Nanothermoelectrics with nanowires

Eric Hoffmann, Henrik Nilsson, Ann Persson, Natt Nakpathomkun, Jason Matthews, Lars Samuelson,

Heiner Linke

The Nanometer Structure Consortium, Lund University, Sweden

former: Materials Science Institute, University of Oregon

Lund University

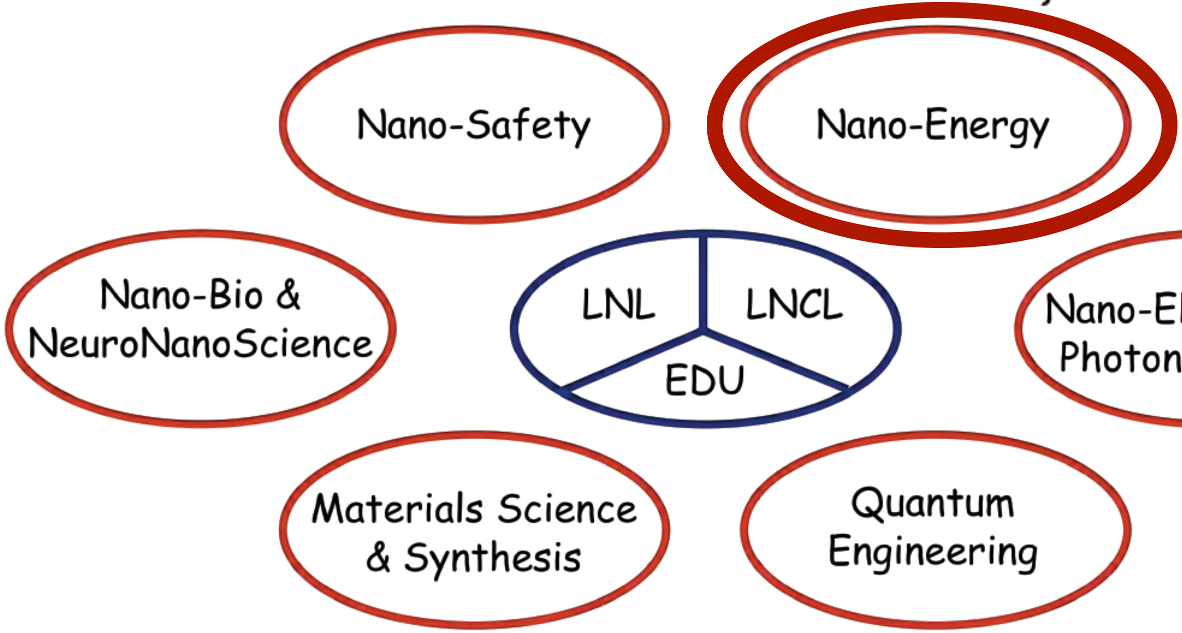
nm structures

ONAMI
OREGON NANOSCIENCE AND MICROTECHNOLOGIES INSTITUTE

UNIVERSITY OF OREGON

Lund Circuit Design Workshop 2010

The Nanometer Structure Consortium, nmC@LU



The illustration above indicates how the six focus areas:

- **Materials Science & Synthesis** (coordinator: Reine Wallenberg, Materials Chemistry)
- **Quantum Engineering** (coordinator: Stephanie Reimann, Mathematical Physics)
- **Nano-Electronics/Photonics for IT** (coordinator: Lars-Erik Wernersson, EIT/Physics)
- **Nano-Bio & NeuroNanoScience** (coordinator: Jens Schouenborg, Neurophysiology)
- **Nano-Energy** (coordinator: Villy Sundström, Chemical Physics)
- **Nano-Safety** (coordinator: Sara Linse, Biophysical Chemistry)

circle around the core facilities providing the resources which all these thrive on:

- **Lund Nano Lab** (coordinator: Lars Montelius, Solid State Physics)
- **Lund Nano Characterization Labs** (coordinator: Anders Mikkelsen, Synchr. Rad. Phys.)
- **Nano-Education** (coordinator: Knut Deppert, Solid State Physics)

Coordinator: Lars Samuelson; **Deputy:** Heiner Linke. **Administrative Director**: Anneli Löfgren

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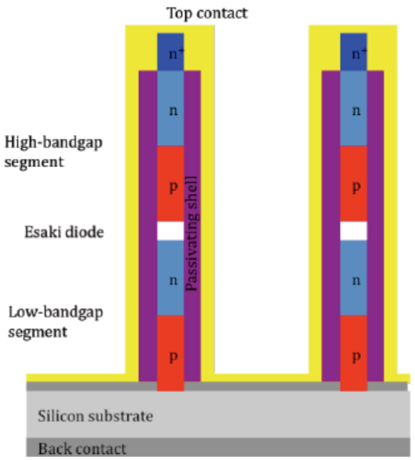
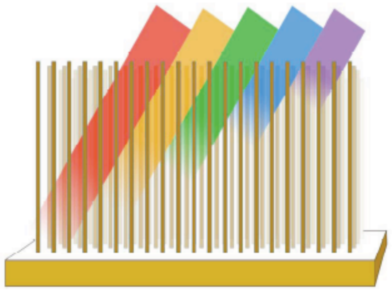
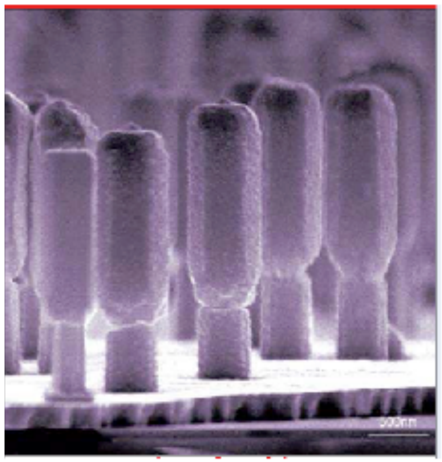
Nanoenergy within nmC@LU

Multi-junction solar cells on Si (K. Deppert)

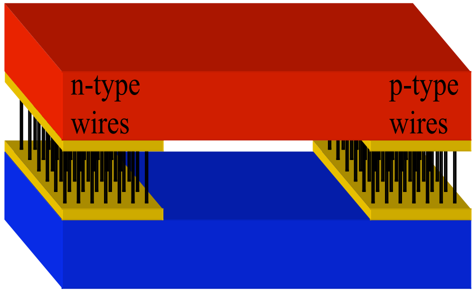


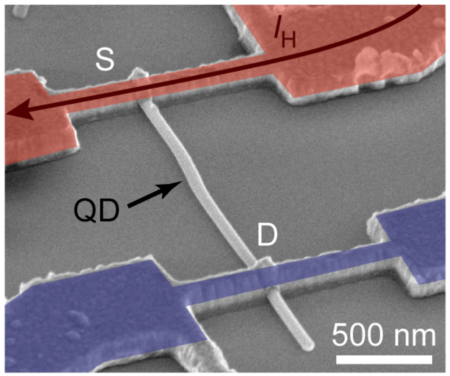


Low-energy lighting (L. Samuelson)

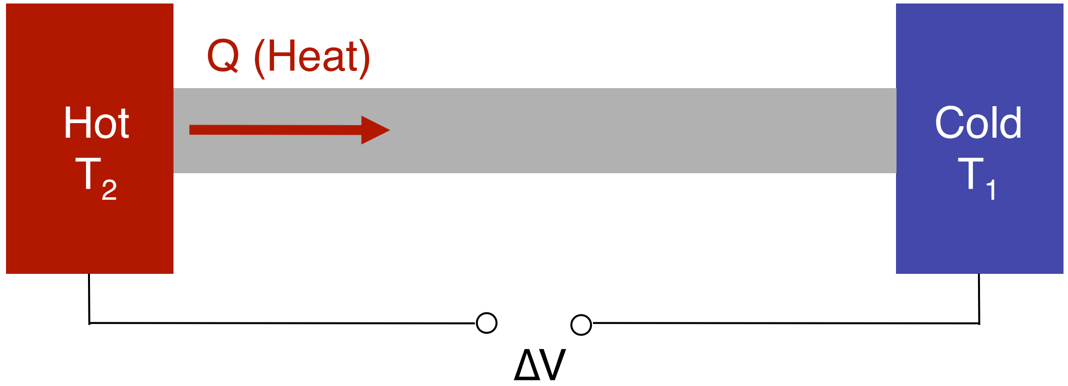


Thermoelectrics (H. Linke)



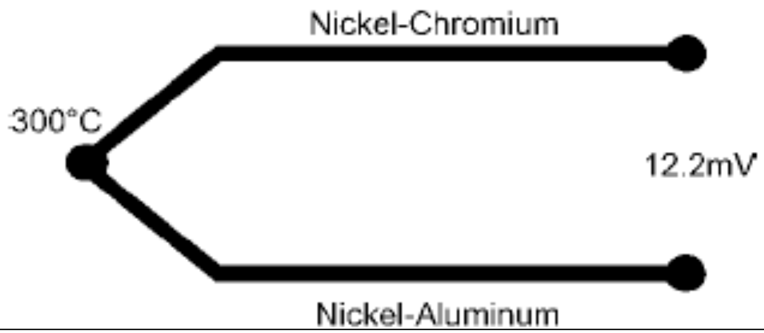


Thermoelectrics

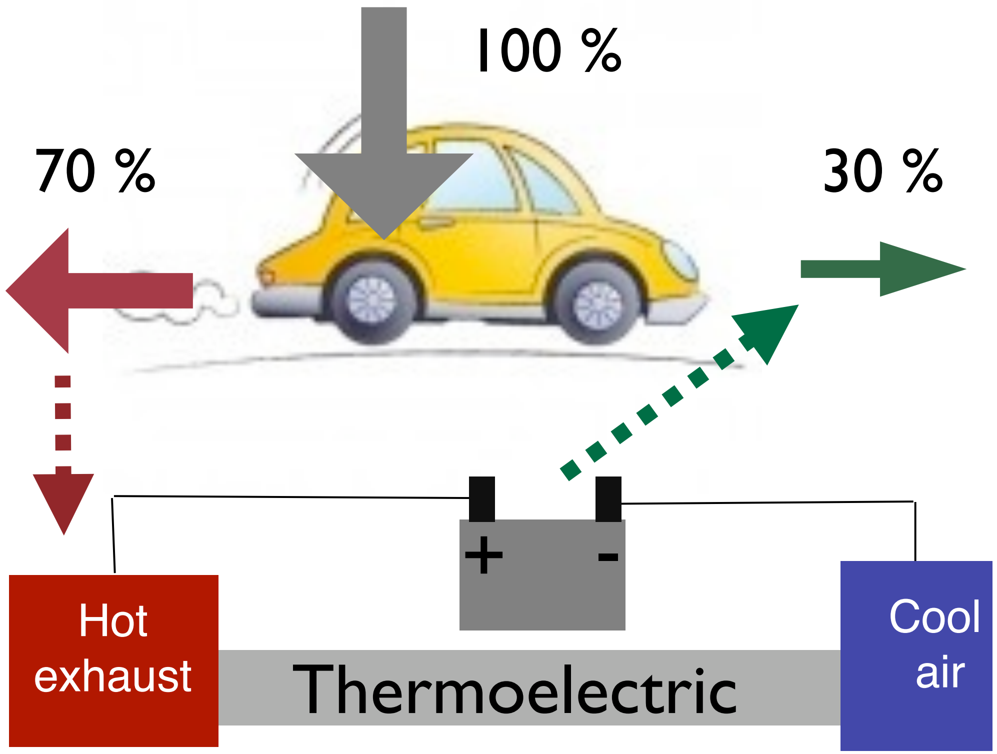


Seebeck coefficient $S = \Delta V/\Delta T$

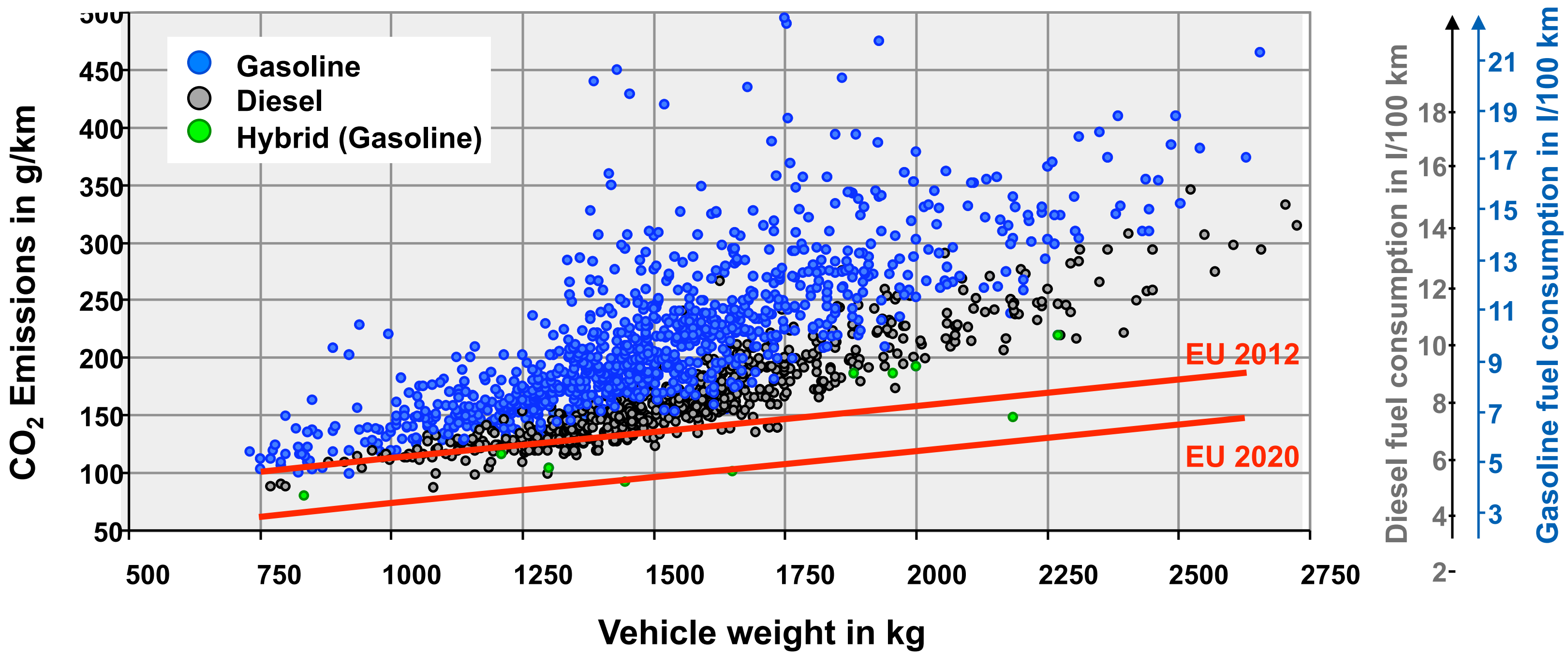
Differential Seebeck effect (difference between two materials):



Thermocouple


100 %
70 %
30 %
+
-
Hot exhaust
Thermoelectric
Cool air

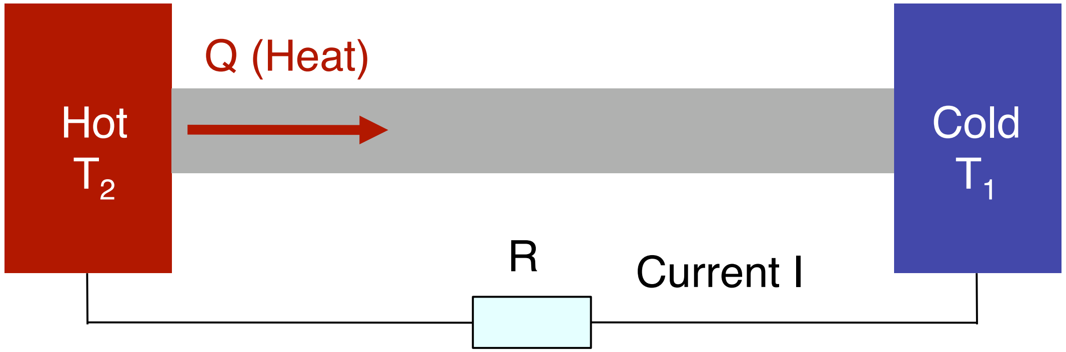
Of interest to the automotive industry...



... and others: - waste heat recovery in ships, industry

- use in hybrid photovoltaics
- cooling (household refrigeration, electronics)
- sensors
- ....

What makes a good thermoelectric ?



- Low parasitic heat conduction by electrons (κ_{el}) and phonons (κ_{ph}).
- High Seebeck coefficient $S = \Delta V / \Delta T$
- Little Joule heating (high conductivity σ)

Figure of merit:

$$Z = \frac{S^2 \sigma}{\kappa_e + \kappa_{ph}}$$

ZT > 1 is good

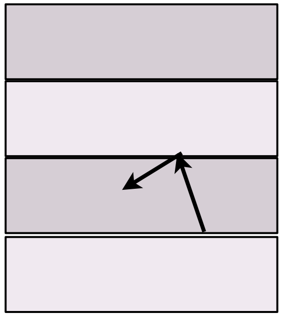
Why *nano*-thermoelectrics?

$$Z = \frac{S^2\sigma}{\kappa_e + \kappa_{ph}}$$

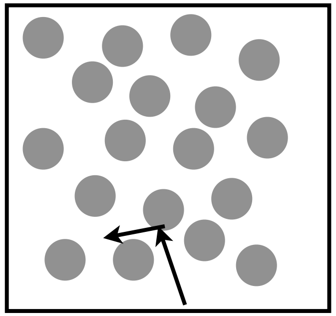
PHONONS

Phonon confinement: Tune phonon DOS and dispersion function

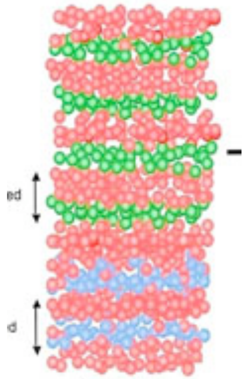
Phonons scatter off interfaces

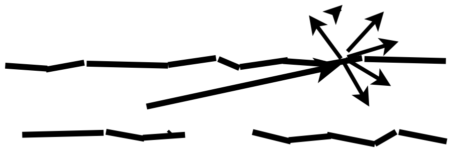


Superlattice



Nanocrystalline materials



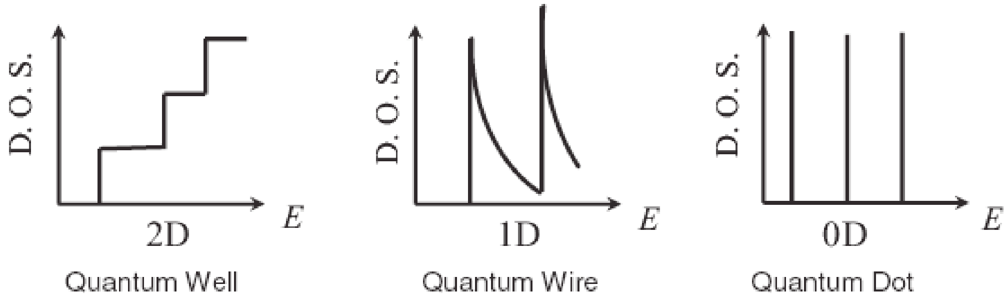


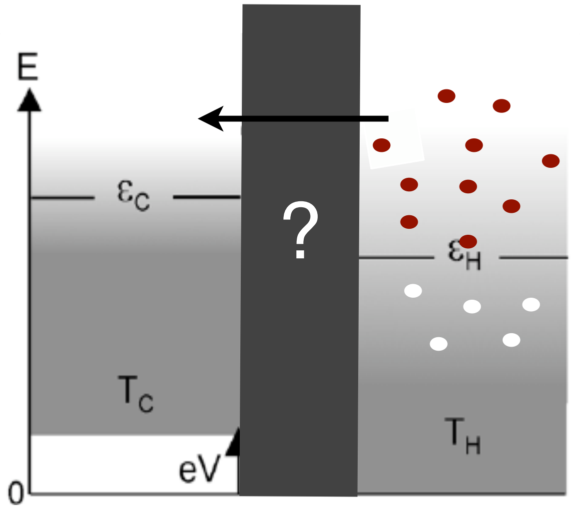
Nanowires

Random stacking (Johnson group)

ELECTRONS

Electron quantum confinement: Optimize electronic properties

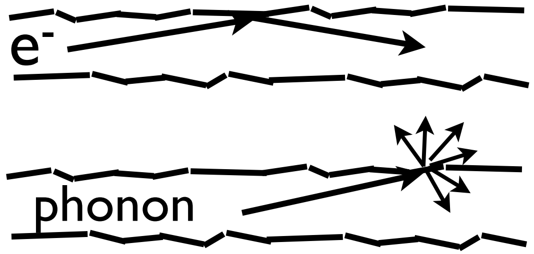




Review: Dresselhaus et al, Adv. Materials **19**, 1043 (2007)

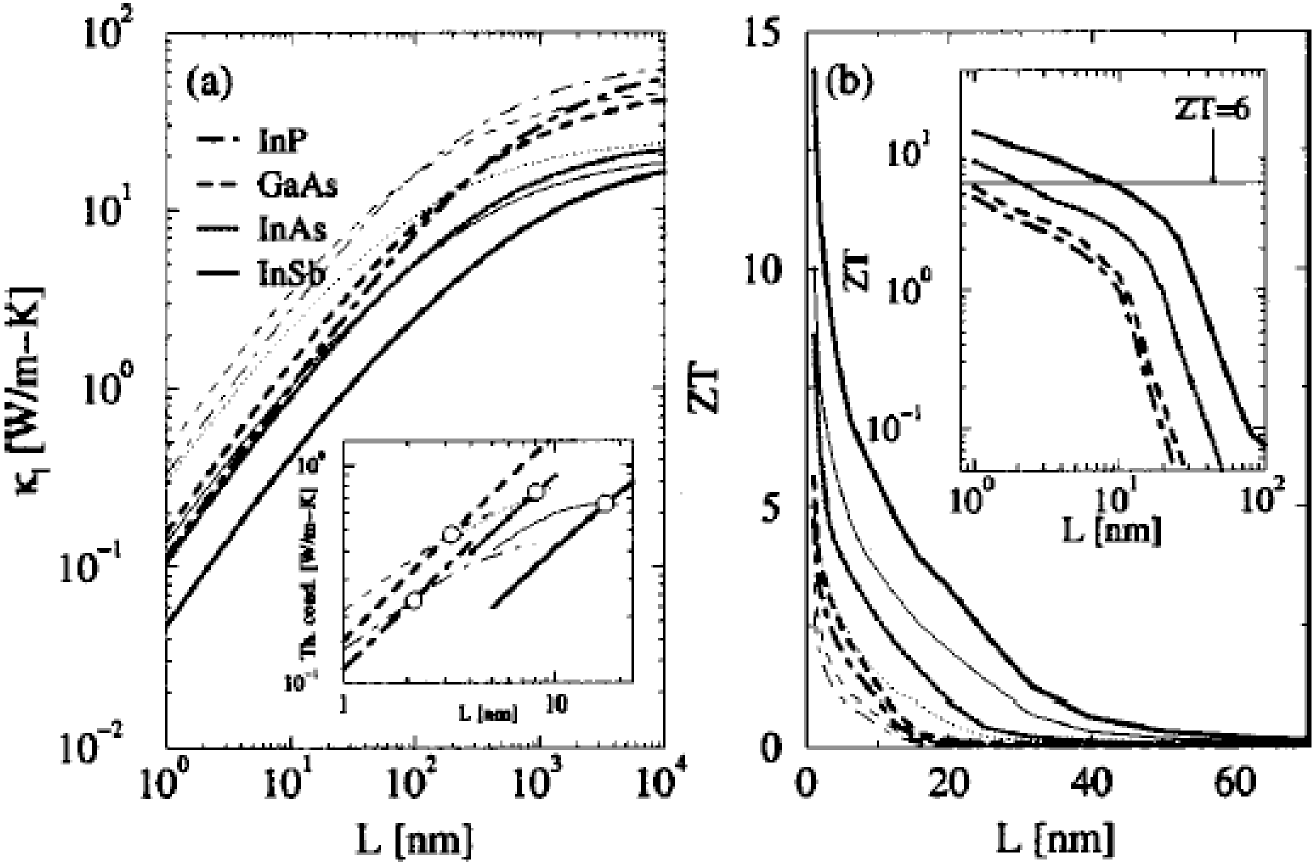
Why nanowires?

Phonons scatter off surface roughness
(more so than electrons)



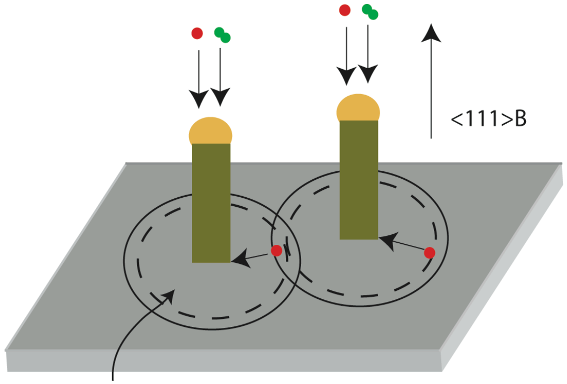
Hicks and Dresselhaus,
PRB **47** (1993)

High ZT predicted in III-V nanowires



Mingo
APL **84**, 2004

Epitaxially grown nanowires, e.g. InAs/InP
(Lars Samuelson group, Lund)

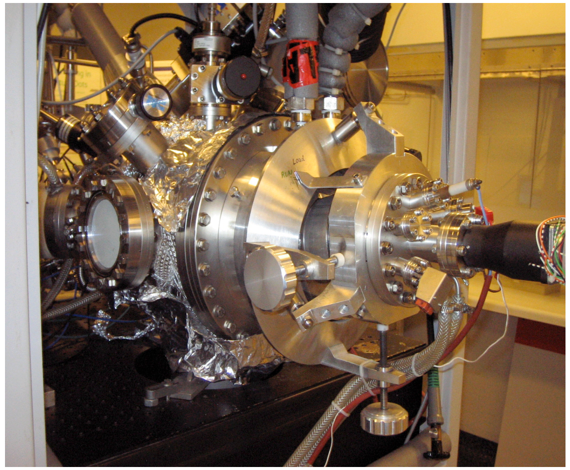


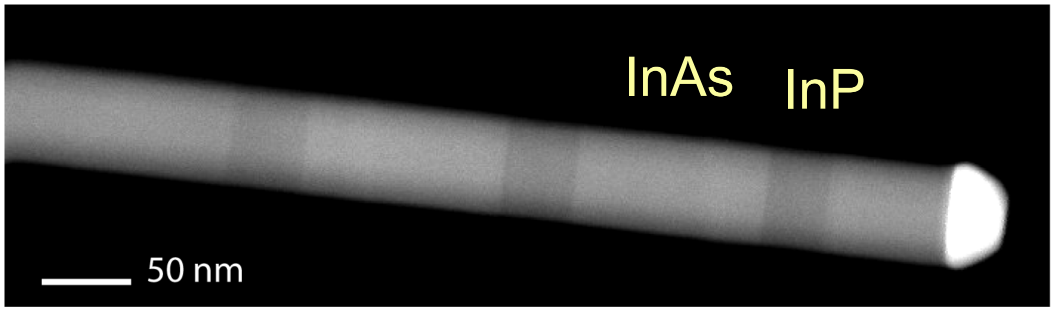
TBAs (group-V)

TMIn (group-III)

Substrate surface
InAs (111)B

CBE

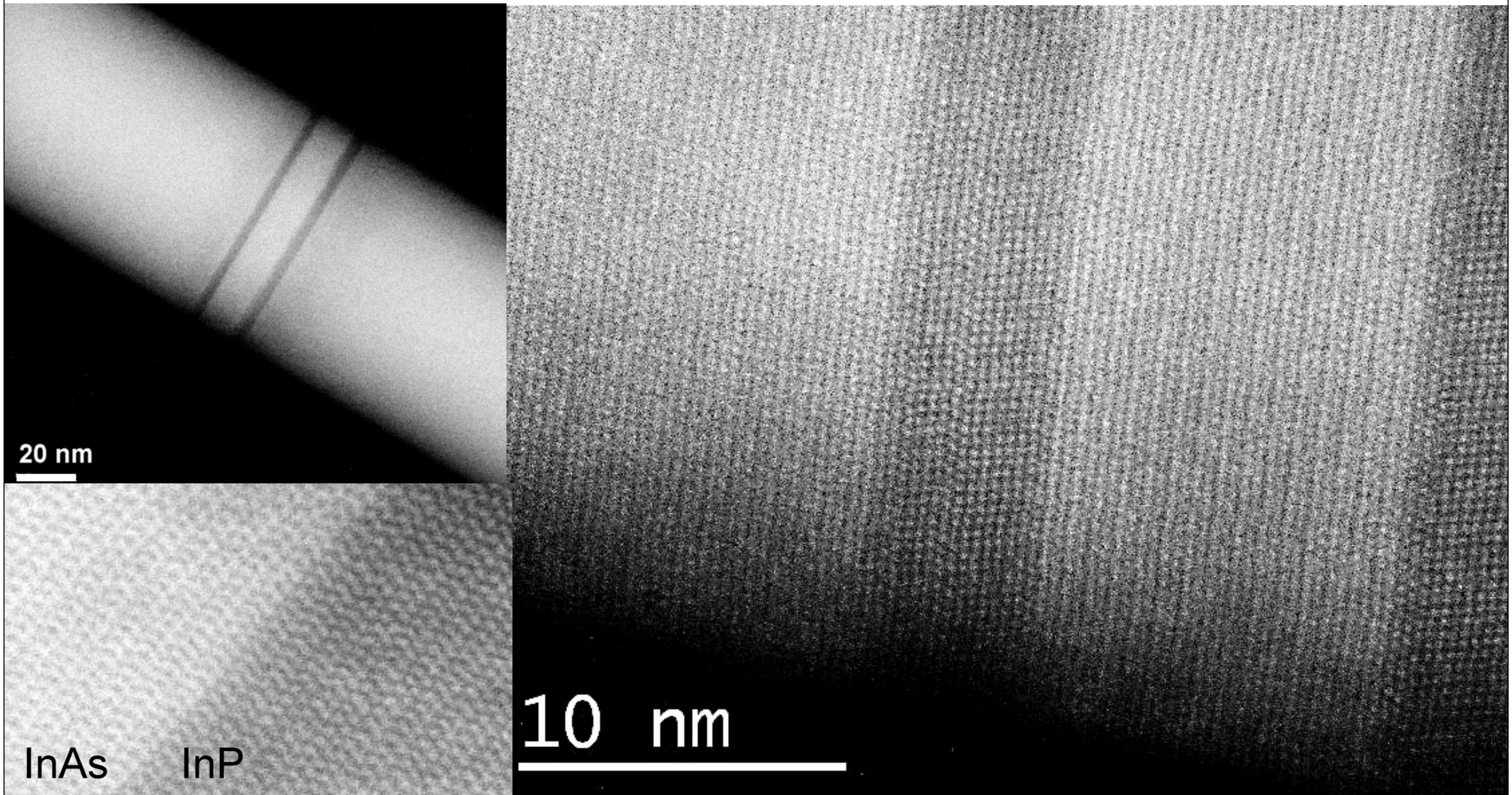




Ann Persson, Linus Fröberg

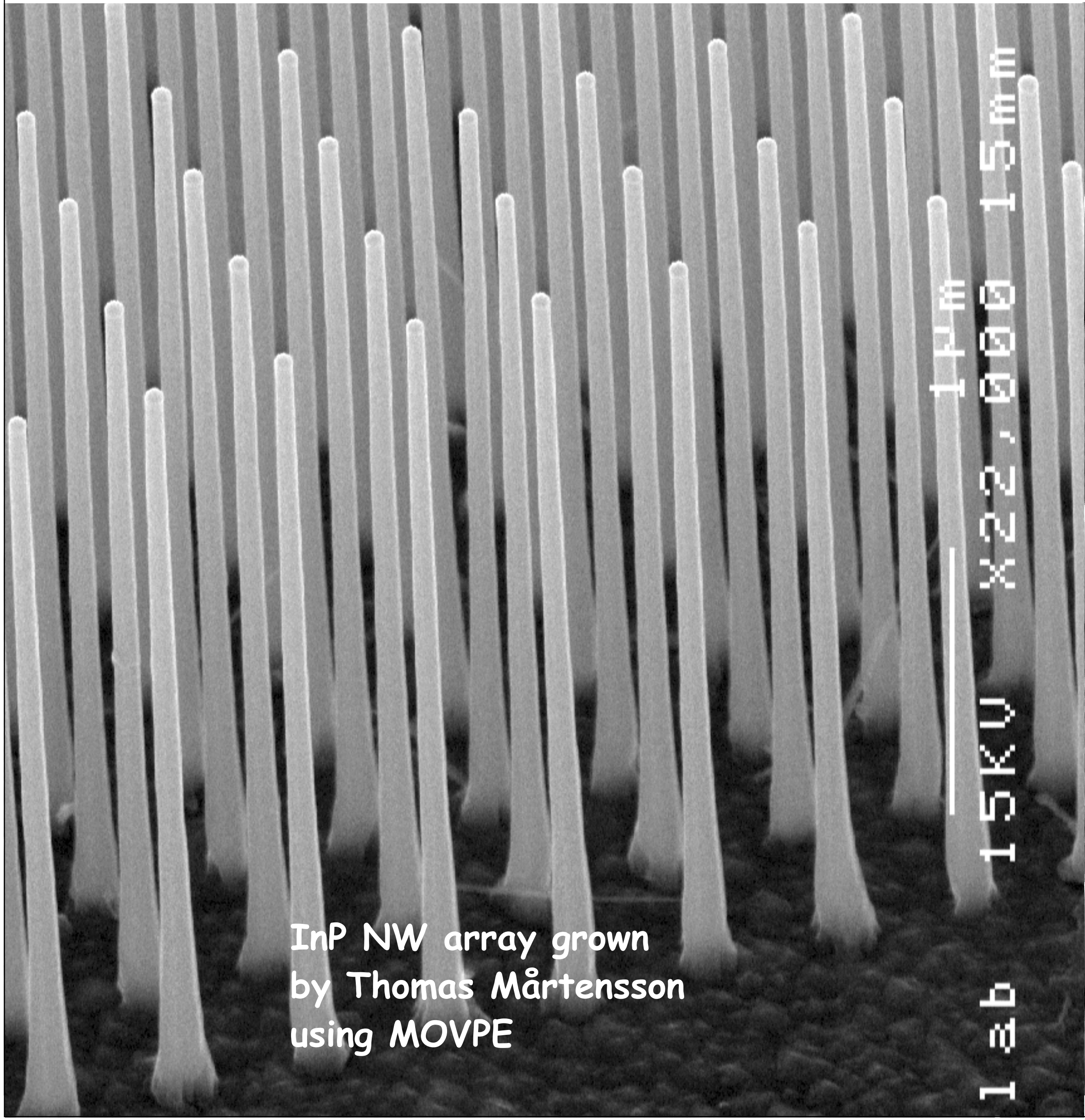
Sharp interfaces

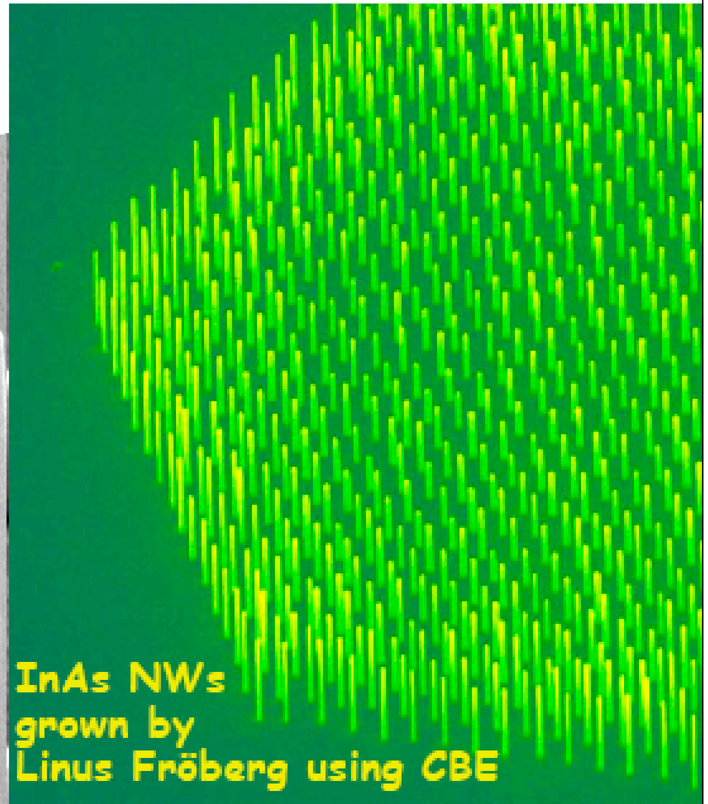
(Imaging: Reine Wallenberg & Magnus Larsson, nCHREM, Lund)



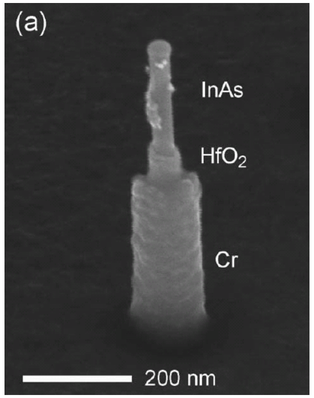
HAADF: High-Angle Annular Dark-Field (in STEM)

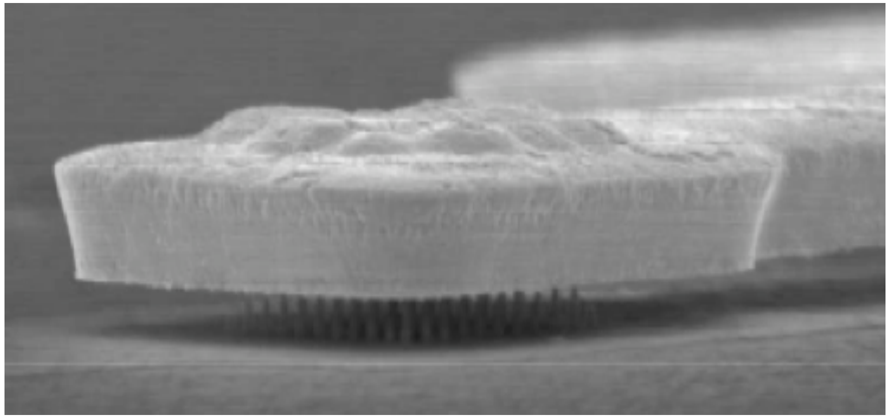
Pattern control





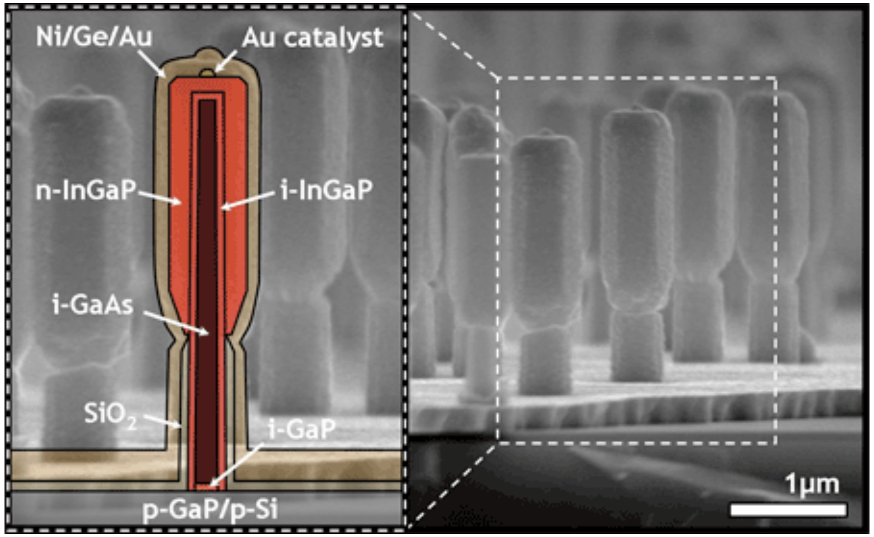
Advanced structures





Vertical field effect transistor
(Lars-Erik Wernersson, T. Bryllert, E. Lind, C. Thelander, L. Samuelson)

IEEE Electron Device Letters, **27**, 323 - 325 (2006)
IEEE Transaction on Electron Devices, **55**, 2008



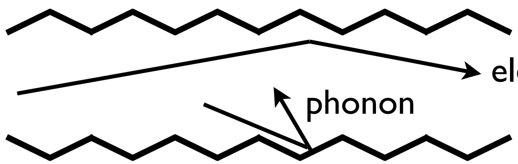
Monolithic Ga/GaInP nanowire LEDs on Si

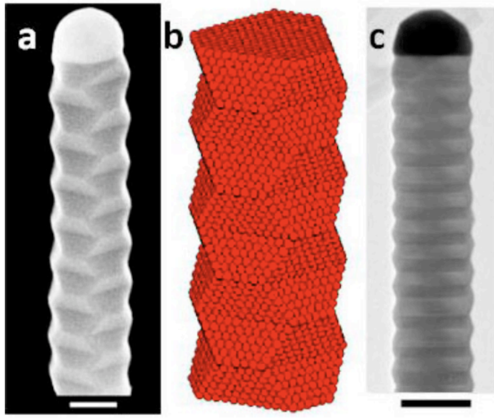
Svensson, Mårtensson, Larsson, Ohlsson, Trägårdh, Hessman, Samuelson
Nanotechnology (2008)

Control of crystal and surface structure

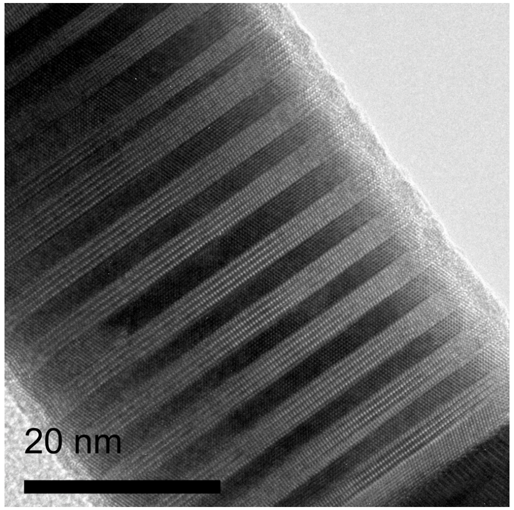
Phonon dispersion, speed of sound in principle depend on:

- composition
- morphology (e.g. ZB, WZ)
- intentional stacking faults
- doping levels and dopants
- core-shell structure
- surface structure





NATURE NANOTECHNOLOGY | VOL 4 | JANUARY 2009 |
P. Caroff*†, K. A. Dick*†, J. Johansson,
M. E. Messing, K. Deppert and L. Samuelson



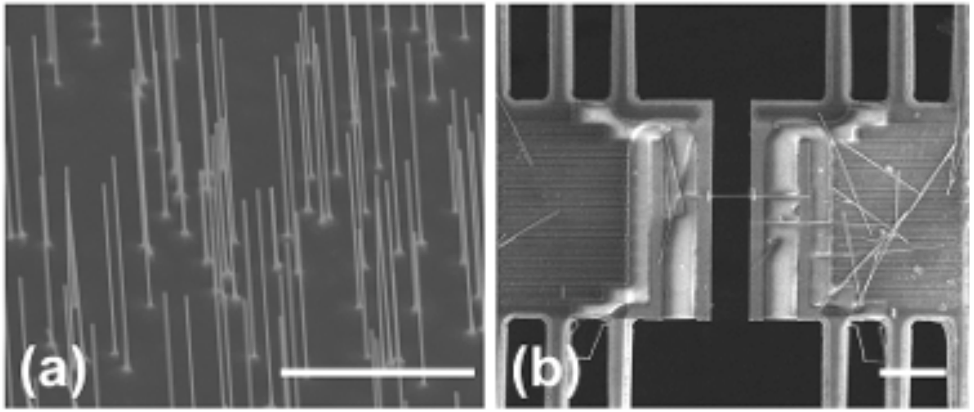
Controlled WZ / ZB superlattice (InAs)

K. A. Dick, P. Caroff, et al. unpublished

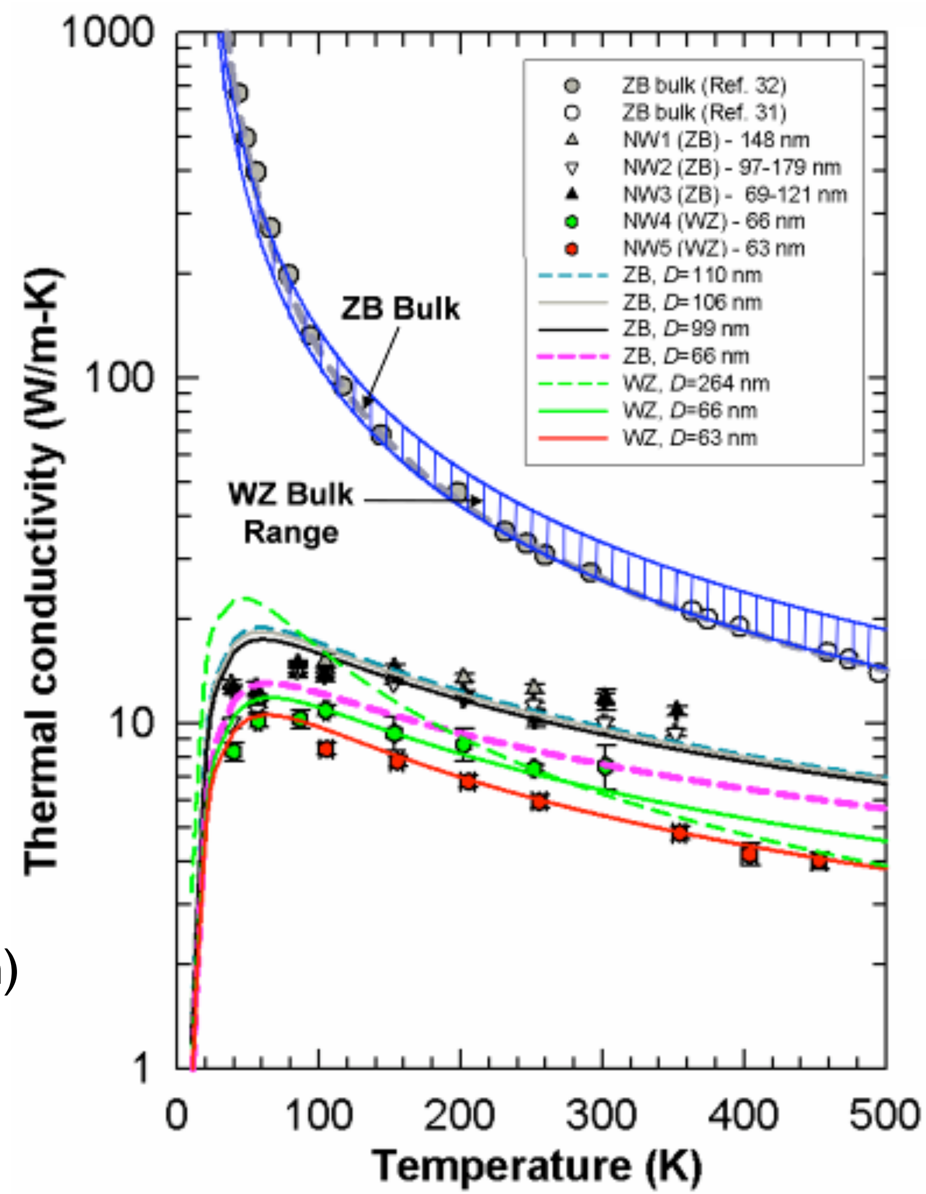
Thermal conductance in WZ, ZB InAs nanowires

with the groups of Li Shi (U Texas, Austin) and Kimberly Dick (Lund)

(in preparation).



Li Shi, Feng Zhou, Arden Moore (U Texas, Austin)



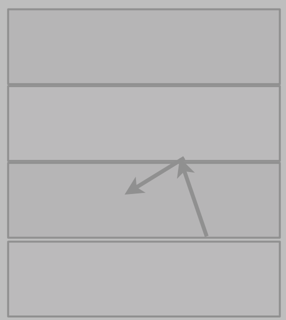
Now we focus on electrons alone.

$$Z = \frac{S^2\sigma}{\kappa_e + \kappa_{ph}}$$

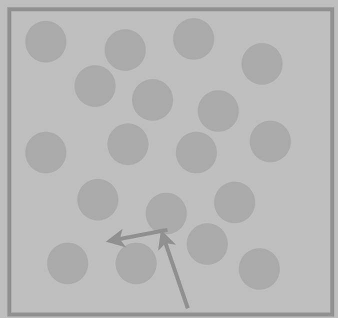
PHONONS

Phonon confinement:
Tune phonon DOS and dispersion function

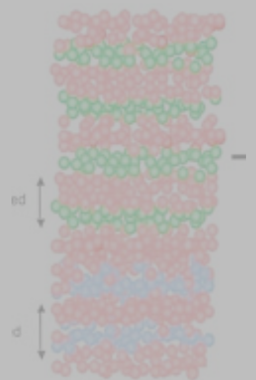
Phonons scatter off interfaces

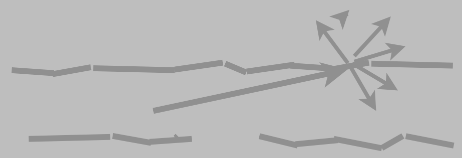


Superlattice



Nanocrystalline materials



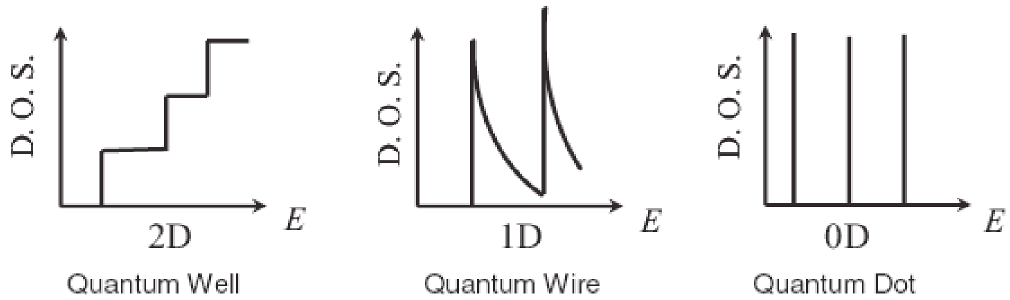


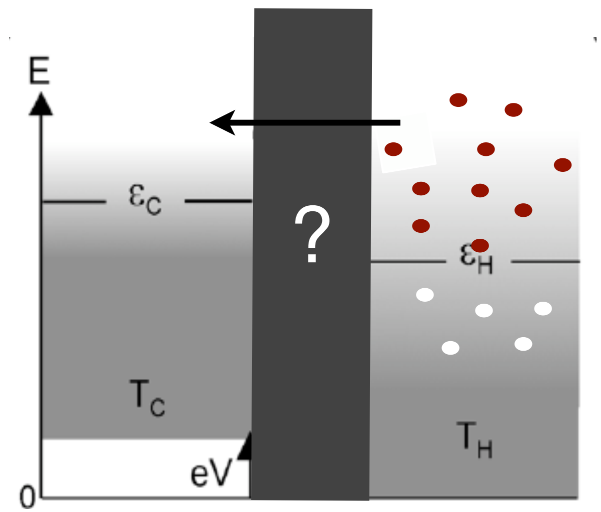
Nanowires

Random stacking (Johnson group)

ELECTRONS

Electron quantum confinement:
Optimize electronic properties



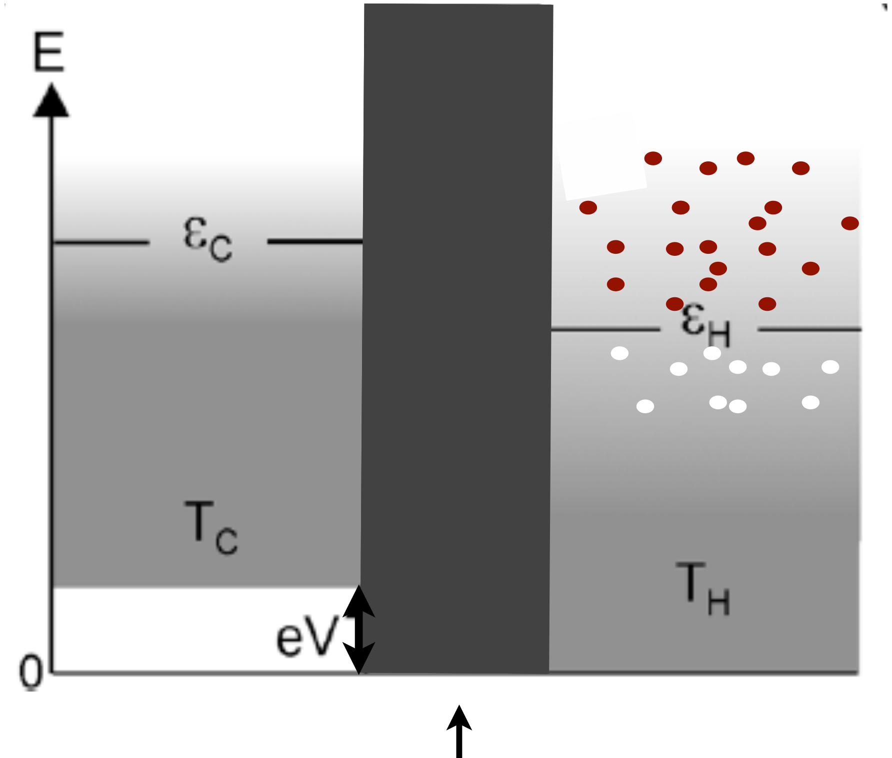


Review: Dresselhaus et al, Adv. Materials **19**, 1043 (2007)

Fundamental elements of thermoelectrics

A cold electron reservoir

A warm electron reservoir

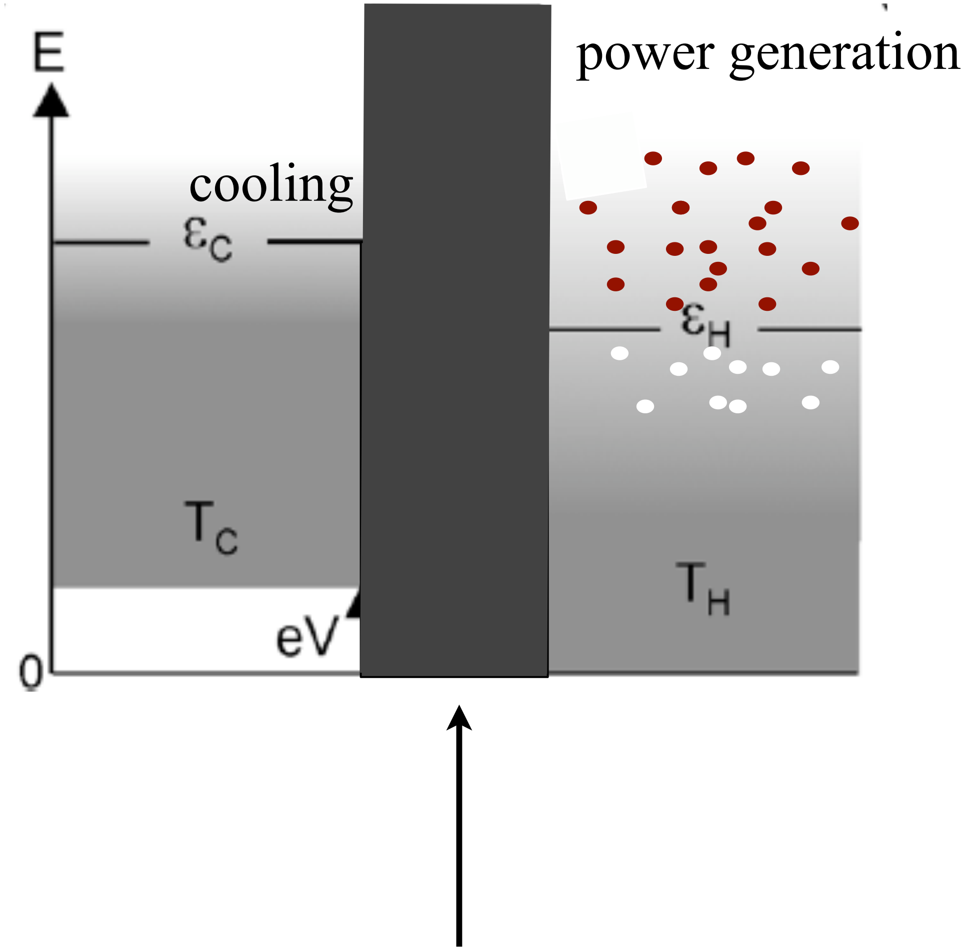


A bias voltage to do work *against.*

... and a magic black box that everything is all about!

A cold electron reservoir

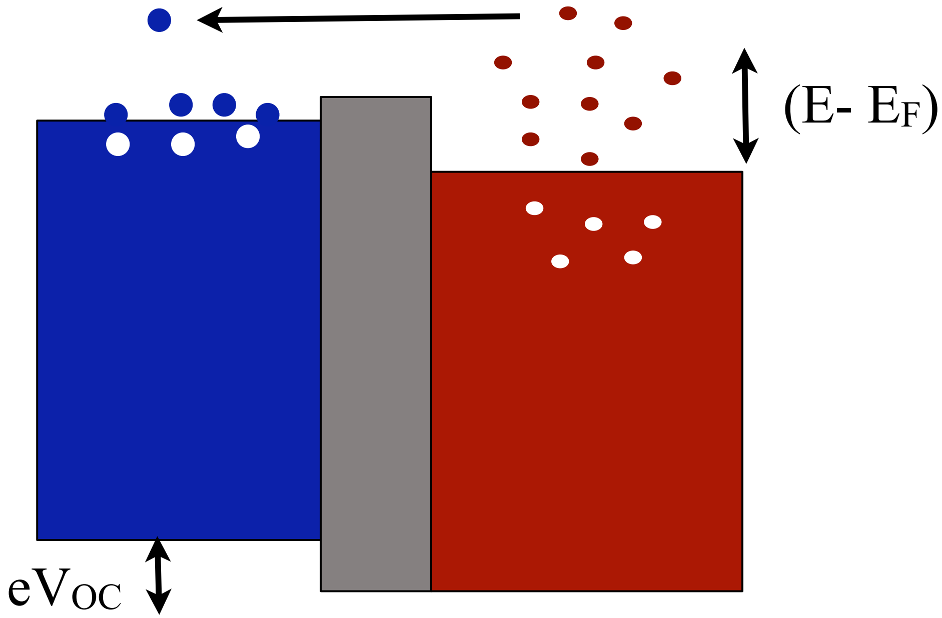
A warm electron reservoir



A bias voltage to do work *against.*

... and a magic black box that everything is all about!

The origin of a thermovoltage (open circuit):



In response to electron transfer, the cold side gets charged, increasing the chemical potential, until net electron flow ceases.

$$S = V_{OC}/T$$
$$\propto - \langle(E-E_F)\rangle/eT$$
$$\approx kT/eT$$
$$= k/e$$
$$\approx 10 - 100\ \mu V/K \quad (k = 86\ \mu eV/K)$$

Outline

(1) TE energy conversion near Carnot efficiency

(2) Experiments with quantum-dot energy filter

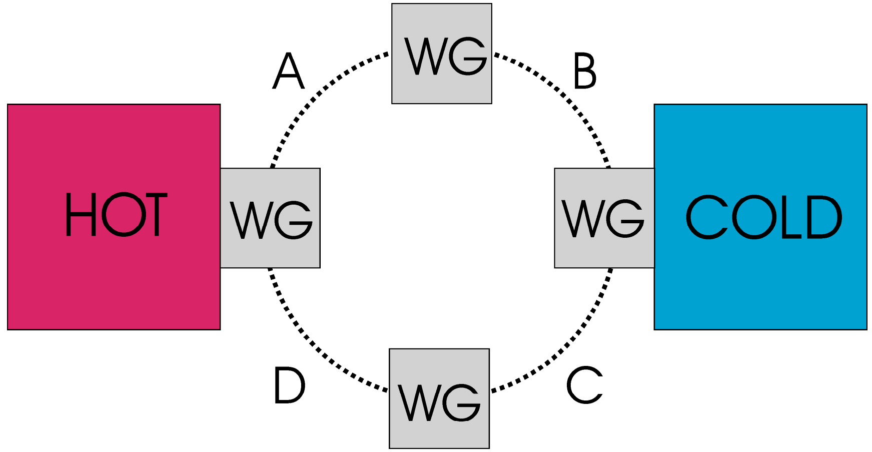
Heat flow assisted by el-ph coupling?

(3) TE efficiency at maximum power

Fundamental efficiency limit of thermoelectrics

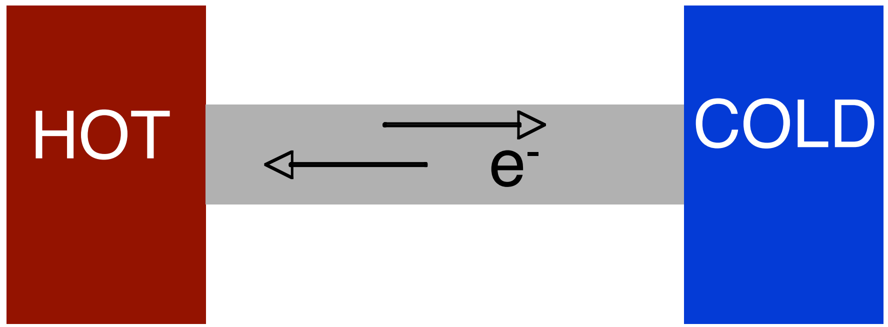
Classic, cyclic Carnot engine:
Working gas (WG) in contact with only one heat reservoir at a time.

$$\eta_C = 1 - \frac{T_C}{T_H}$$

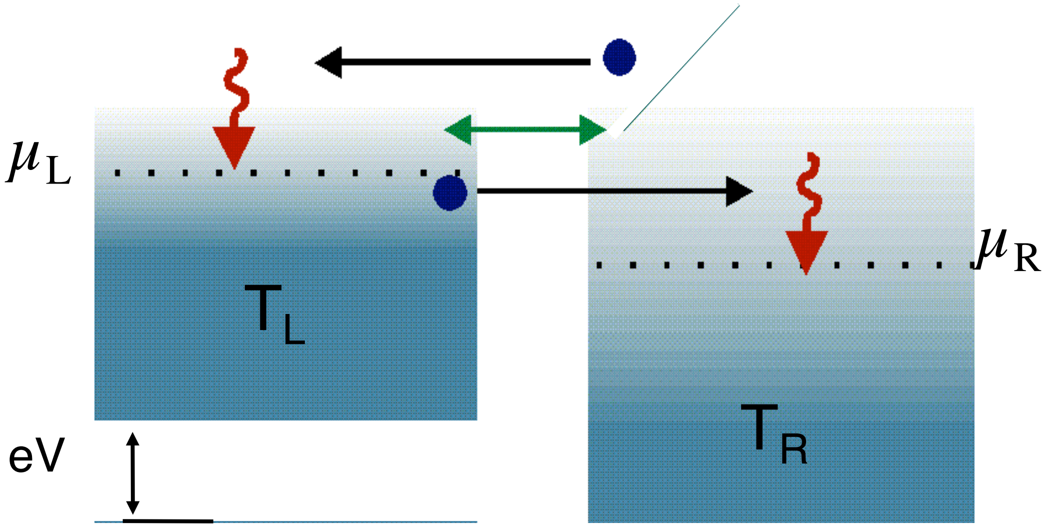


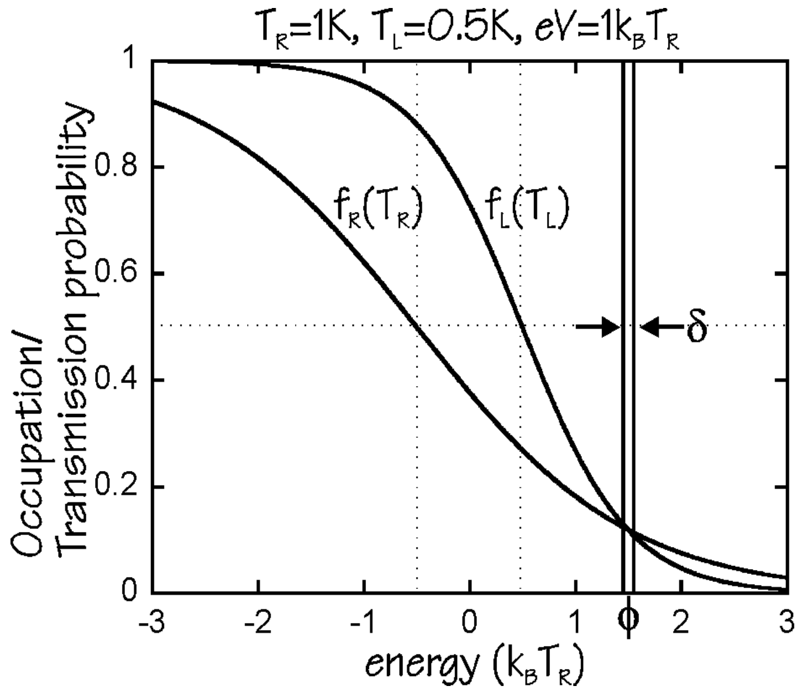
Thermoelectric:
In contact with both reservoirs at all times.

$$Z = \frac{S^2\sigma}{\kappa_e + \kappa_{ph}}$$



Reversible electron transfer





Transfer of one electron at energy ε from L to R:

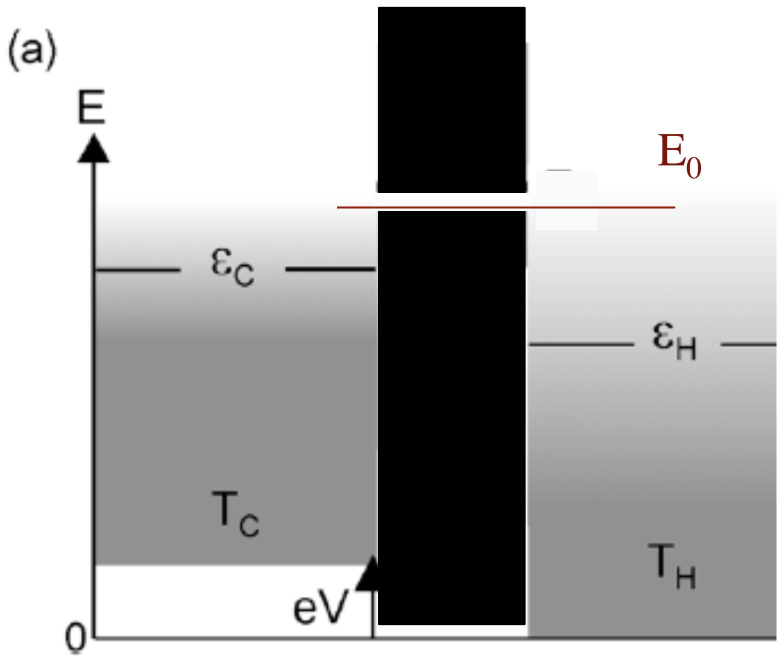
$$\Delta S = \frac{-(\varepsilon - \mu_L)}{T_L} + \frac{(\varepsilon - \mu_R)}{T_R}$$

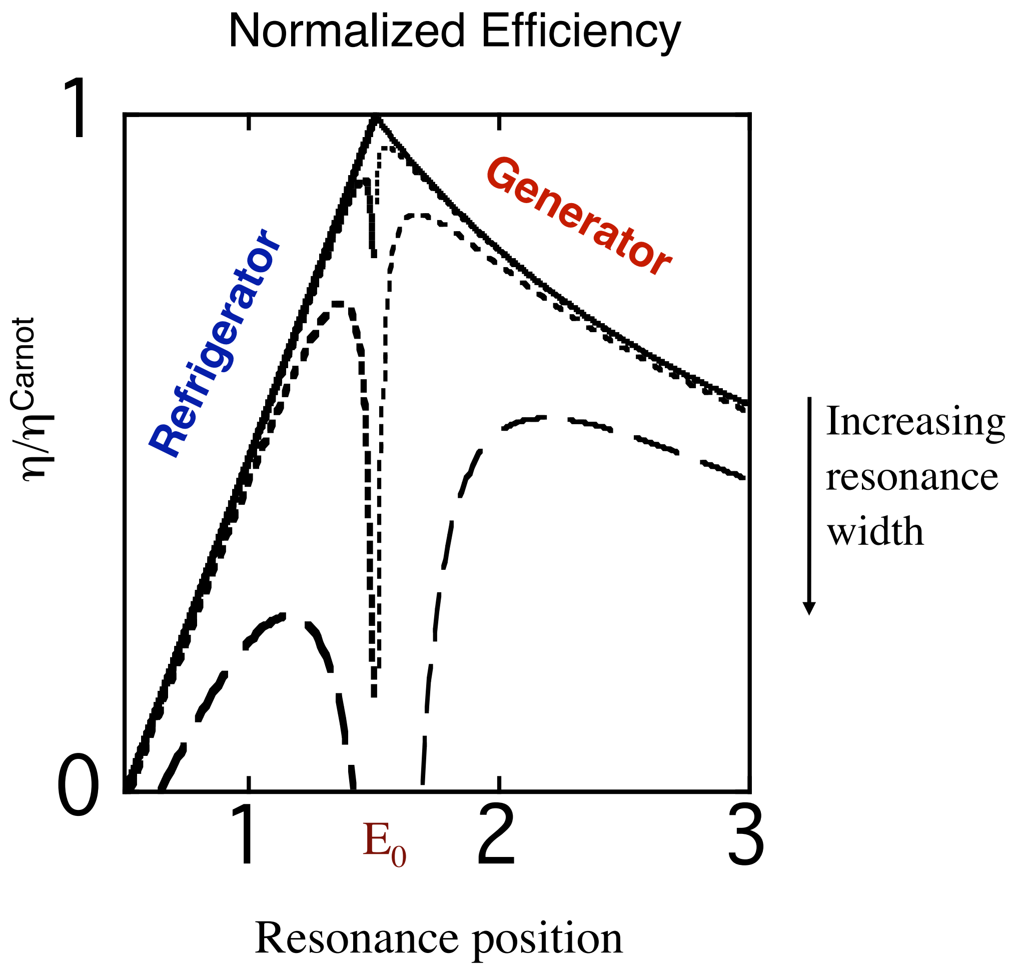
$$\Delta S = 0 \quad for \quad \varepsilon = \left(\frac{\mu_L T_R + \mu_R T_L}{T_R - T_L} \pm \right)$$

"Energy-specific equilibrium"

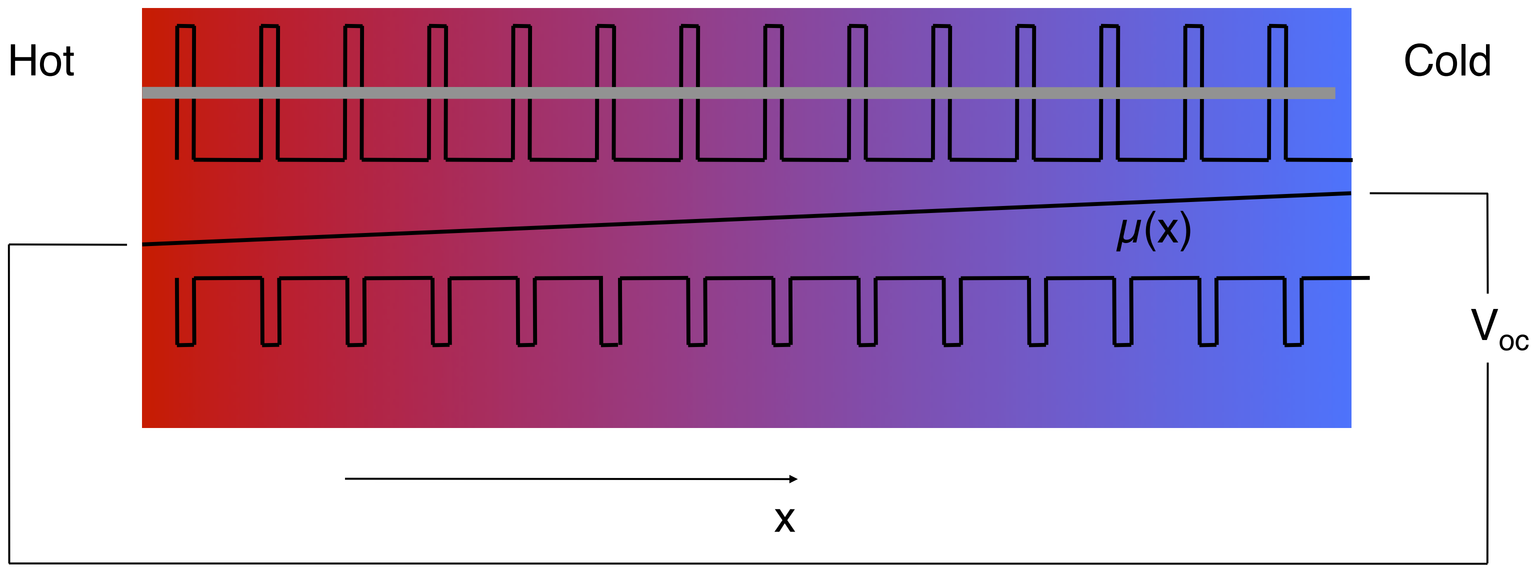
T. E. Humphrey and H. Linke, PRL **89,** 116801 (2002)

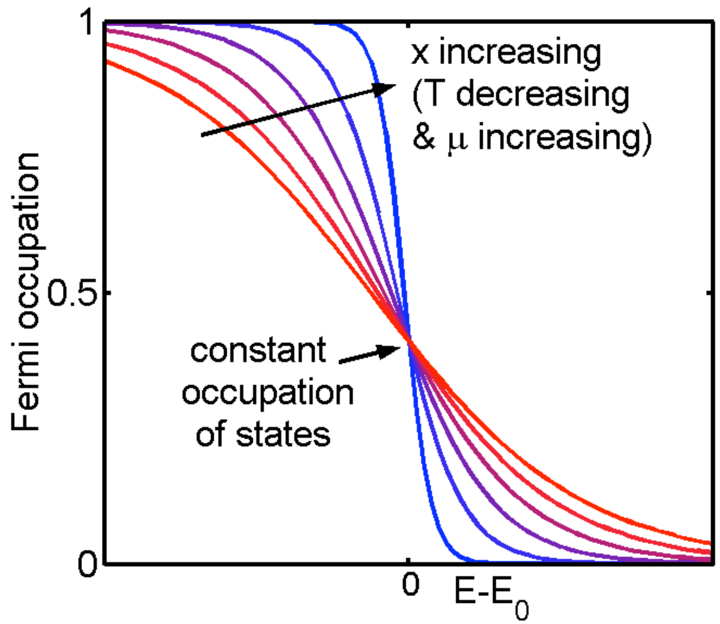
Power generation or Refrigeration near Carnot efficiency





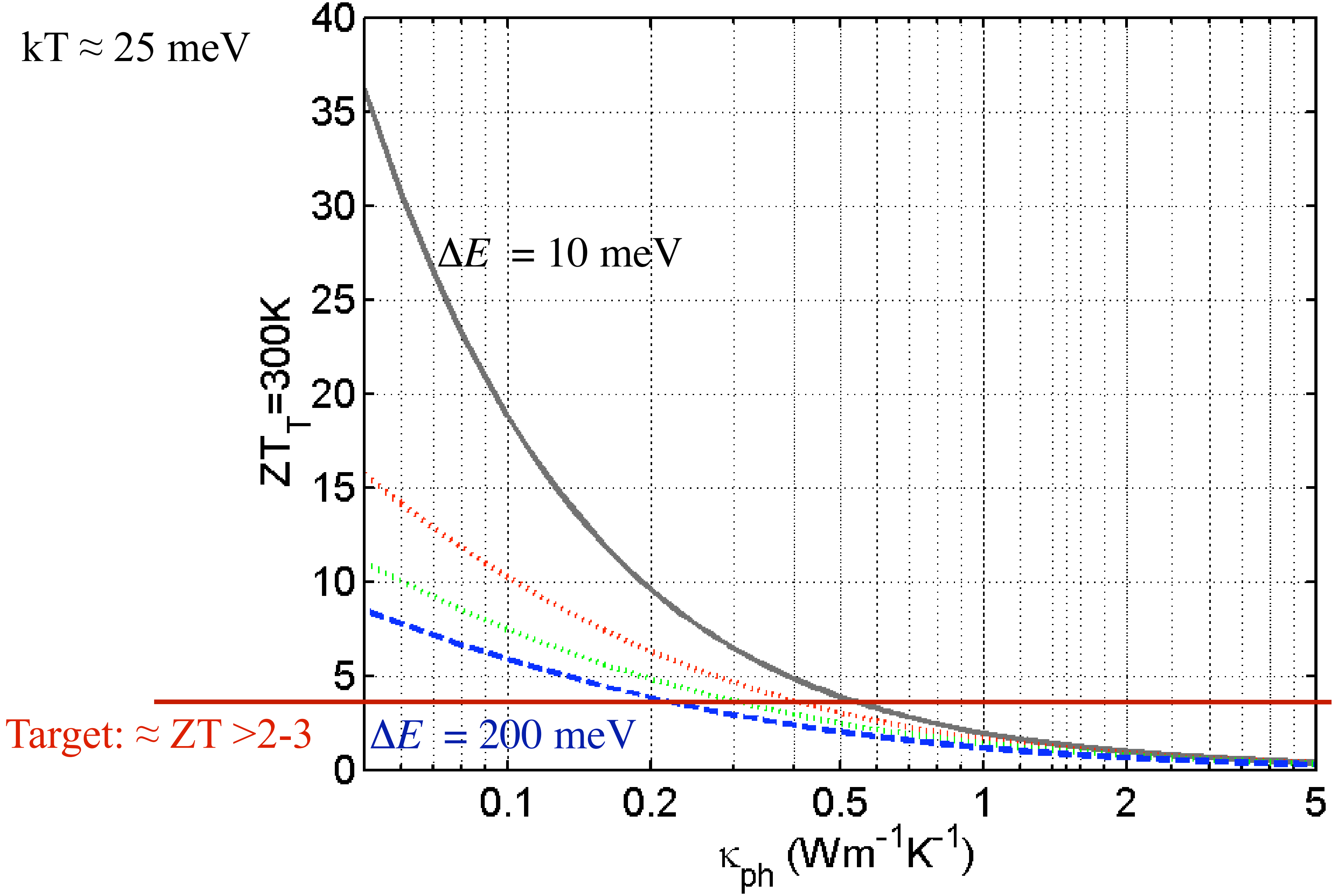
Reversible thermoelectric materials





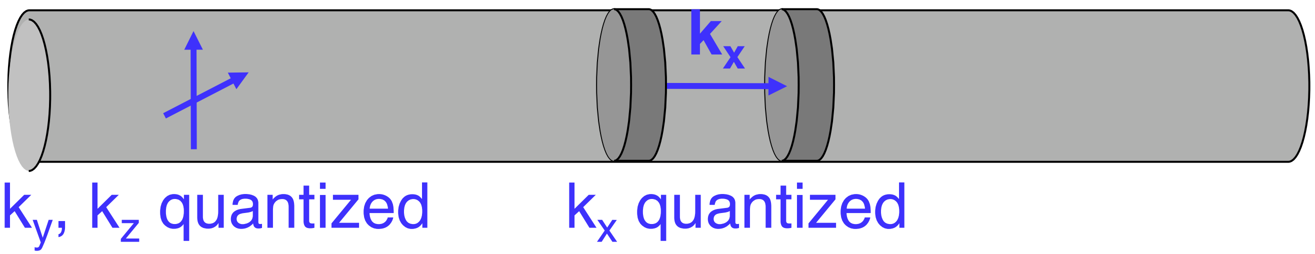
T. Humphrey, H Linke,
PRL **94**, 096601 (2005)

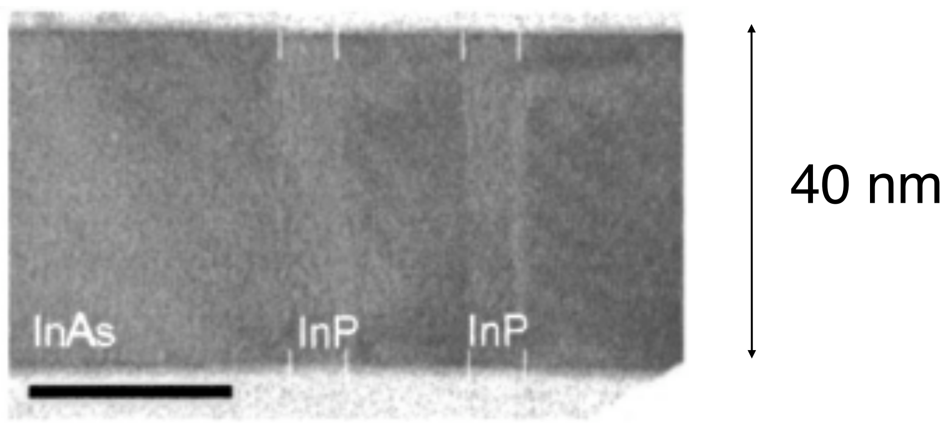
Performance of a thermoelectric nanomaterial



Energy-filtering using nanowires

1D - 0D -1D resonant tunneling in a heterostructure nanowire.

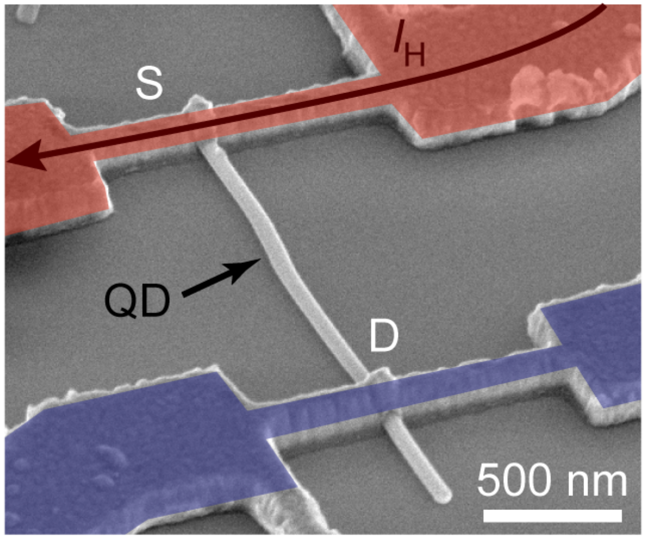


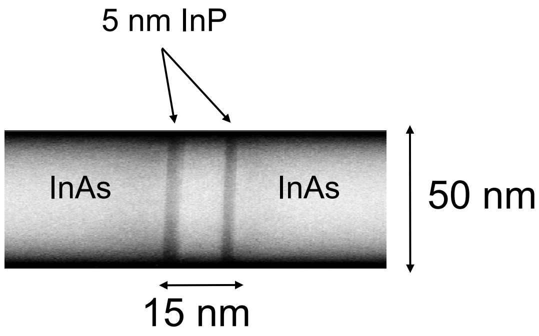


Björk *et al.*

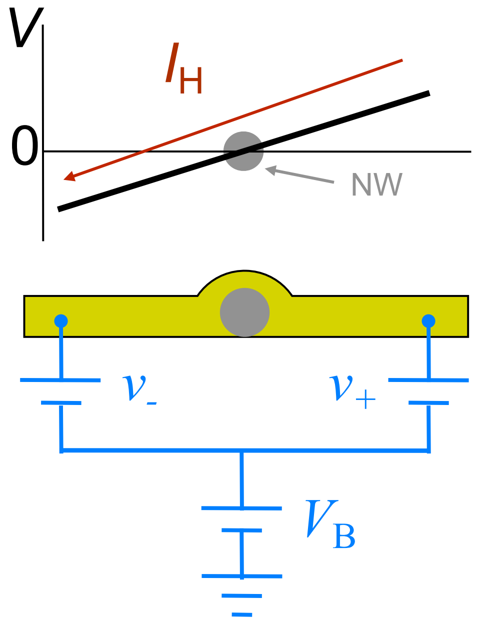
Appl. Phys. Lett., Vol. 81, No. 23, 2 December 2002

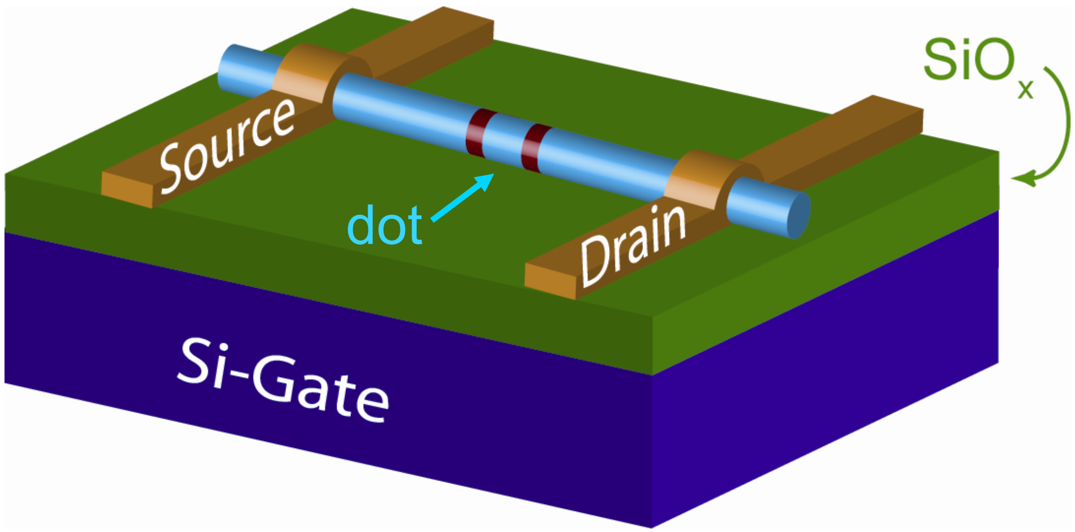
Thermal and electrical biasing



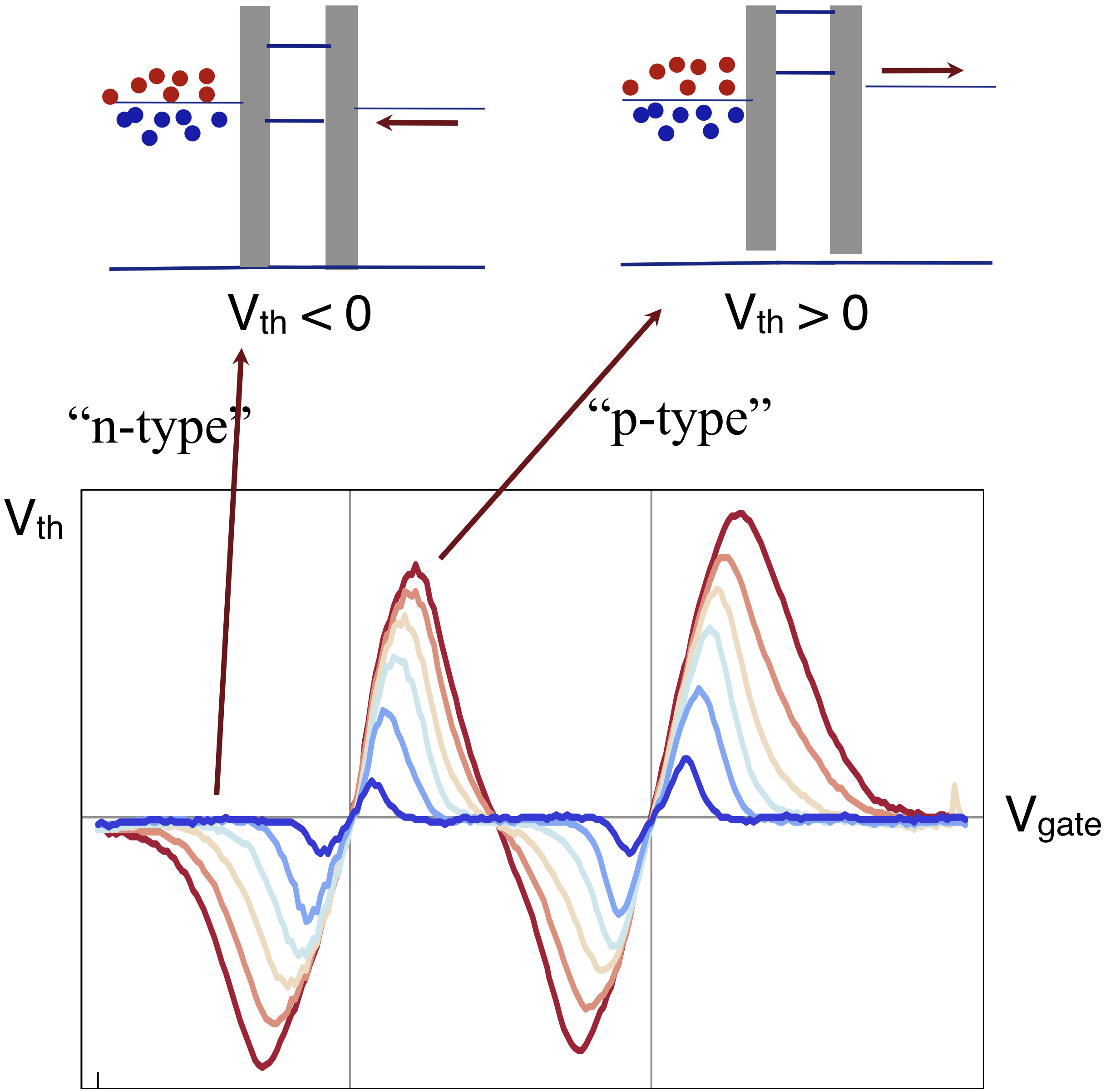


T = 250 mK to 10 K



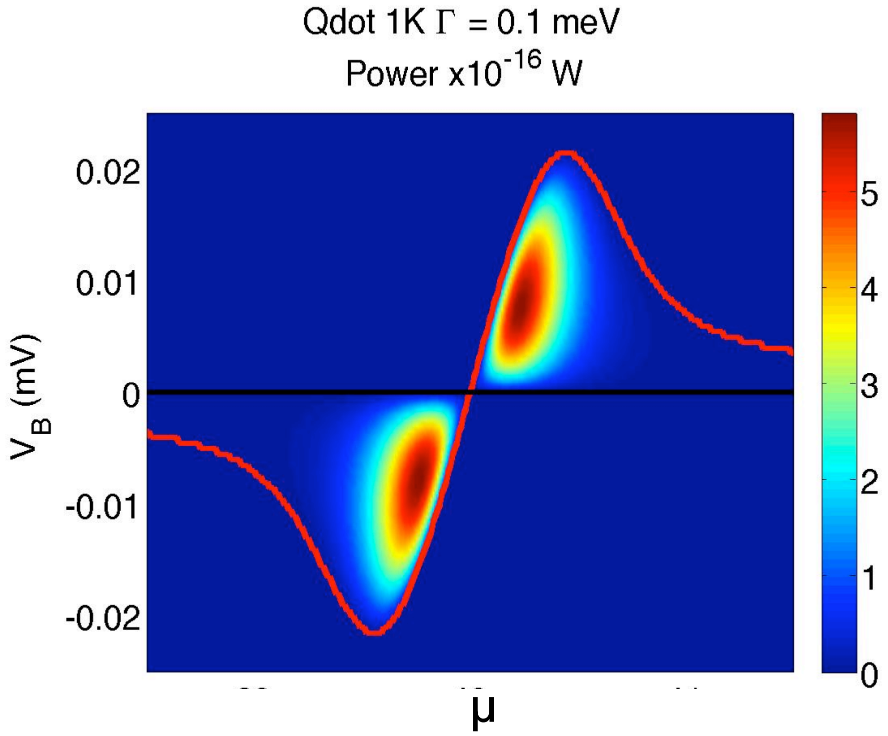


Thermovoltage lineshape



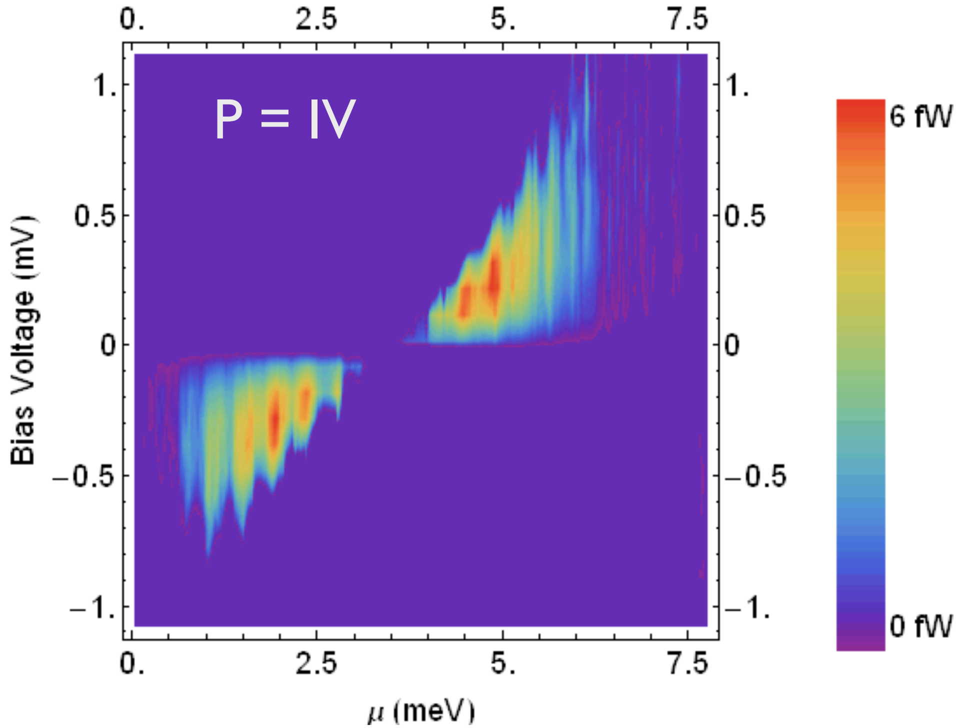
Thermoelectric power production

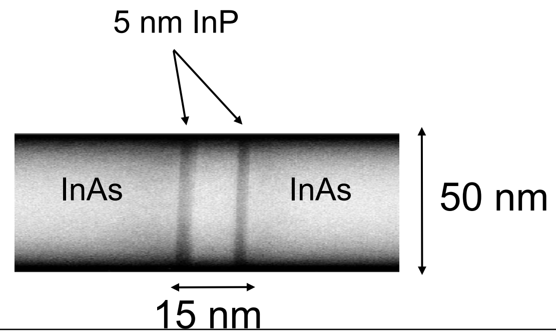
Power: Model
(Natt Nakpathomkun)



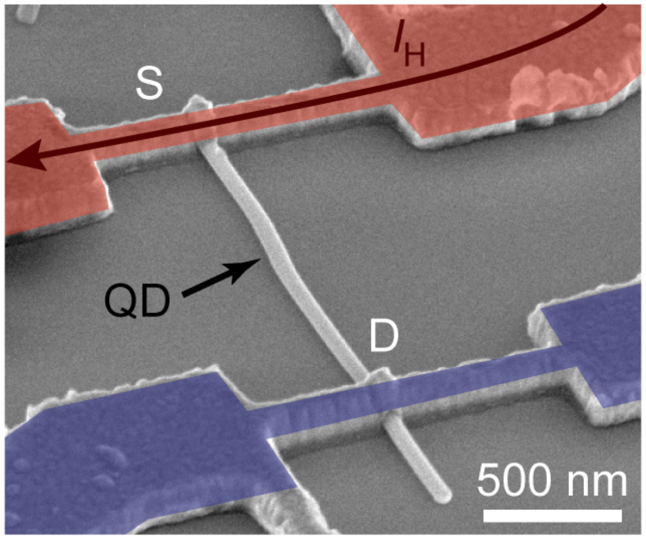
$$P = IV = \frac{2eV}{h}\int \left(f_C - f_H\right)\tau\left(E\right)dE$$

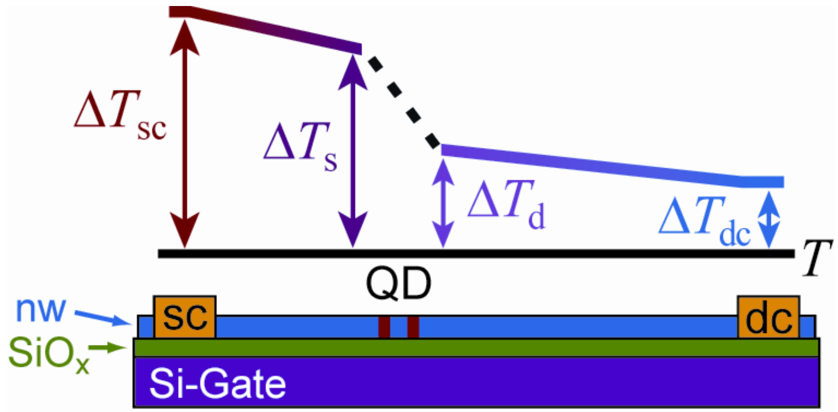
Power: Experiment
(Eric Hoffmann)

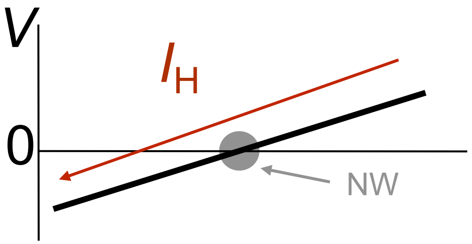


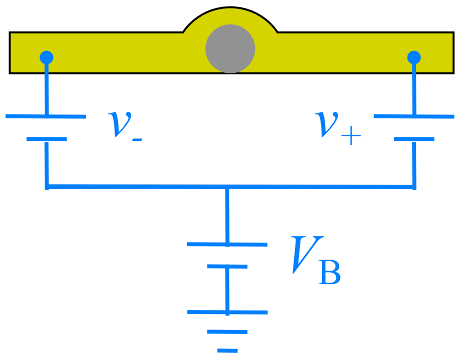


Quantum-dot thermometry









Quantum-dot thermometry:

Measure $\Delta T_{s,d}$ as a function of I_H.

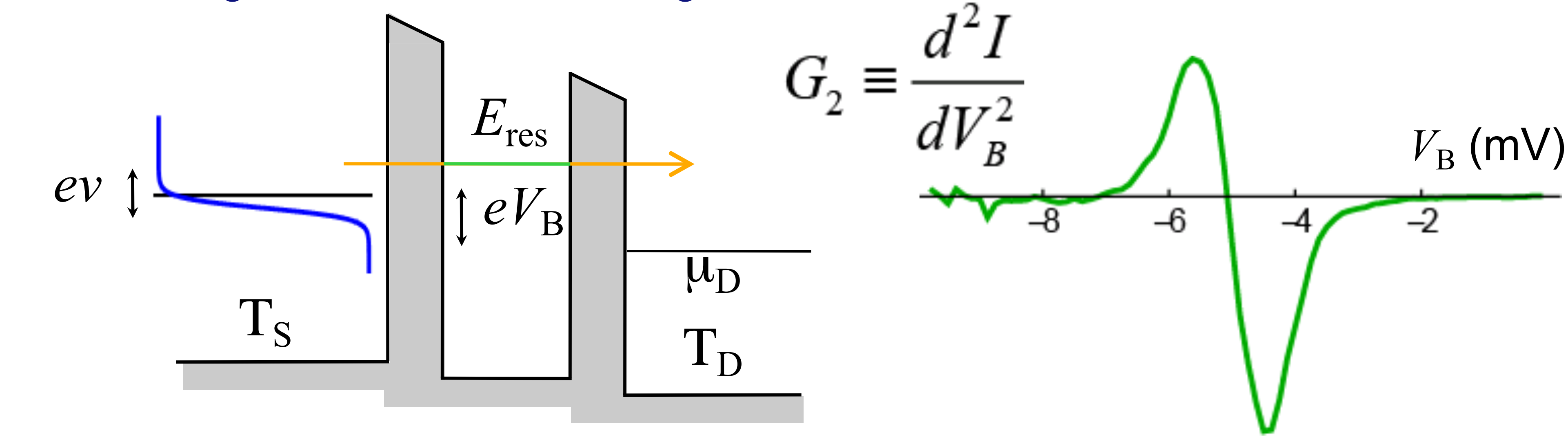
Hoffmann *et al*., App. Phys. Lett., **91**, 252114 (2007)

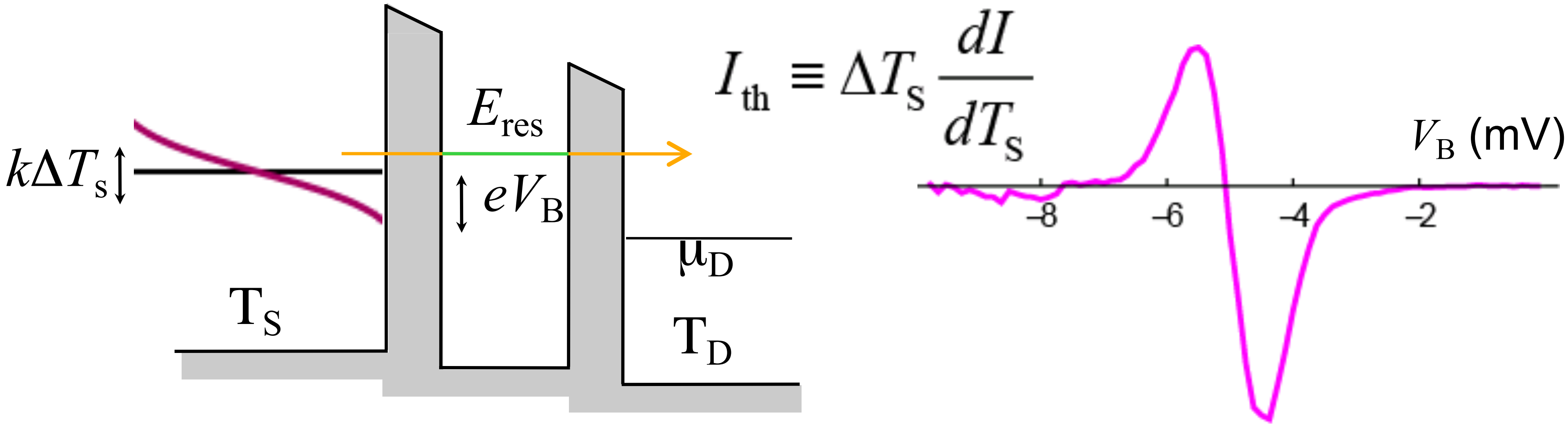
Hoffmann and Linke, J. of Low Temp. Phys., **154**, 161-171 (2009)

Hoffmann *et al*., Nano Letters, **9**, 779 (2009)

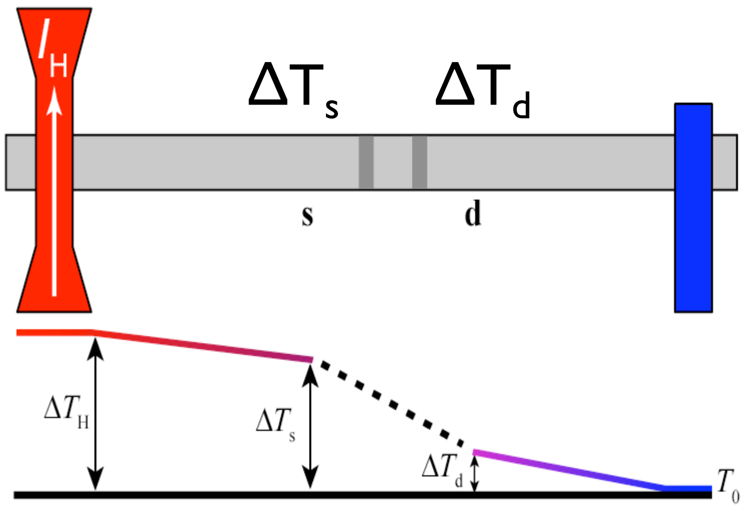
Quantum-dot thermometry

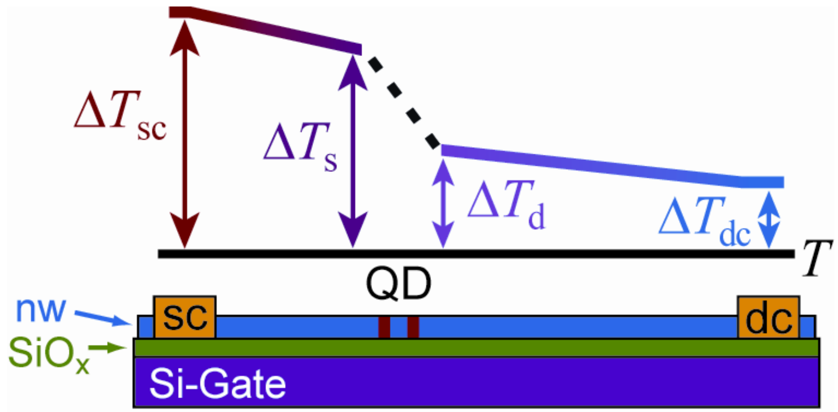
Current responses to two different perturbations:
Thermal gradient and bias voltage

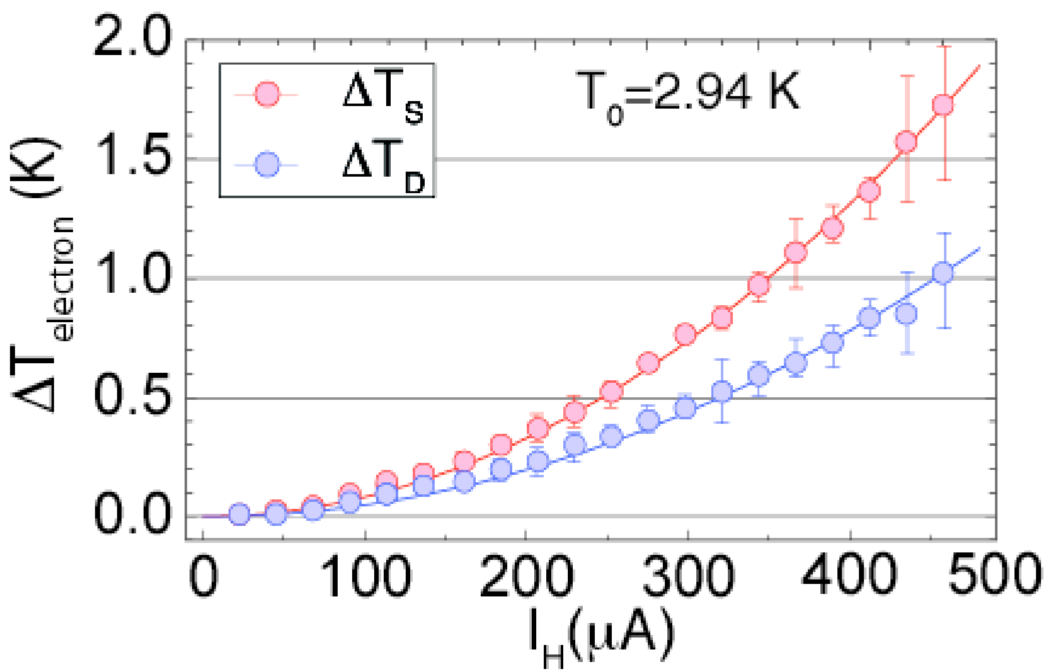




Experiment







nature nanotechnology

Research Highlights

Nature Nanotechnology
Published online: 6 February 2009 | doi:10.1038/nnano.2009.34

Subject Categories: Nanometrology and instrumentation | Nanomaterials

Thermoelectrics: Drops across dots
Michael Segal

Hoffmann *et al*., APL (2007)

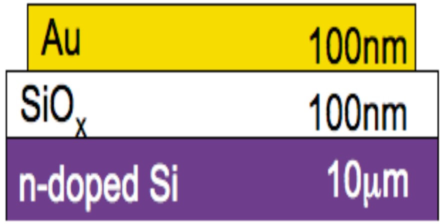
Hoffmann and Linke, J. Low Temp. Phys.

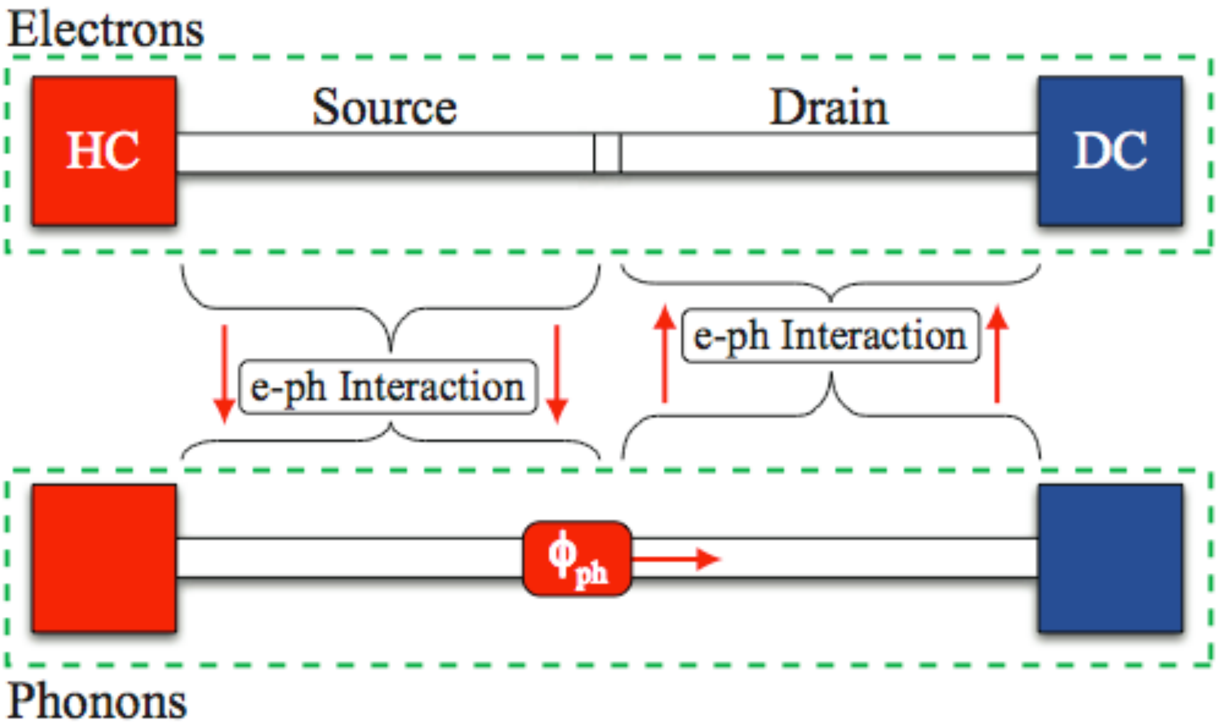
Hoffmann *et al*., Nano Lett., (2009)

Eric Hoffmann

Why do electrons in the drain heat up?

Electronic heat flow might bypass the electrically insulating quantum dot by coupling to the NW phonons.





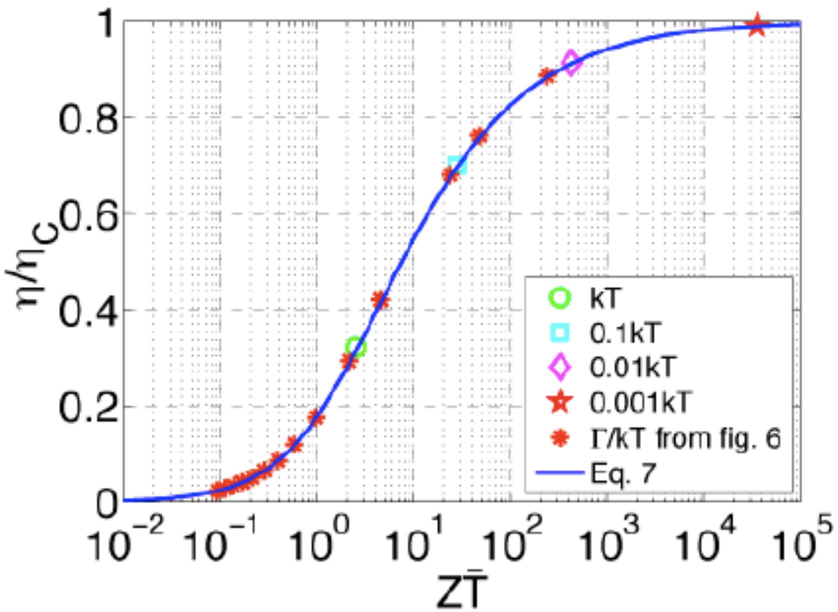
How to measure efficiency?

$$\eta = \frac{P}{\dot{Q}_H}$$

$$P = IV = \frac{2eV}{h}\int (f_C - f_H)\tau(E)\,dE$$

$$\dot{Q}_H = \int (E - \mu_H)(f_C - f_H)\tau(E)\,dE$$

Figure of merit ZT can be related to efficiency relative to Carnot:



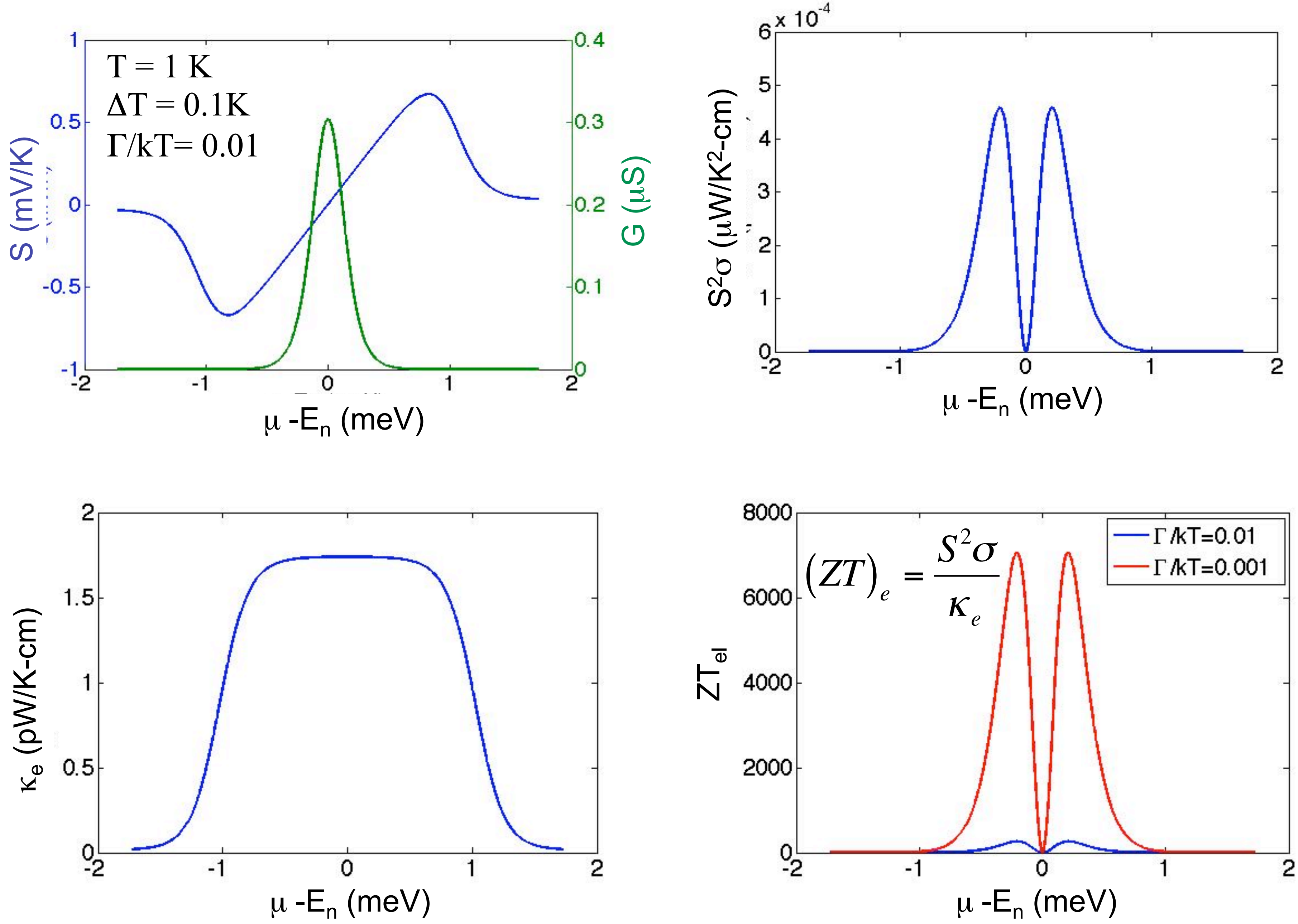
We choose:

$$(ZT)_{\mathrm{el}} \equiv \lim_{\kappa_{\mathrm{ph}}=0} Z\bar{T} = \frac{S^2 G\bar{T}}{\kappa_{\mathrm{el}}}$$

$$\kappa_{\mathrm{el}} = L_0 G\bar{T} \qquad S = V_{th}/\Delta T$$

$$(ZT)_{\mathrm{el}} = \frac{S^2 G\bar{T}}{L_0 G\bar{T}} = \frac{S^2}{L_0}$$

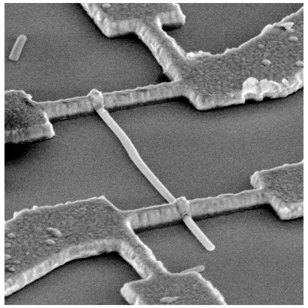
Electronic ZT of quantum dots (model)



Conclusions

Key results:

- Heterostructure III-V nanowires highly controllable system
- Extremely high *electronic* ZT measured for quantum dot.
- Thermometry and mapping of heat flow.



Conclusions:

- Low-d systems can vastly enhance electronic ZT.

  but
- exceedingly sensitive to fine tuning of energy states.
- smaller k_{ph} still a pre-requisite.

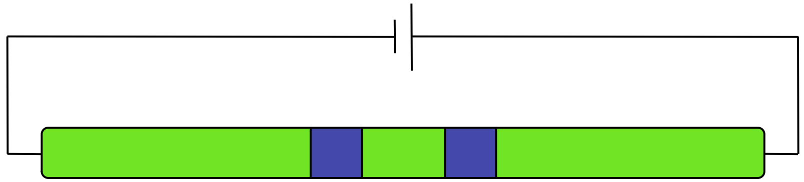
Outlook

Efficiency near maximum power: beyond ZT.

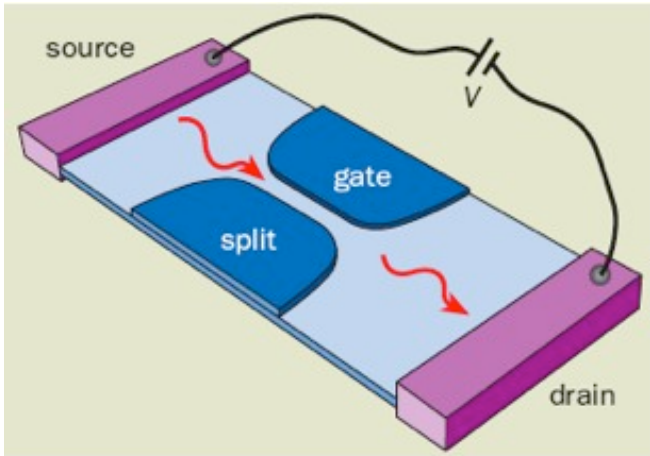
Efficiency at maximum power

Curzon-Ahlborn limit: $\eta_{CA} = 1 - \sqrt{T_C/T_H} \approx \frac{\eta_C}{2} + \frac{\eta_C^2}{8} + \mathcal{O}(\eta_C^3) + \ldots,$

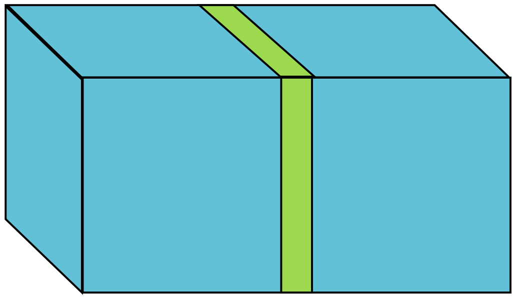
- Quantum dots (0D)



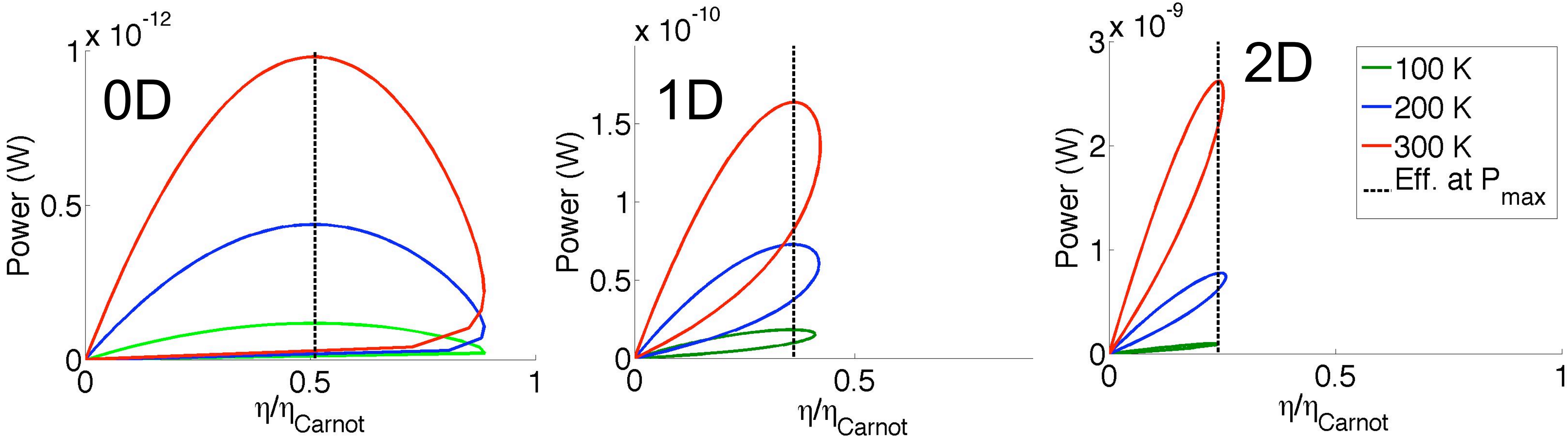
- Ideal Nanowires (1D)

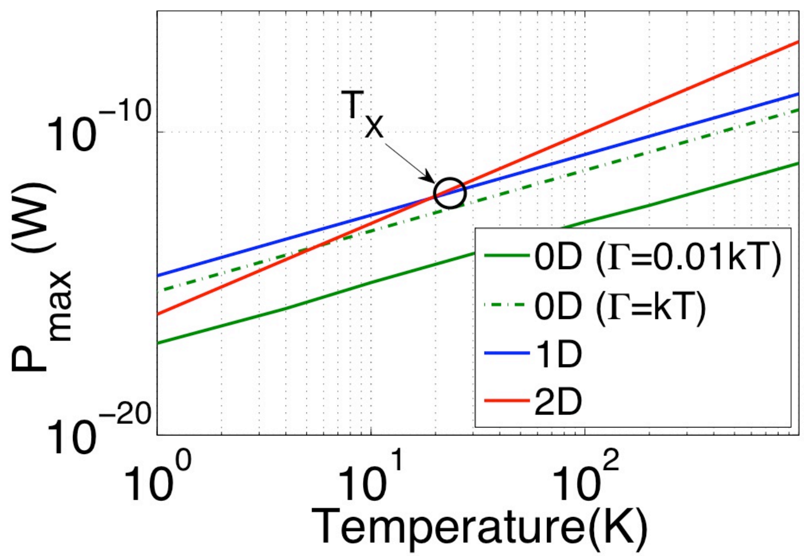


- Thermo-ionic generator (2D-barrier)



Power - Efficiency trade off in 0D, 1D, 2D/3D:





2D: η @ $P_{max} \sim 24\%$

1D: η @ $P_{max} \sim 36\%$

0D

$\Gamma/kT = 1$: η @ $P_{max} \sim 29\%$

$\Gamma/kT = 0.01$: η @ $P_{max} \sim 50\%$

Natthapon Nakpathomkun

Contributors

LUND UNIVERSITY

UNIVERSITY OF OREGON

Students & Postdocs

Eric Hoffmann, Henrik Nilsson, Tammy Humphrey, Ann Persson, Jason Matthews, Natthapon Nakpathomkun

Collaborators

Lars Samuelson, Kimberly Dick, Knut Deppert (Lund)
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