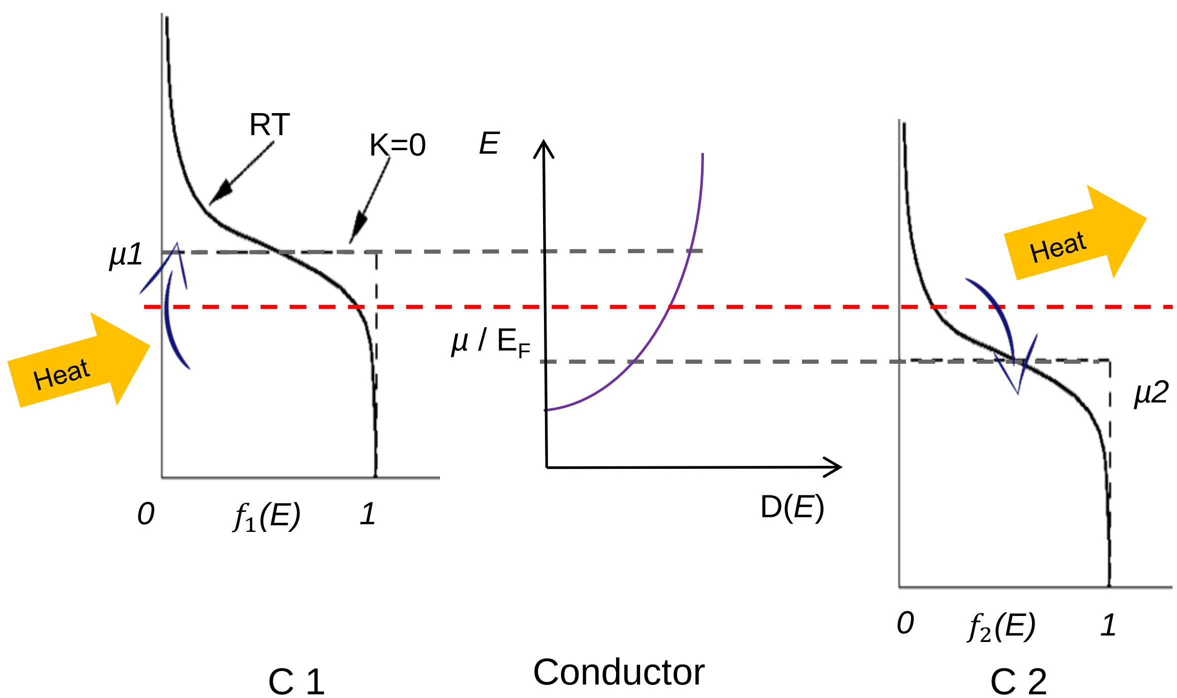
$$A = \begin{cases} 1 \; for \; G \\ \frac{E-\mu}{qT} \; for \; G_s \end{cases}$$

Temperature difference changes charge Fermi distribution

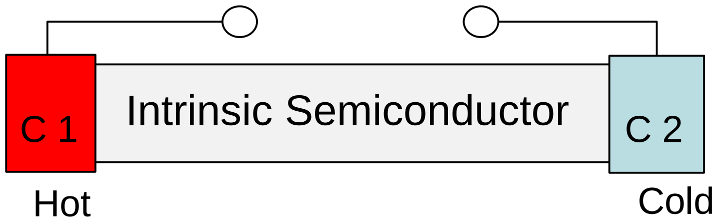
Thermoelectric phenomena - Landauer

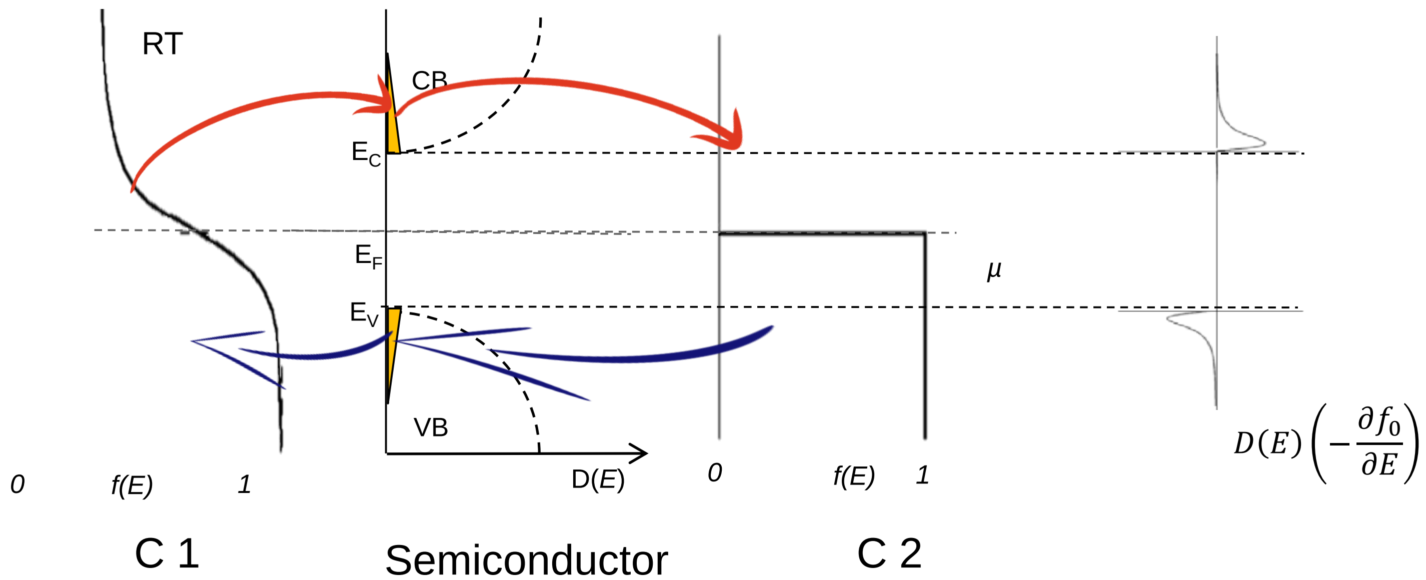


- Peltier effect



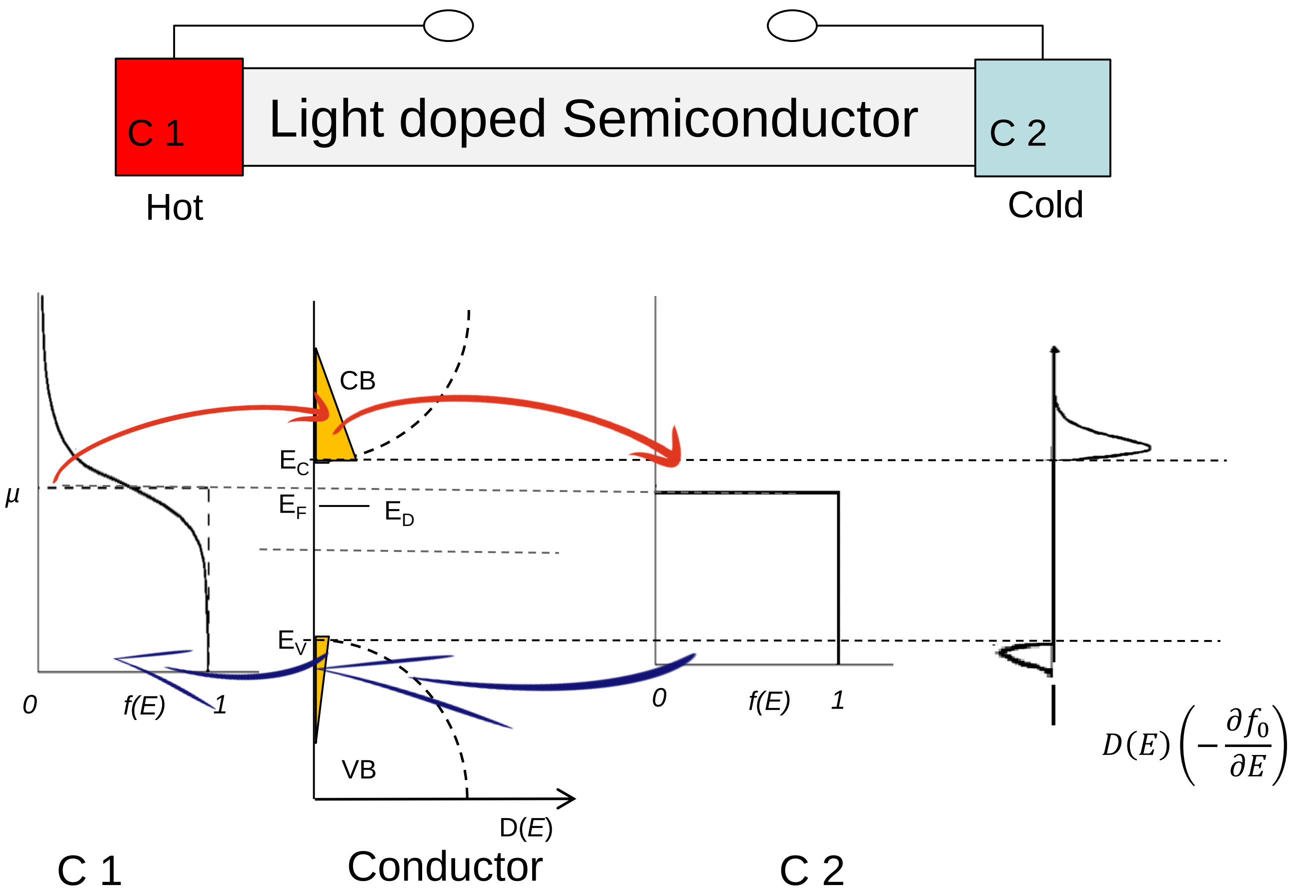
Thermoelectric phenomena - Landauer





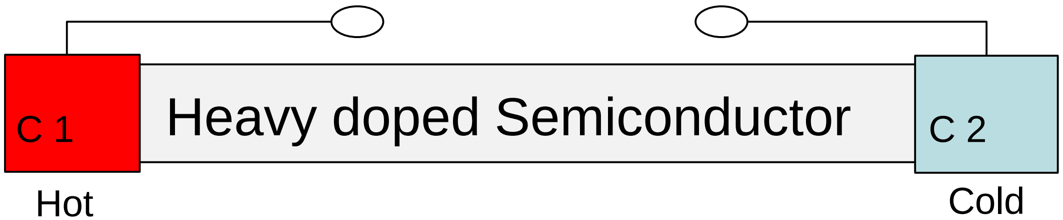
Intrinsic semiconductor has zero seebeck

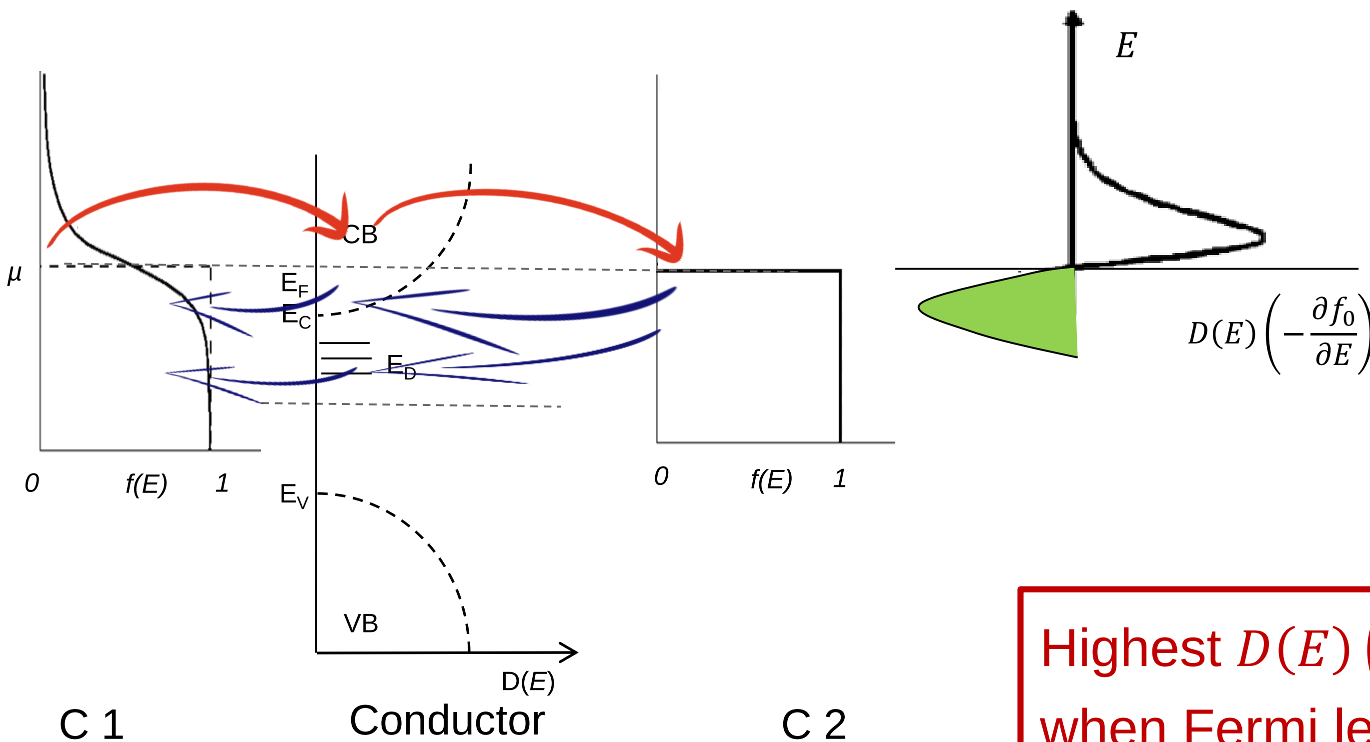
Thermoelectric phenomena - Landauer



Asymmetric DOS -> higher Seebeck

Thermoelectric phenomena - Landauer

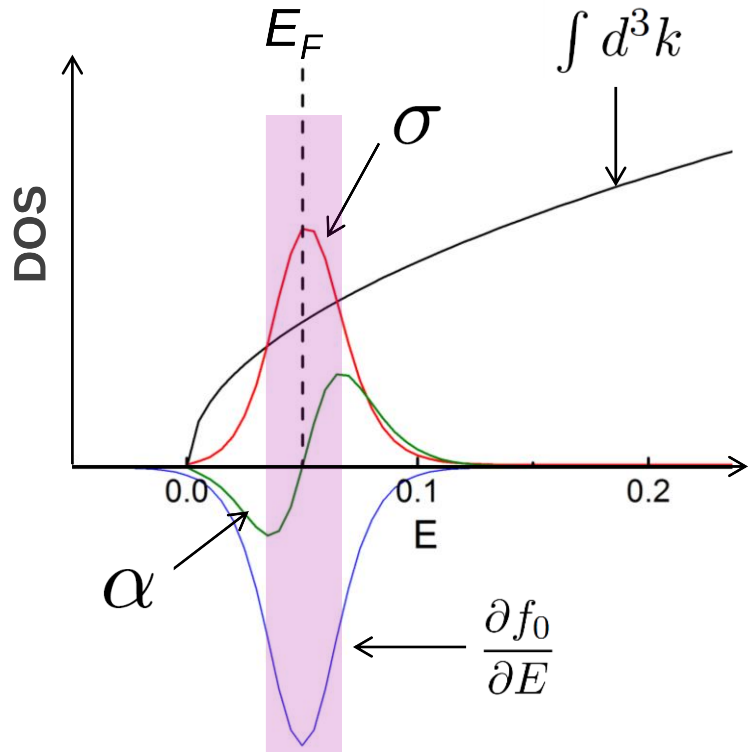




Highest $D(E)\left(-\frac{\partial f_0}{\partial E}\right)$ occurs when Fermi level is close to band edge.

Transport coefficients - Boltzmann

- Optimizing power factor



Seebeck coefficient

$$\alpha = \frac{1}{qT} \frac{\int \tau v^2 (E - E_F)(-\frac{\partial f_0}{\partial E}) d^3k}{\int \tau v^2 (-\frac{\partial f_0}{\partial E}) d^3k}$$

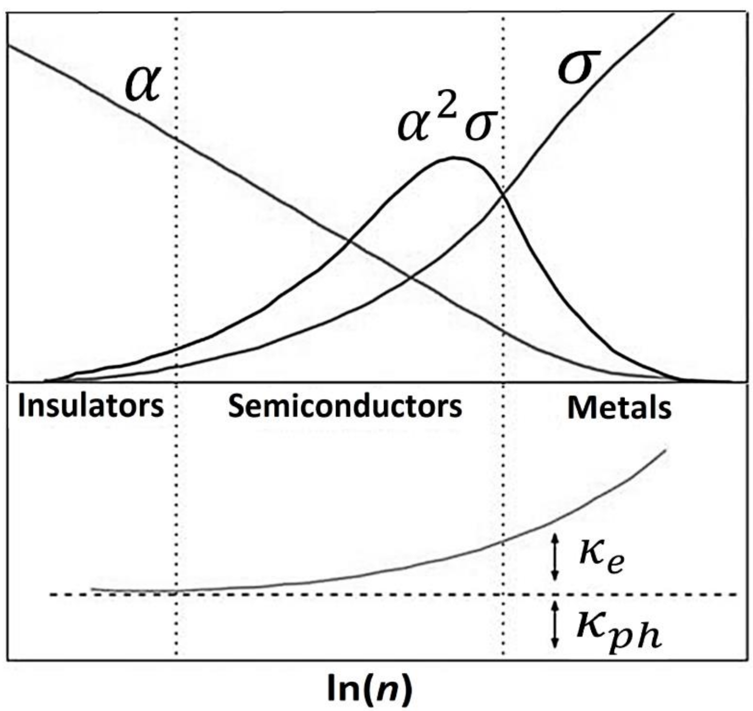
Electrical conductivity

$$\sigma = \frac{q^2}{4\pi^3} \int \tau v^2 (-\frac{\partial f_0}{\partial E}) d^3k$$

$$zT = \frac{\alpha^2 \sigma}{\kappa_e + \kappa_{ph}} T$$

Transport coefficients - Boltzmann

- Optimizing power factor



Seebeck coefficient

$$\alpha = \frac{8\pi^2 k_B^2}{3qh^2} m^* T \left(\frac{\pi}{3n}\right)^{\frac{2}{3}}$$

Electrical conductivity

$$\sigma = qn\left(\frac{q\tau}{m^*}\right)$$

$$zT = \frac{\alpha^2 \sigma}{\kappa_e + \kappa_{ph}} T$$

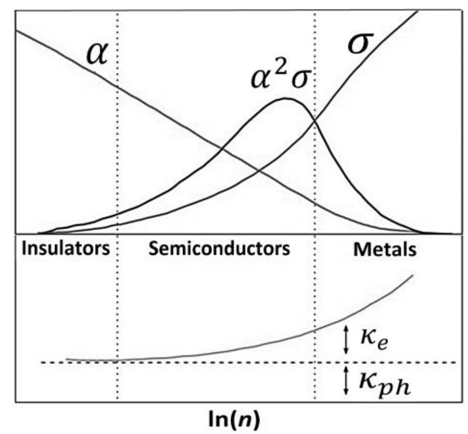
Wiedemann-Franz law

$$\kappa_e = nq\mu\mathcal{L}T$$

- Optimize the interaction between transport coefficients
- Doping, defect scattering, energy filtering

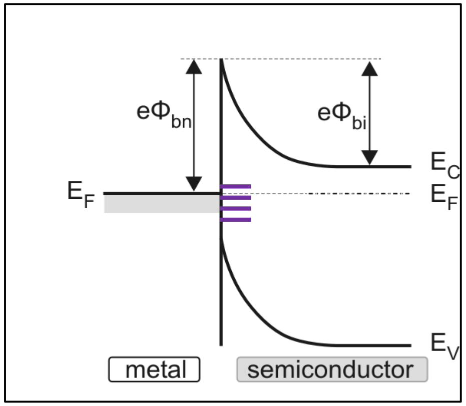
- Bulk transport properties

  - How much electrons/ holes, α, n
  - The ability electrons/ holes move, σ, μ, n
  - The ability heat propagate, κ
  - Expect $zT > 1$

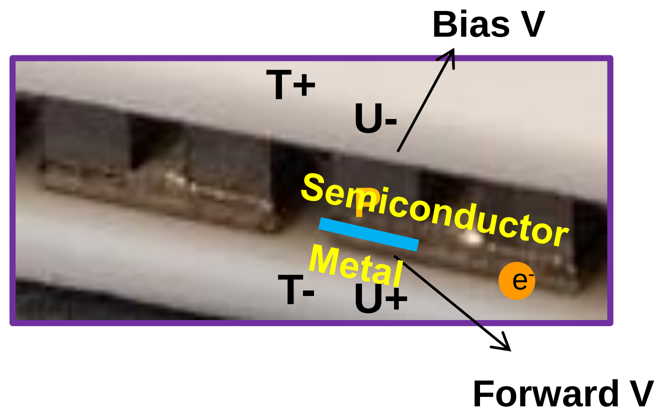


- Interface transport properties

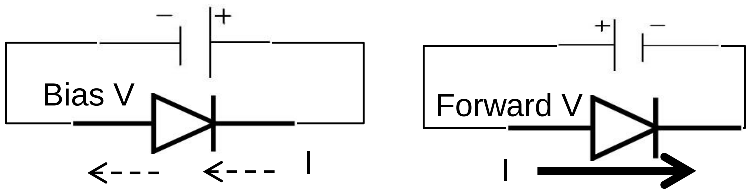
  - Non-rectifying contact
  - Rectifying contact, R_C
  - Interface states, N_a



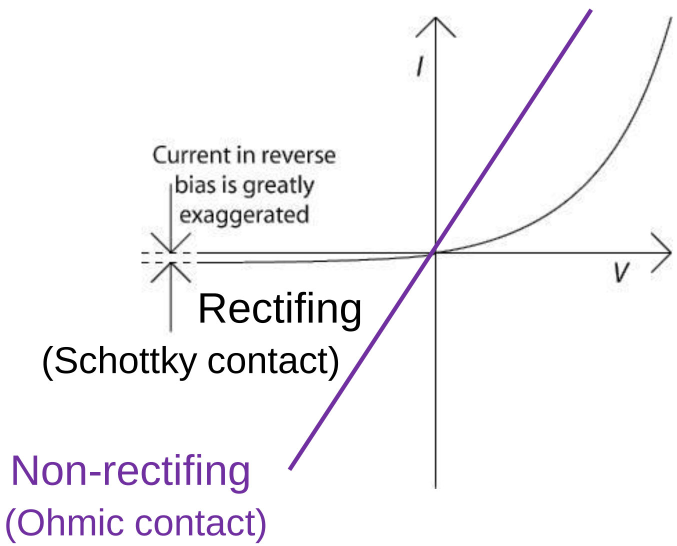
Interface transport properties

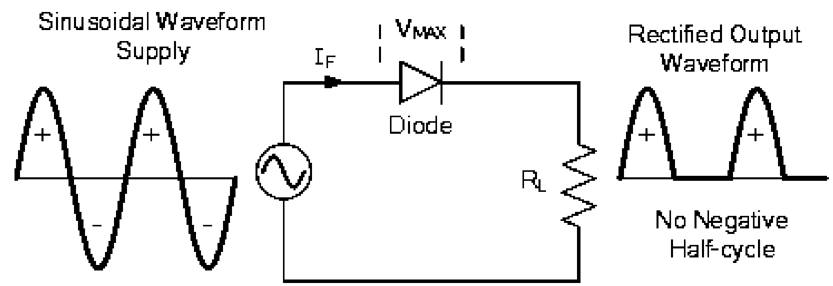


Rectification



High contact resistance R_C !!

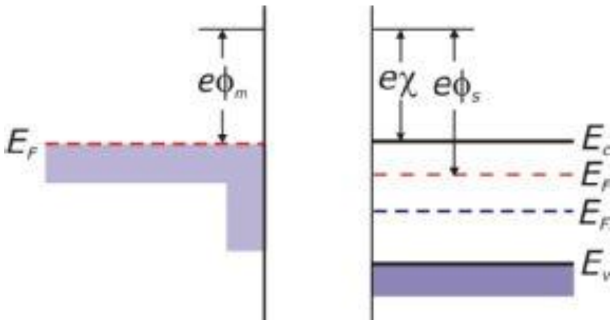


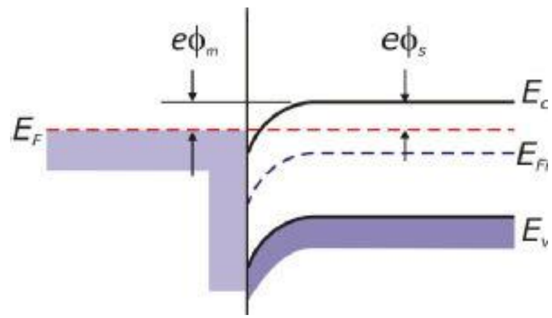


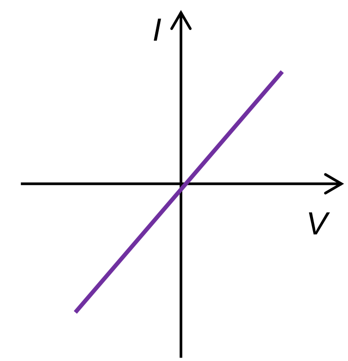
Interface transport properties

The ideal non-rectifying barriers (Ohmic contact)

Metal work function $\phi_m \approx$ Semiconductor electron affinity χ

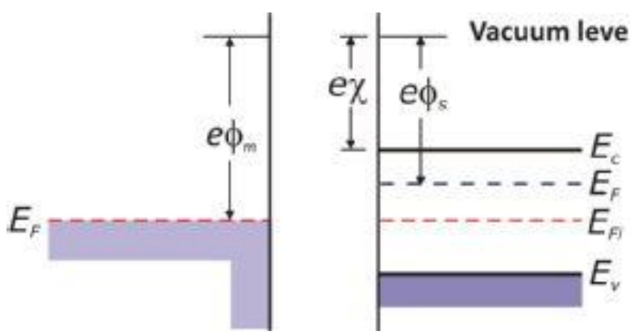


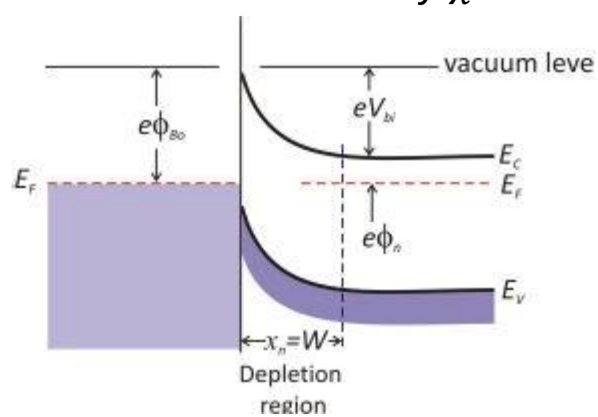


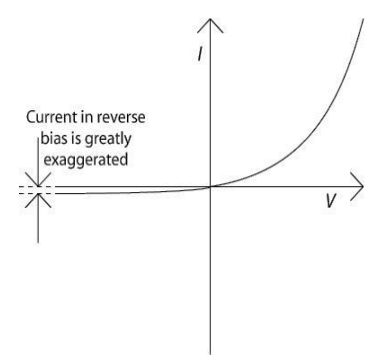


Rectifying barriers (Schottky contact)

Metal work function ϕ_m >> Semiconductor electron affinity χ



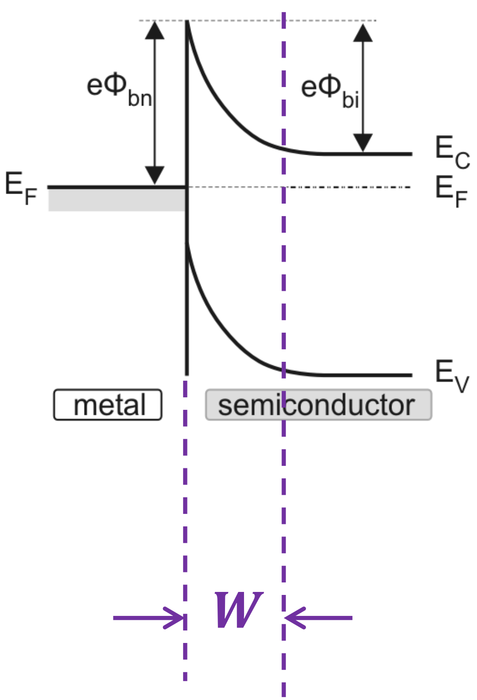




Barrier height $\phi_{bo} = \phi_m - \chi$

Interface transport properties

The Tunneling Barriers



Depletion region

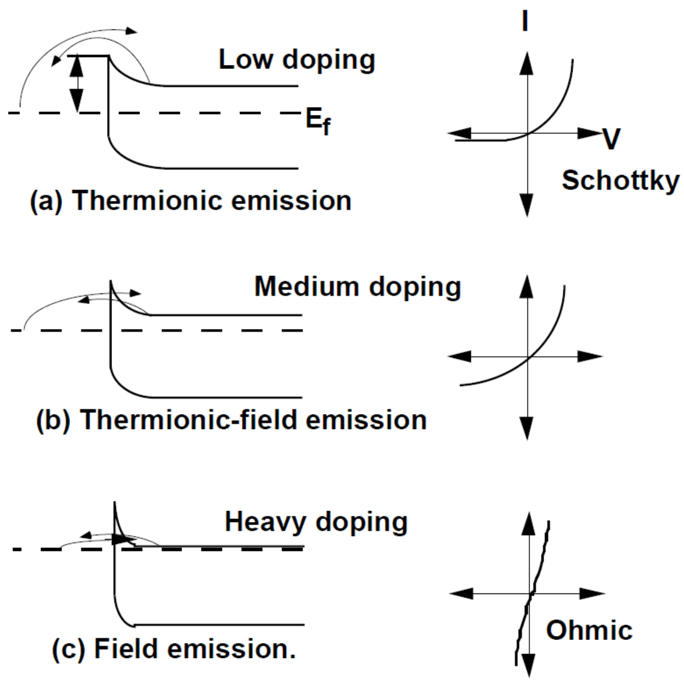
$$W = \sqrt{\frac{2\epsilon_s(e\phi_{bi} + V - \frac{kT}{e})}{eN_d}}$$

ϵ_s -- Dielectric constant **-- Fixed**

$e\phi_{bi}$ -- Build-in potential **-- Fixed**

N_d -- Doping concentration **-- Manipulative ☺**

For most semiconductors



$N_d < 10^{17}\ cm^{-3}$

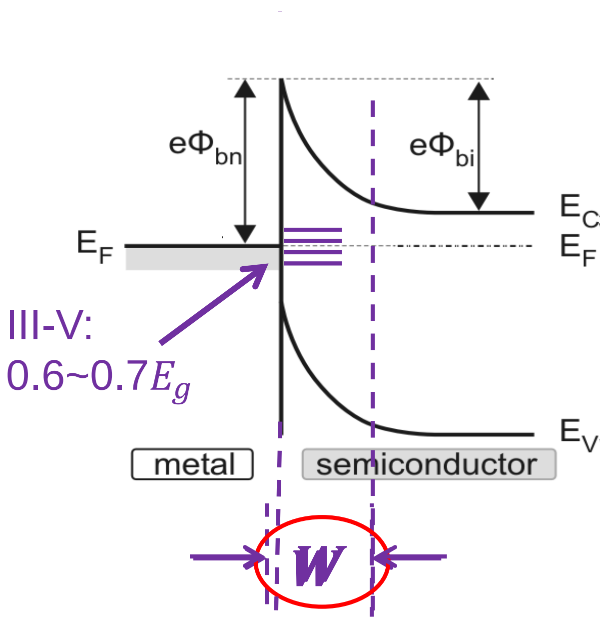
$N_d = 10^{17}\sim10^{18} cm^{-3}$

$N_d = 10^{19}\sim10^{20} cm^{-3}$

W small enough for tunneling

Interface transport properties

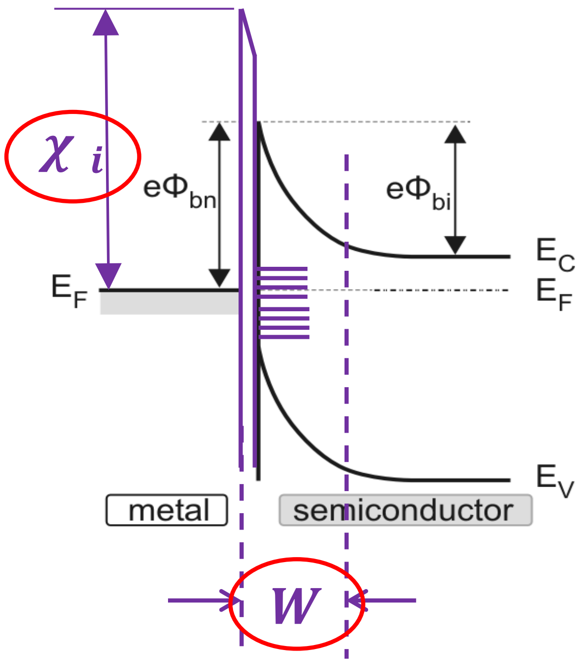
More complicated- interface states in reality



- Pinning the Fermi level
- High density of surface states
  - → Dielectric barrier χ_i, dominating!
- In real world, M-S interface is about
  - Selection of metal
  - Epitaxial growth

Interface transport properties

More complicated- interface states in reality



- Pinning the Fermi level
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- In real world, M-S interface is about
  - Selection of metal
  - Epitaxial growth

Sum up:

- **Bulk transport – two approaches**

  Laudauer approach – illustrative for phenomena

  BTE – describtive for correlations between $\alpha, n, \sigma, \mu, \kappa$

- **Transport at interface**

  Non-rectifying contact

  I need learn more from you