Thermoelectric effects in ultra-scaled semiconductor devices
Role of electronic and lattice properties

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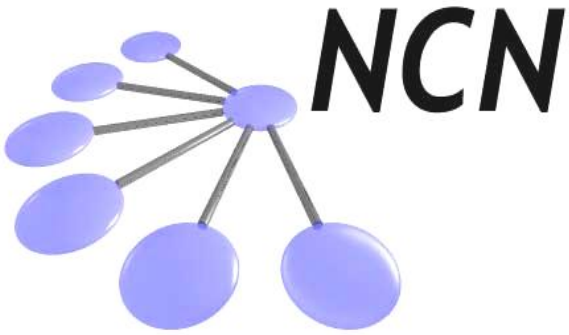
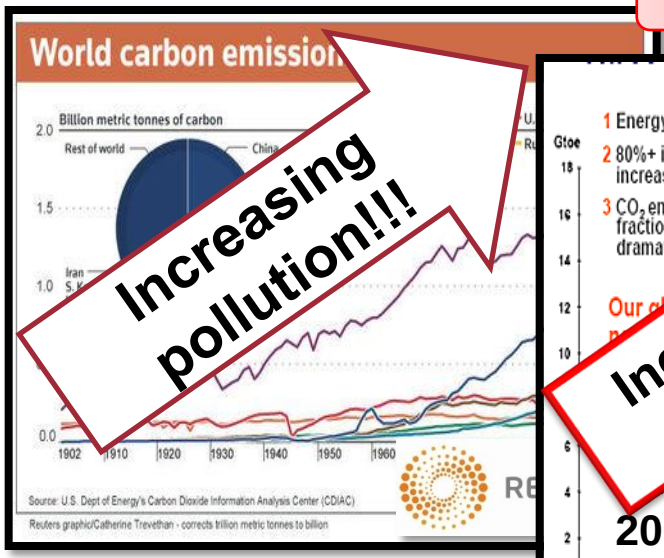
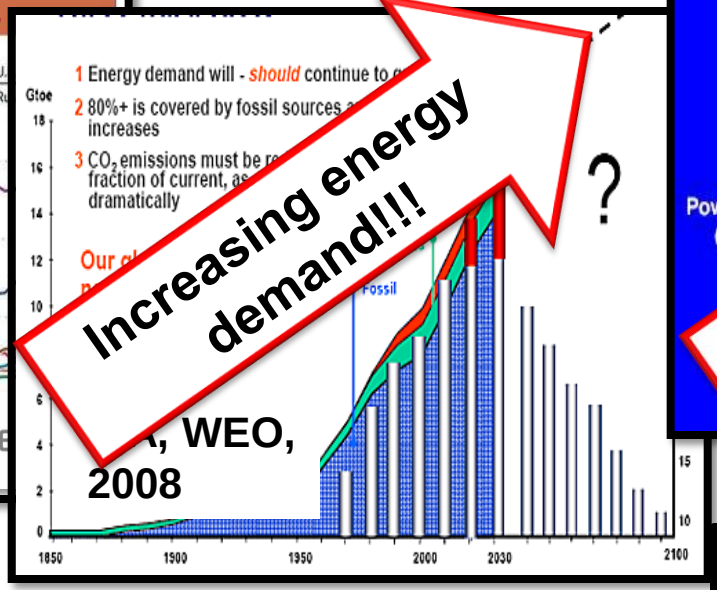


Why thermoelectricity ???

Nasty Problems

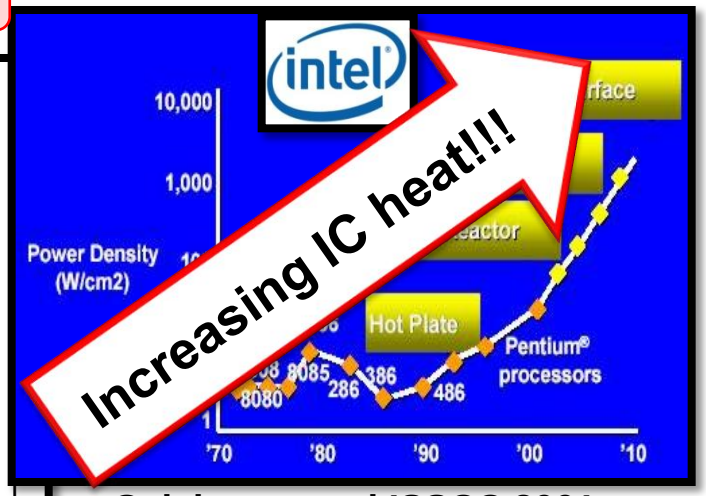


Increasing pollution!!!



Increasing energy demand!!!

, WEO, 2008

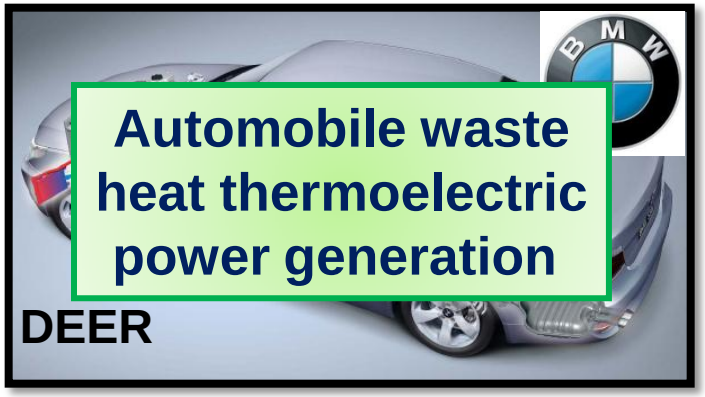


Increasing IC heat!!!

Gelsinger et. al ISSCC 2001

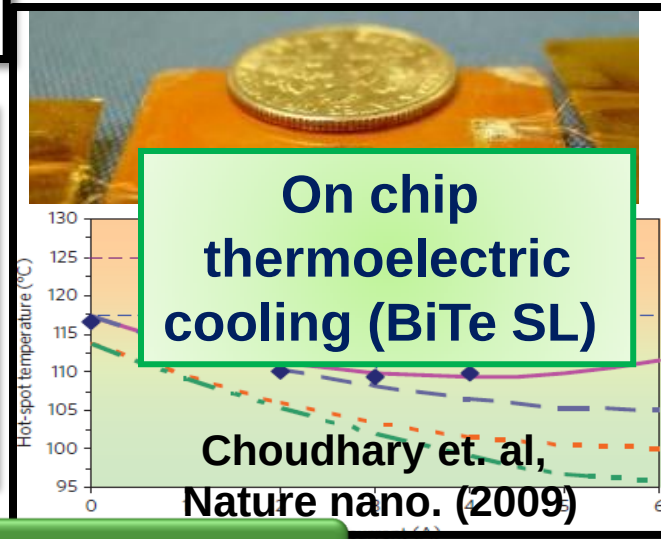
Green energy Production by thermoelectricity

www.tellure



Automobile waste heat thermoelectric power generation

DEER



On chip thermoelectric cooling (BiTe SL)

Choudhary et. al, Nature nano. (2009)

Green Solutions from thermoelectricity !!!

What inspired present research ???

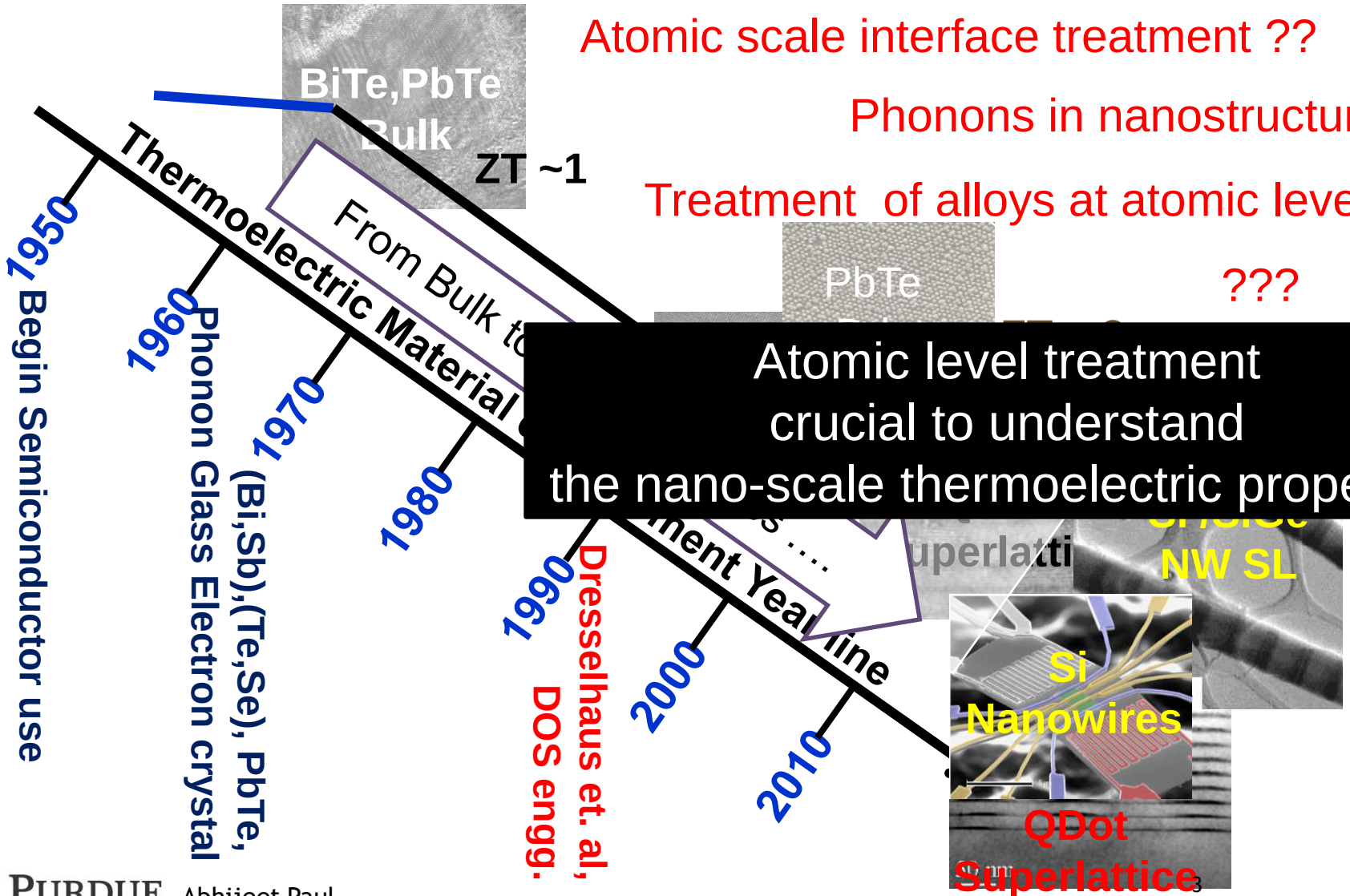
Electronic structure in nanostructures?

Atomic scale interface treatment ??

Phonons in nanostructures ??

Treatment of alloys at atomic level ??

???



Outline of the talk

- Introduction to Thermoelectricity
  - Basics
  - Material Development
  - Research vectors
- Approach for thermoelectric (TE) analysis.
- Research milestones
  - Results for Silicon nanowires
  - Scientific Outreach
- Future Proposal
  - Investigation of SiGe nanowire superlattices as TE material.
- Summary

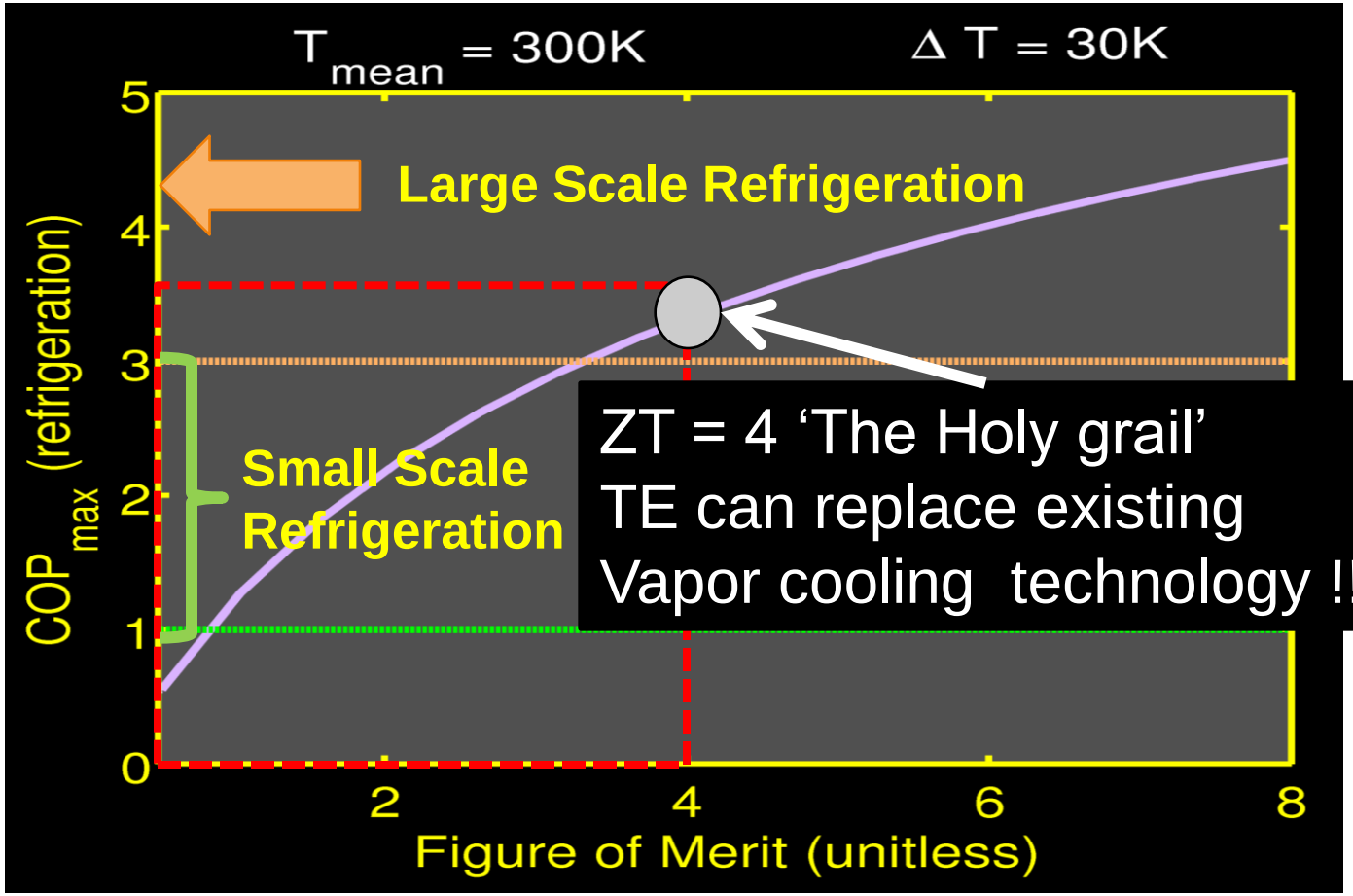
Assessing thermoelectric efficiency: ZT

Coefficient of Performance

$$= \left[\frac{T_{hot}}{T_{hot}-T_{cold}}\right]\cdot\left[\frac{\sqrt{1+ZT}-T_{hot}/T_{cold}}{\sqrt{1+ZT}+1}\right]$$

Heat energy removed from cold side

Heat energy added to hot side



Composition of Figure of Merit (ZT)

Generation of potential difference due to applied temperature difference → **`Seebeck Coefficient'**.

$$S = \frac{\Delta V}{\Delta T}$$

Measure of thermoelectric power generation (High)

Generation of temperature difference due to applied potential difference → **`Peltier Coefficient'**

$$\Pi = T\frac{\Delta V}{\Delta T}$$

Measure of thermoelectric cooling (High)

$$ZT = \frac{GS^2T}{\kappa_l + \kappa_e}$$

'Thermoelectric Figure of Merit' unitless quantity obtained at temp `T'. Defined by Ioffe in 1949.

Ability of material to conduct electricity → **`Electrical Conductance'**

$$G = \frac{\Delta I}{\Delta V}$$

Measure of charge flow (High)

Ability of material to conduct heat energy → **`Thermal Conductance'**

$$\kappa = \frac{1}{T}\frac{\Delta Q}{\Delta d}$$

Measure of heat flow (Low) Both electrons (k_e)and lattice(k_l) carry heat.

Large COP → High ZT → large G ↑ large S ↑ and small κ ↓ desired !!!

Material of choice for thermoelectricity

TE Parameters → / Materials ↓		Electrical Conductivity (G) ↑	Seebeck Coefficient (S) ↑	Thermal Conductivity (κ) ↓
Metals	✗	Very High ↑ ~10^7 S/m	Low ↓ ~ 10μV/K	High ↑ ~10^2 W/m-K
Insulators	✗	Extremely low (~10^{-10}S/m) ↓	High ↑	Low ↓ ~10^{-2}-10^{-4} W/m-K
Semiconductors	✓	Moderate ↑ 10^{-3}S/m	High ↑ ~120 μV/K	Low ↓ ~10 W/m-K

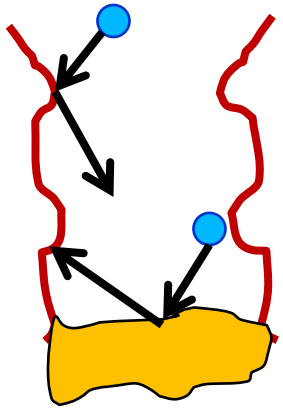
Semiconductors most suitable TE material.
Allow separate control of G (electrons) and κ (phonons).

ZT enhancement…

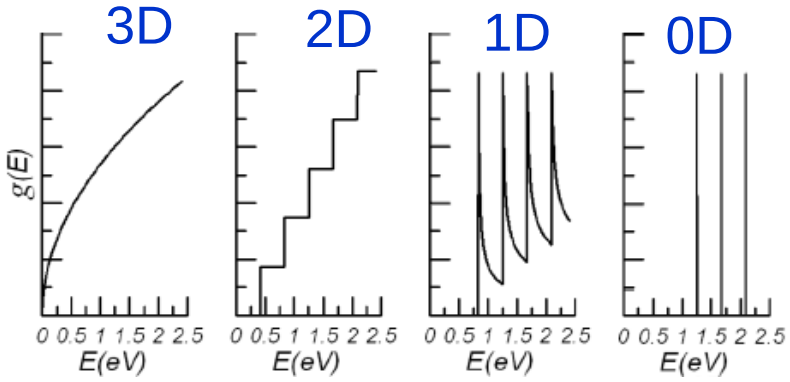
1990s ⟶ Enhance Power factor (S^2G) by electronic structure modification.

Nanostructures provide DOS modification.

$$ZT = \frac{TGS^2}{\kappa_e + \kappa_l}$$



Phonon scattering



DOS engineering

1960s ⟶ Reduce thermal conductivity by phonon scattering.

Nanostructures and alloys increase phonon scattering.

Nanostructures allow tuning of G, S and κ !!!

Material Research → ??? → Market

Promising TE Materials

Making research Economically viable

Potential Markets [1]

Crucial R&D vectors

- Fabrication of nanostructures.
- Robust thermoelectric characterization
- Higher reliability
- Better structural stability.
- Efficient thermoelectric modules.
- Bulk and low cost production.
- Better simulation and analysis tools.

- Thin Films
- Nano-particles
- Super Lattices
- Nano-composites
- Nanowires
- Quantum Dots

Research

- Consumer (35%)
- Automobile (14%)
- Telecom (16%)
- Medical and Bio (12%)
- Industry (9%)
- Semicon. Process (8%)
- Defense & space (6%)

Economy $$$

Computer simulation an integral part to develop better TE materials and modules

[1]Hachiuma & Fukuda ECT, 2007

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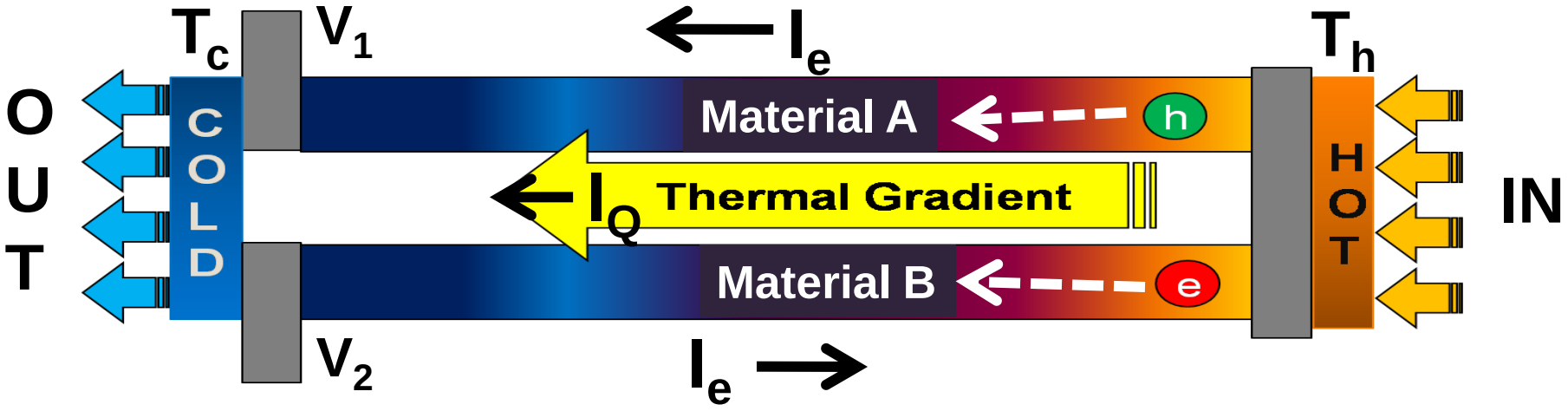
How to analyze thermoelectric properties of materials ?



Steady-state linear thermoelectric (Onsager's) relations [1,2]

Electric current

$$I_e = G.\Delta V - (GS).\Delta T$$

Heat current

$$I_Q = \left(GS\bar{T}\right).\Delta V + \left(\kappa - S^2 G\bar{T}\right).\Delta T$$

Landauer's Formula can be used to evaluate the transport parameters

$$|\Delta V| < \frac{k_B \bar{T}}{q}$$

$$\Delta T << \bar{T}$$

$$\Delta V = V_1 - V_2, \Delta T = T_h - T_c, \bar{T} = T_h + T_h/2, \kappa = \kappa_e + \kappa_l$$

[1] L. Onsager, Phys. Rev. 37 405 (1931).
[2] G. D. Mahan, Many-body Physics.

Calculation of thermoelectric parameters

G,S κ_e (Electronic)

κ_l (Lattice)

$$= \text{Pre-factor} \times f(L_m^{e/l})$$

Landauer's Integral

Under zero current condition

$$G \propto L_0^e \qquad S \propto L_1^e / L_0^e \qquad \kappa_l \propto L_1^l$$

Landauer's approach →
A suitable approach to calculate thermoelectric transport parameters in nanostructures.

$$L_m^l = \int_0^{\omega_{max}} \omega^m \left[\frac{<\lambda_{ph}(\omega)>}{L}\right]\left(\frac{\partial F_{BE}(\omega)}{\partial T}\right) M(\omega) d\omega$$

Phonon Integral

Phonons need

- No Fermi Level
- Bose Einstein distribution (bosons!!)
- M(ω) → Phonon dispersion.

$L_m^{e/l}$

Both need

- No. of modes, M(E).
- Mean free path (λ).

Accurate electronic & phonon dispersions must !!!.

Electrons need

- Moment calculation near Fermi Level
- Fermi Dirac distribution (fermions!!)
- M(E) → Electronic bandstructure.

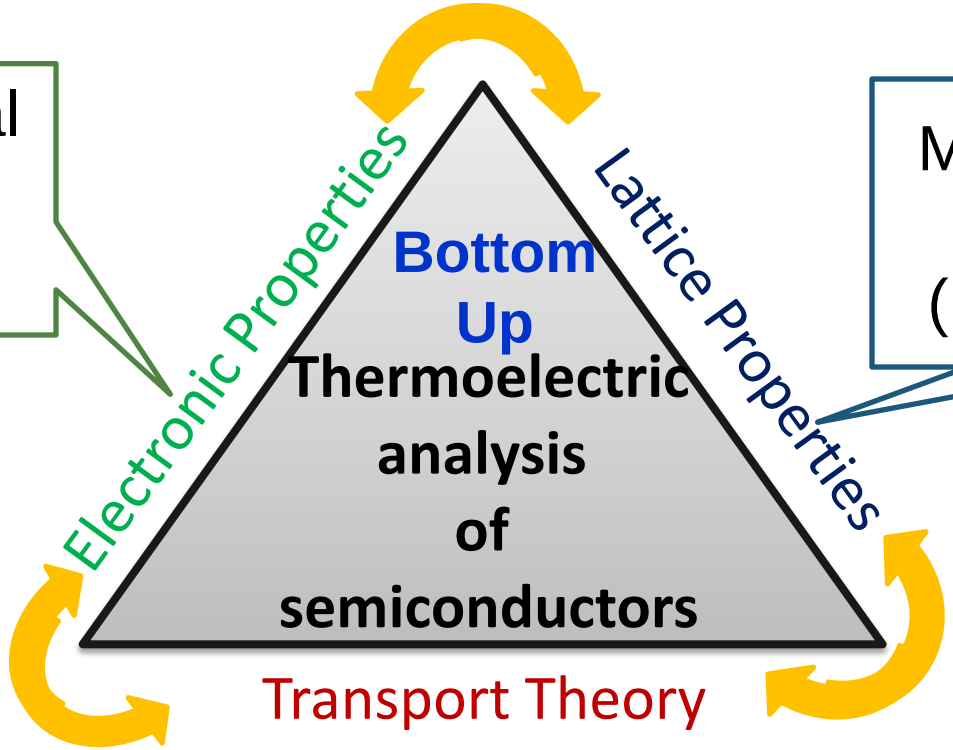
$$L_m^e = \int_{-\infty}^{Etop} \left(\frac{E - Ef}{k_B T}\right)^m \left[\frac{<\lambda_{el}(E)>}{L}\right]\left(-\frac{\partial F_{FD}(E)}{\partial E}\right) M(E) dE$$

Electron Integral

The approach for TE analysis

Semi-empirical Tight-Binding (TB) method.

Modified Valence Force Field (MVFF) method.



Landauer's approach and Green's function method

Three ingredients for TE analysis in nanostructures

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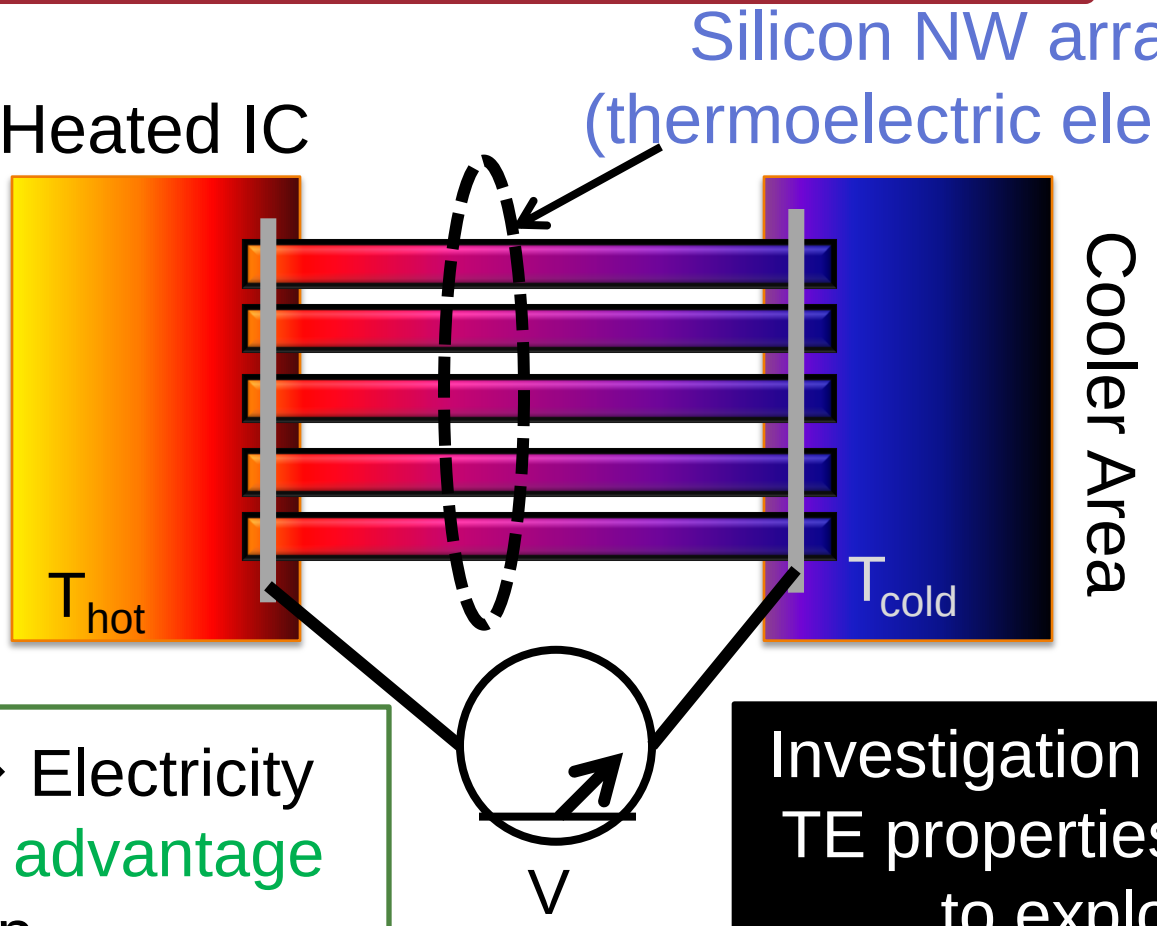
Why thermoelectric analysis of Si Nanowires (SiNW) ???

How to cool the heating ICs ??



Waste heat → Electricity

Two pronged advantage

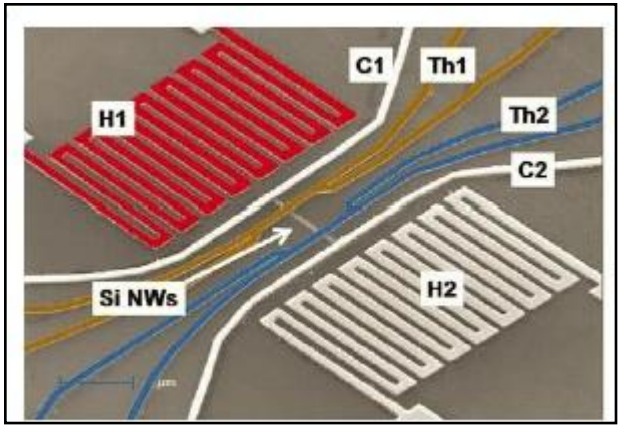
- Cool the chip.
- Obtain electricity

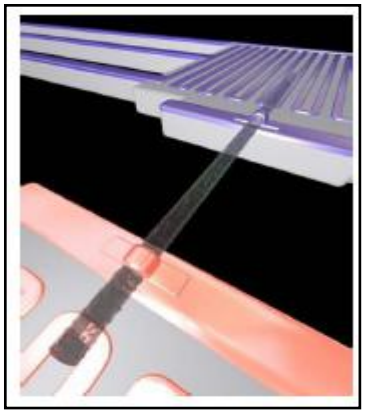
Investigation of SiNW TE properties crucial to explore more ideas !!!

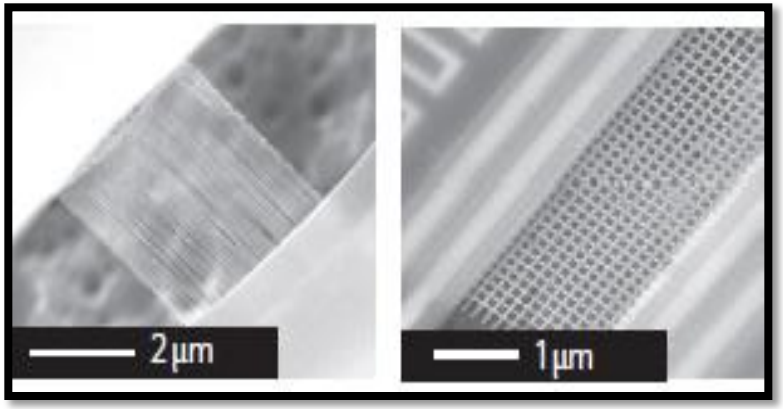
Experimental realizations…

High ZT p-type SiNW waste heat conversion

Thermal conductance reduction Silicon phonon mesh







ZT ~1 @ 200K
Caltech, Nature, 451,168, 2008

ZT ~0.6 @ 300K
Berkeley, Nature, 451,163, 2008

κ ~ 1.9 W/m-K
Caltech, Nature nano.2010, doi:10.1038/nnano.2010.149

100 fold rise in SiNW ZT compared to Bulk Si ZT (0.01 @ 300K)!!!

100 fold reduction in Si nanomesh κ compared to Bulk Si (~148 W/m-K @ 300K)!!!

Nanostructuring (SiNW) turns 'lousy bulk Si' to better TE material !!

Role of electronic structure on Thermoelectric properties

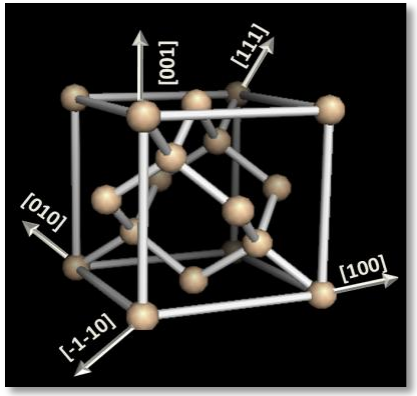
1. Atomistic confinemenet effects on the Seebeck coefficient (S) in SiNWs.
2. Atomistic and uniaxial strain effect on thermoelectric power-factor (S^2G) of SiNWs.

DEVICE DETAILS:
- Rectangular SiNW → [100], [110] and [111] channels.
- Width (W) and height (H) varied from 2 to 14nm.

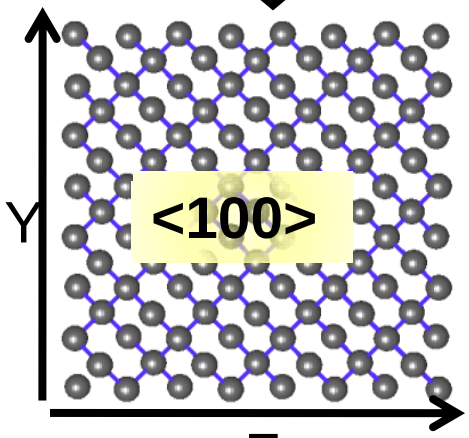
Electronic structure using Atomistic Tight Binding method.

S and G calculation using Landauer's approach.

Atomistic Tight binding Approach : A short introduction

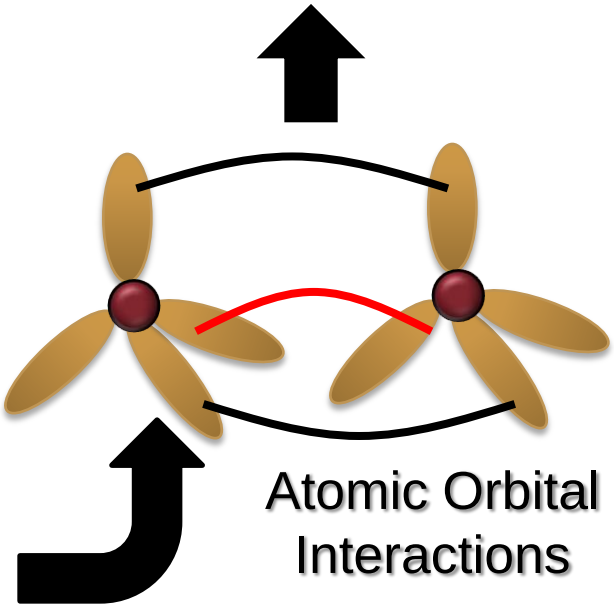


Zinc blende unitcell



Nano-structure

Assemble
TB Hamiltonian
and
obtain eigen energies



Atomic Orbital Interactions

ADVANTAGES

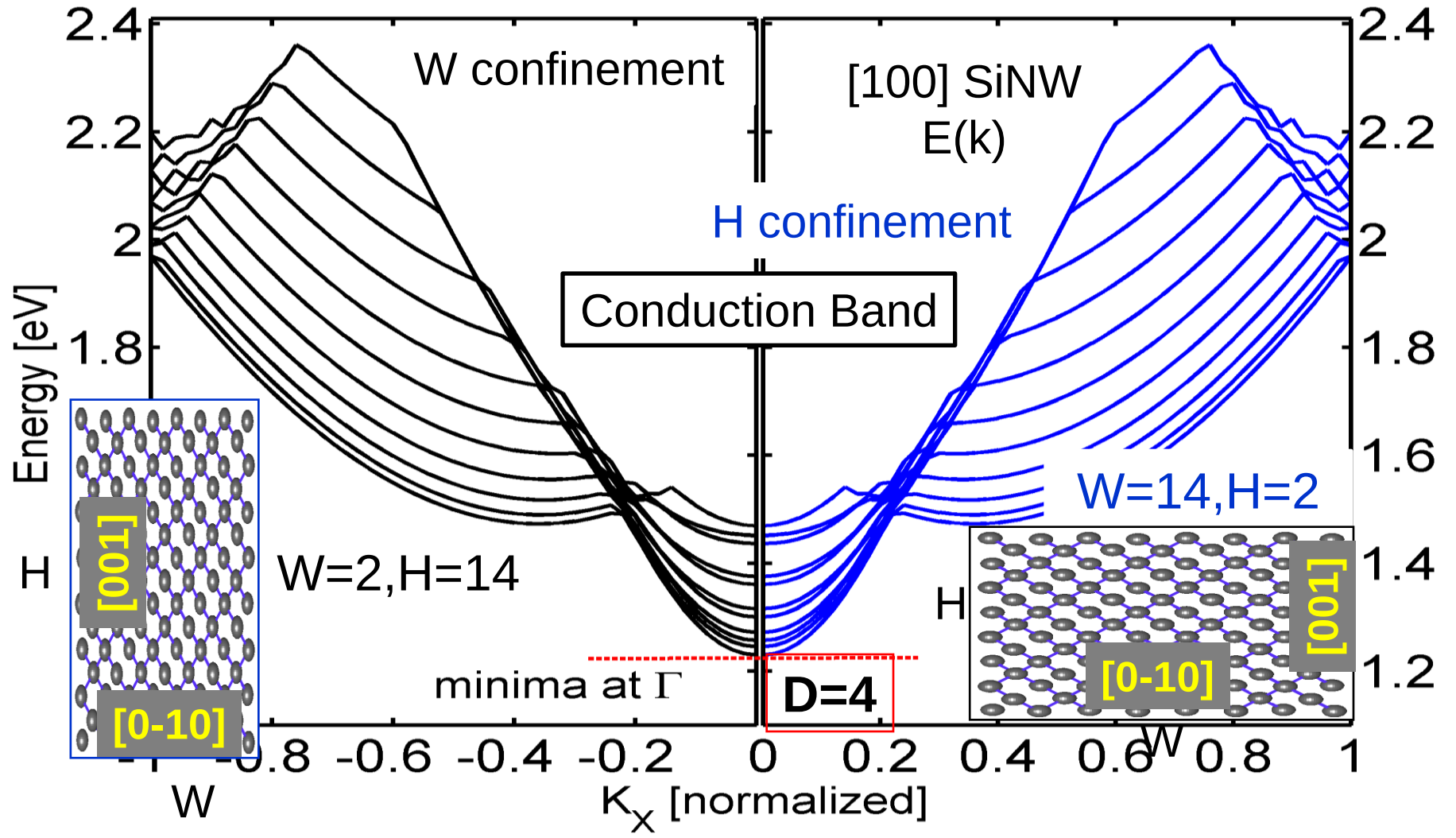
- ✓Appropriate for treating atomic level disorder.
- ✓Strain treatment at atomic level.
- ✓Structural, material and potential variation at atomic level treated.

10 band nearest neighbor $sp^3d^5s^*$ model with spin orbit coupling.

Electronic structure calculation in SiNWs using Tight Binding [1] (TB)

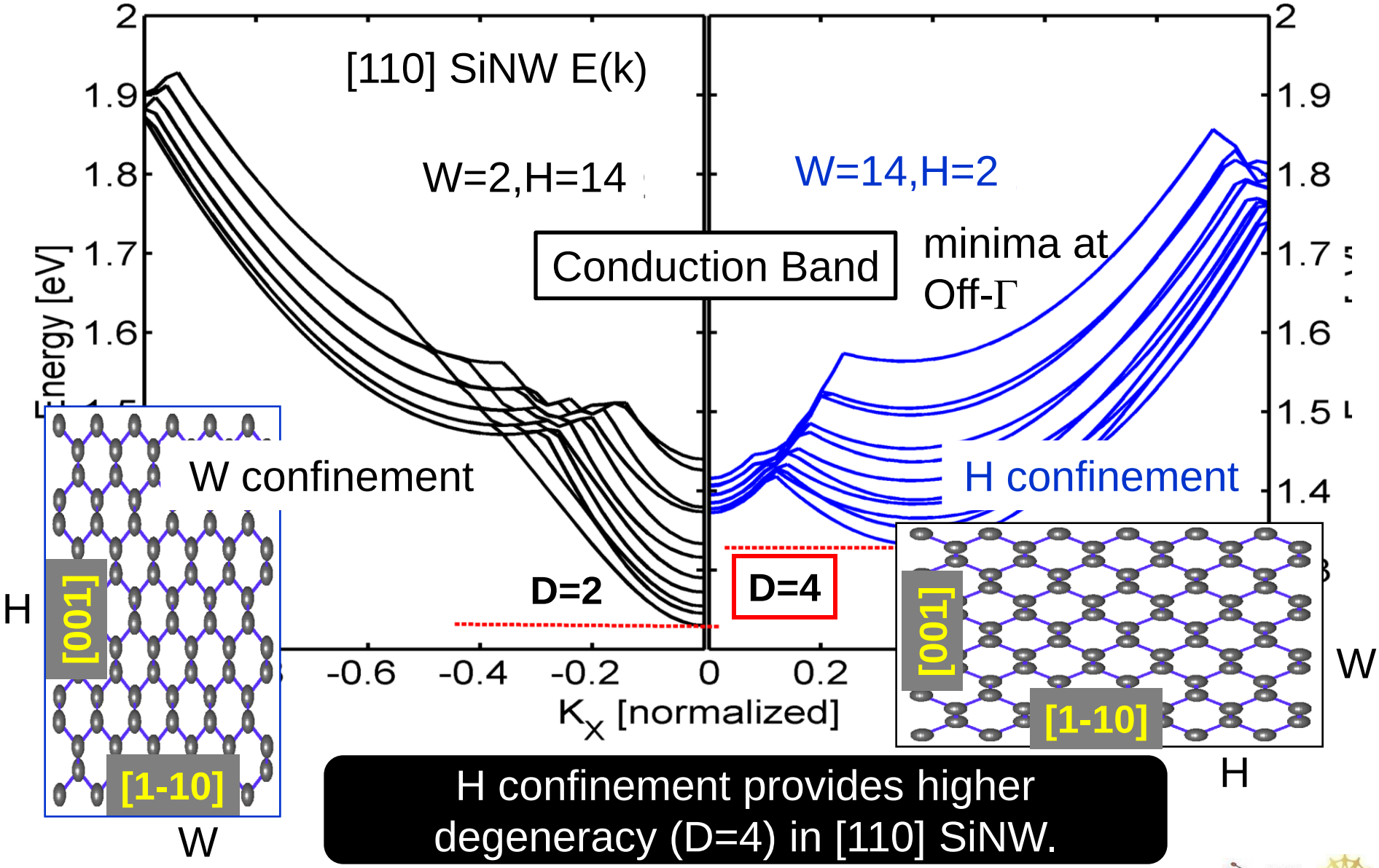
[1] Klimeck et. al CMES, 3, No. 5 (2002);

Effect of atomistic confinement on E(k): [100] SiNW



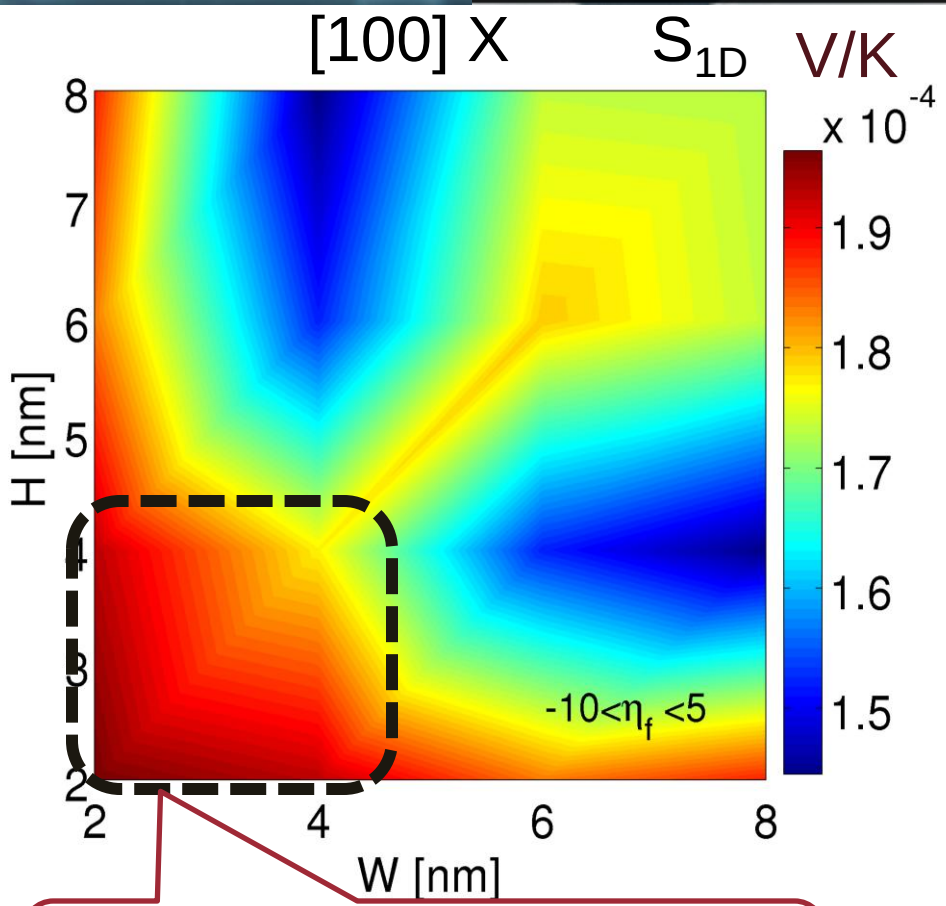
H and W confinement symmetric for [100] oriented wires

Effect of atomistic confinement on E(k): [110] SiNW

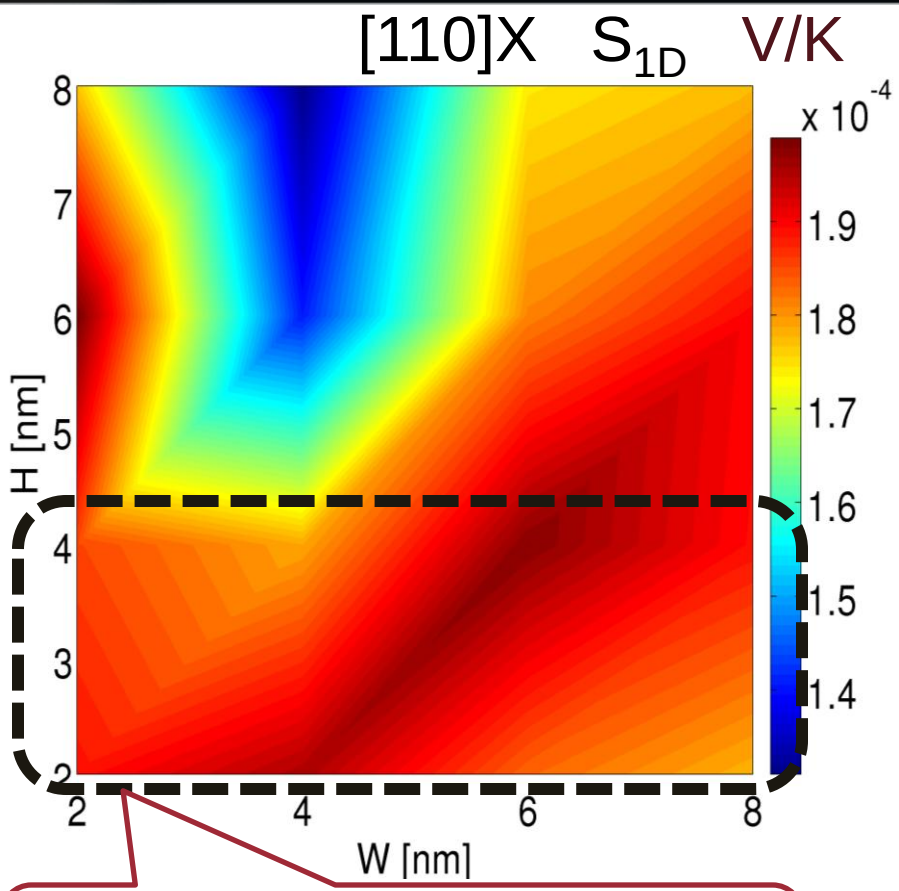


H confinement provides higher degeneracy (D=4) in [110] SiNW.

Tuning S by confinement



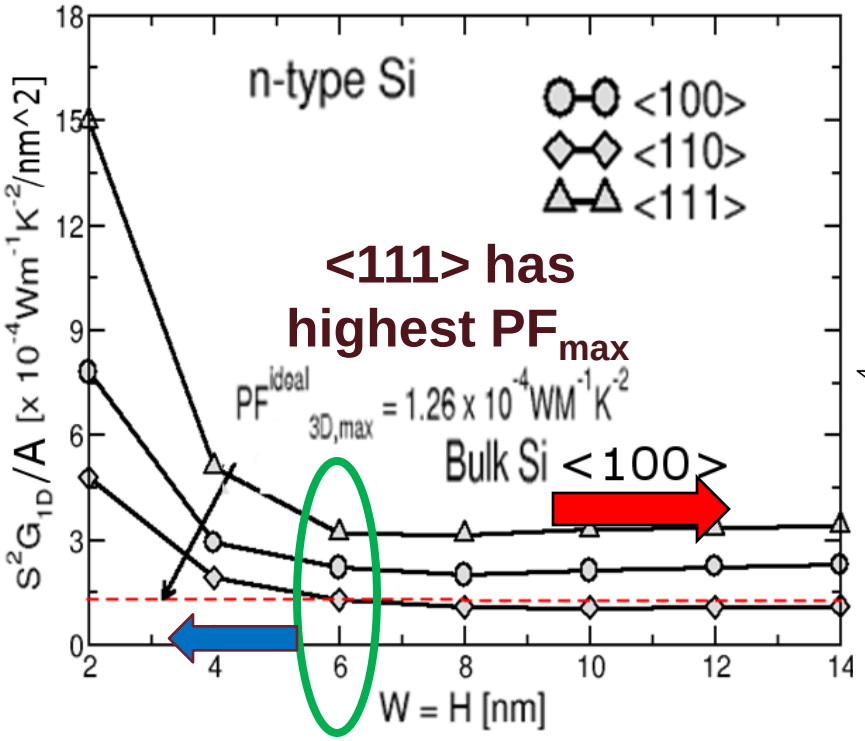
Both H and W confined for high S



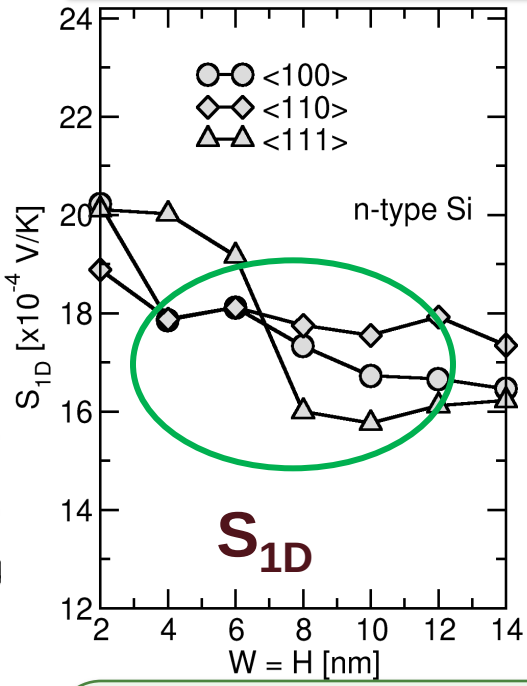
Only H confinement increases S

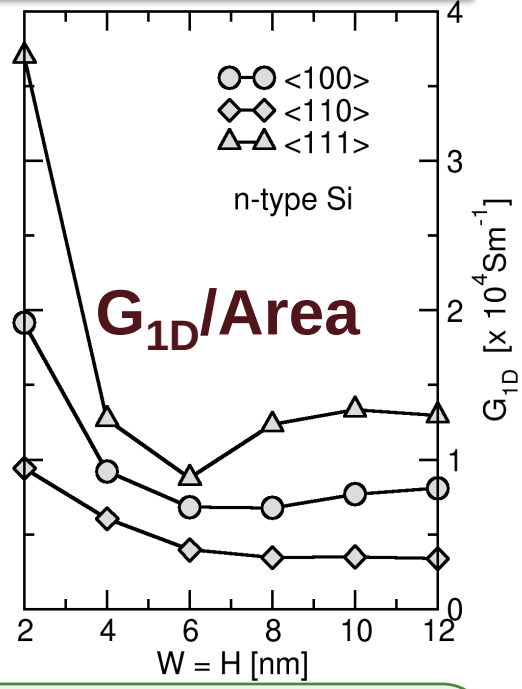
Geometrical confinement a nice way to tune 'S' in SiNWs.

Maximum Ballistic Power Factor (PF_{max})



Components of Power Factor



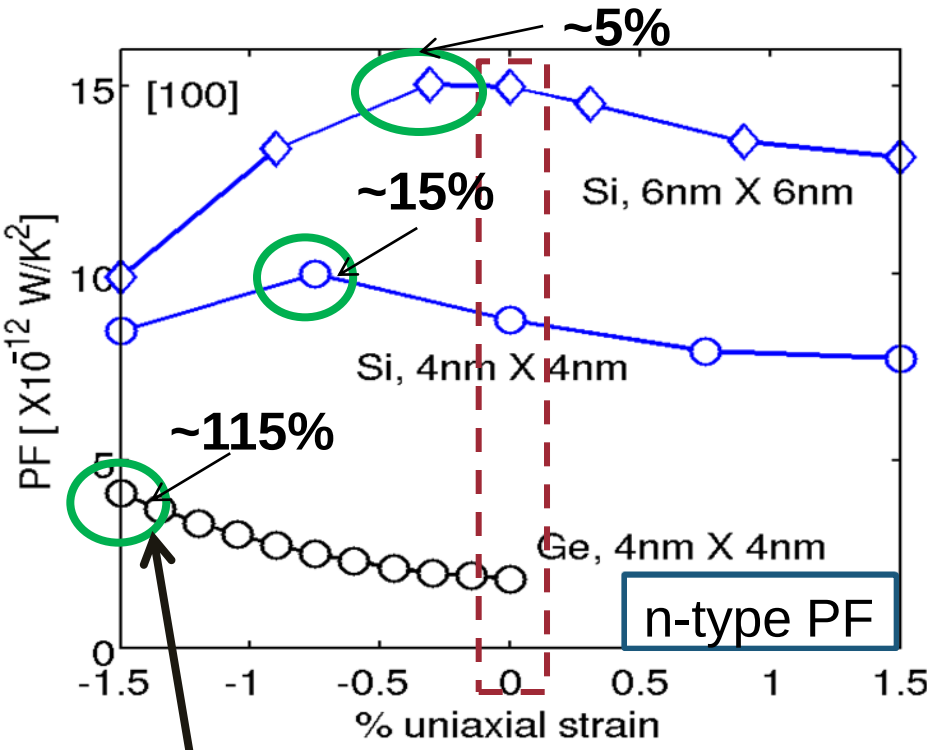


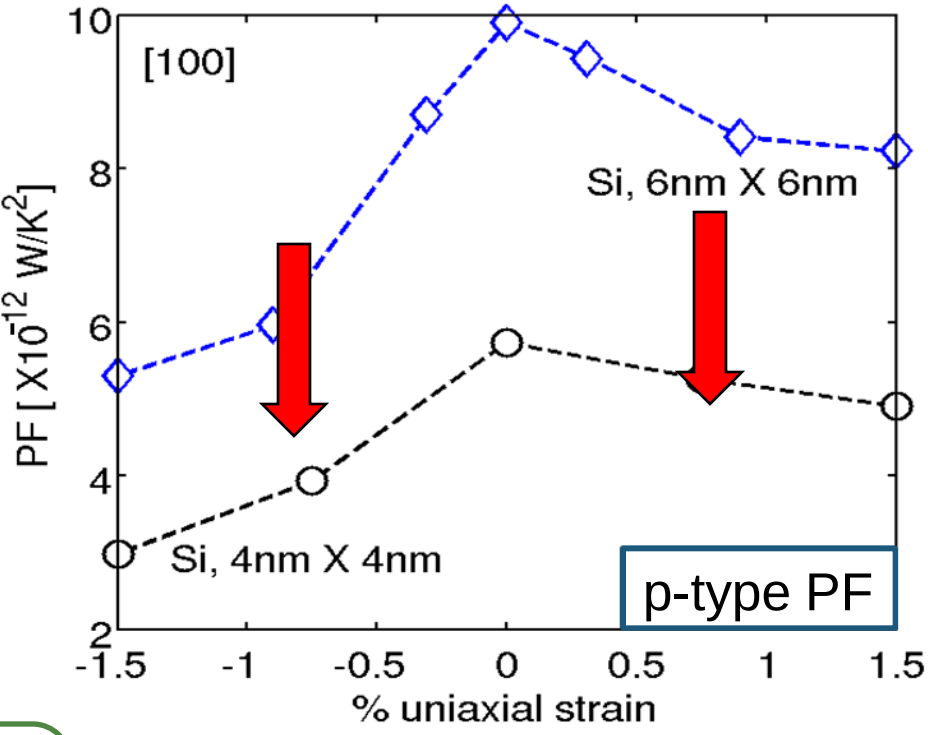
- PF/Area improved for SiNW with W/H < 6nm.
- PF_{max} saturates in larger SiNW.

- Seebeck Coefficient is almost constant at PF_{max}.
- G per area shows a saturation with <111> showing highest G/area value.

<111> shows maximum PF
W/H < 6nm improves PF

Improvement in PF: Role of uniaxial strain





GeNW better due higher DOS L-valley.

Compressive strain → inc. DOS near Fermi level → Improves PF.

Compressive/Tensile strain split VB→ dec. DOS near Fermi level → degrades PF.

Compressive uniaxial strain improves n-type ballistic PF.

New results from the work

- ✓ Atomistic approach shows:
  - ➢ Width and height confinement → not equivalent at atomic scale.
  - ➢ Crystal transport orientation crucial.
- ✓ Confinement direction important → design high S devices.
- ✓ SiNWs with W & H < 6nm → improvement in Ballistic PF.
- ✓ <111> orientated SiNW → best ballistic PF.
- ✓ Uniaxial Compressive strain → improves n-type PF.

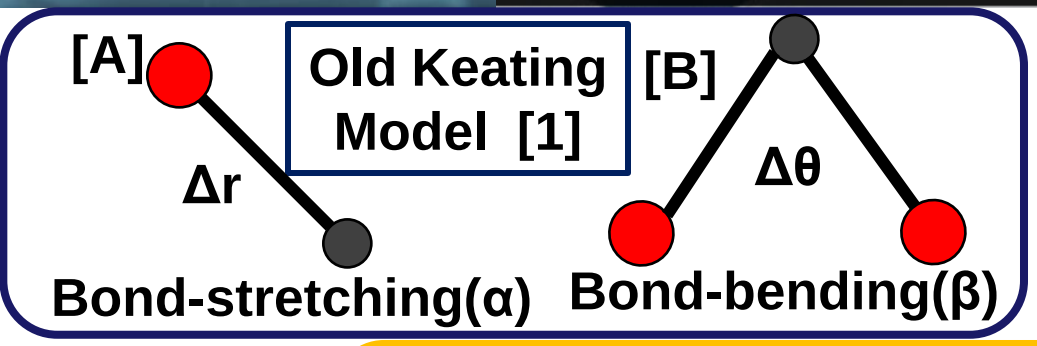
Role of phonon dispersion on Thermoelectric properties

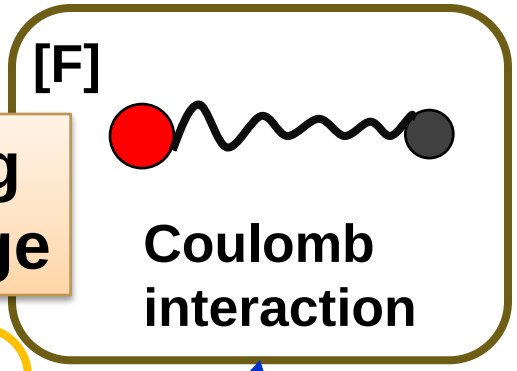
1. Phonon dispersion in bulk Si using Modified VFF.
2. Phonon dispersion in calculation in SiNWs.
3. Effect of phonon dispersion on SiNW lattice thermal properties.

SiNW DETAILS:

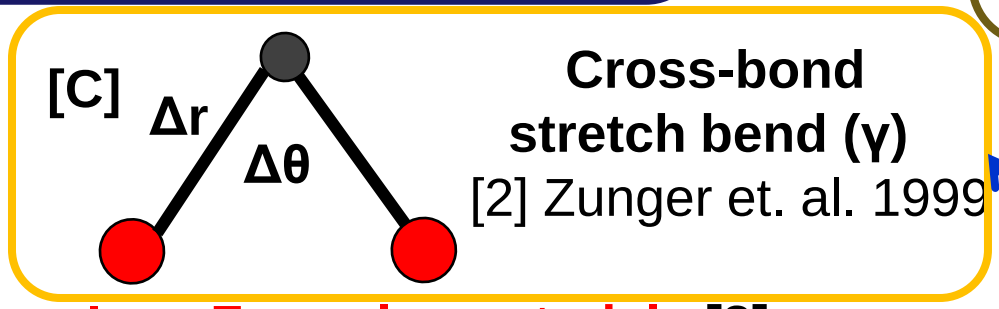
- Rectangular SiNW → [100] channels
- Width (W) and height (H) varied from 2 to 6nm.

Phonon dispersion calculation: Modified VFF (MVFF) model

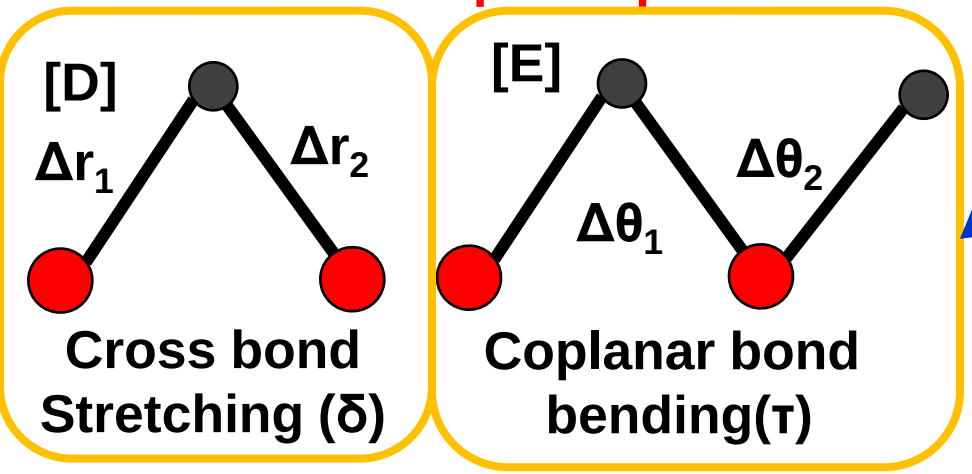




Imp. for polar materials [2]



Imp. For polar materials [2]



New combination of Interactions:
Modified Valence Force Field
Calculate phonons in zinc-blende materials.

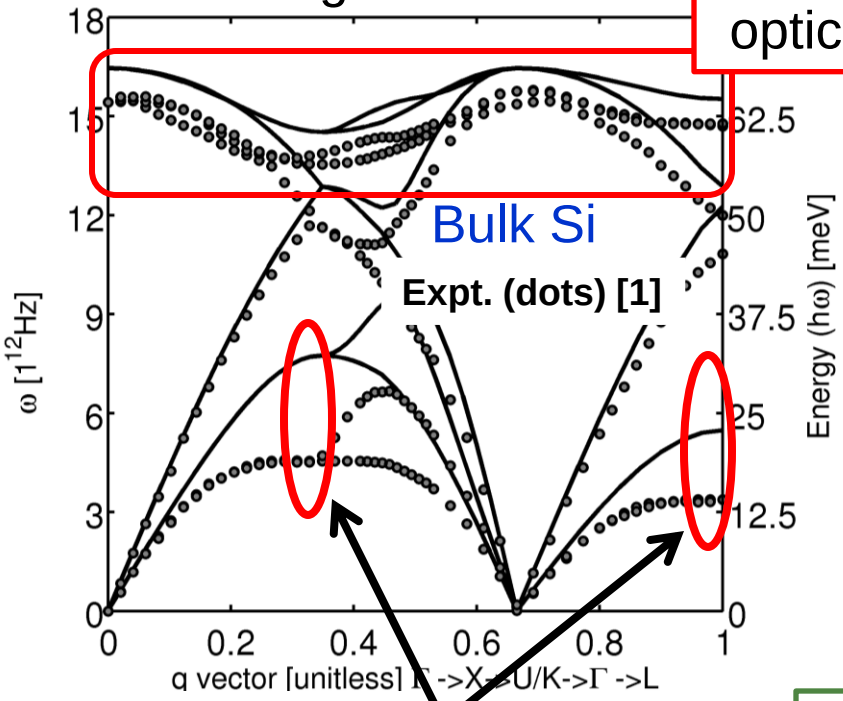
Imp. for non-polar materials

([3] Sui et. al, 1993)

[1] Keating. Phys. Rev. 145, 1966.
[2] PRB, 59,2881, 1999.
[3] PRB, 48, 17938,1993

What is the need for a new model??

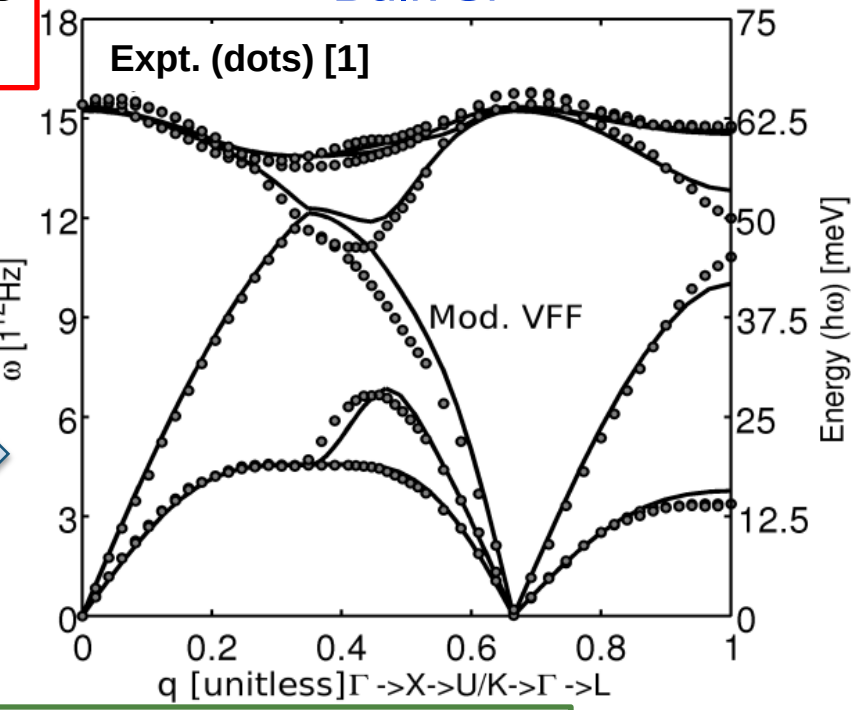
Keating VFF Model



Over estimates optical modes

Over estimates acoustic modes at zone edges.

Bulk Si



New MVFF model matchs the dispersion very well in the entire Brillouin zone !!!

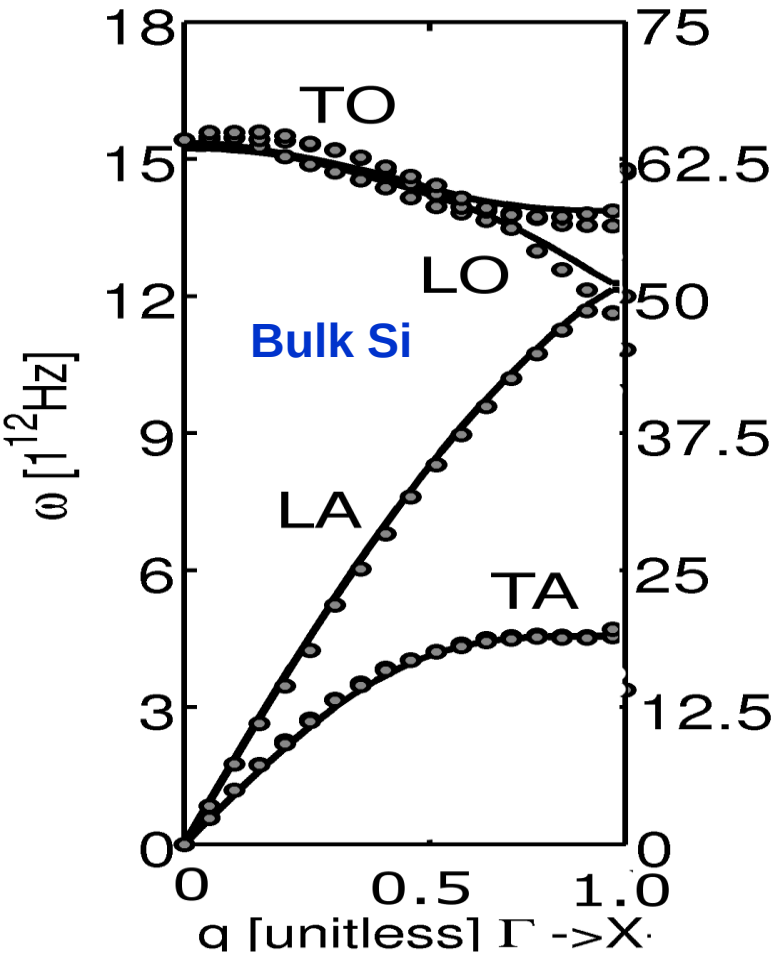
Expt. Data, inelastic neutron scattering (80K and 300K).

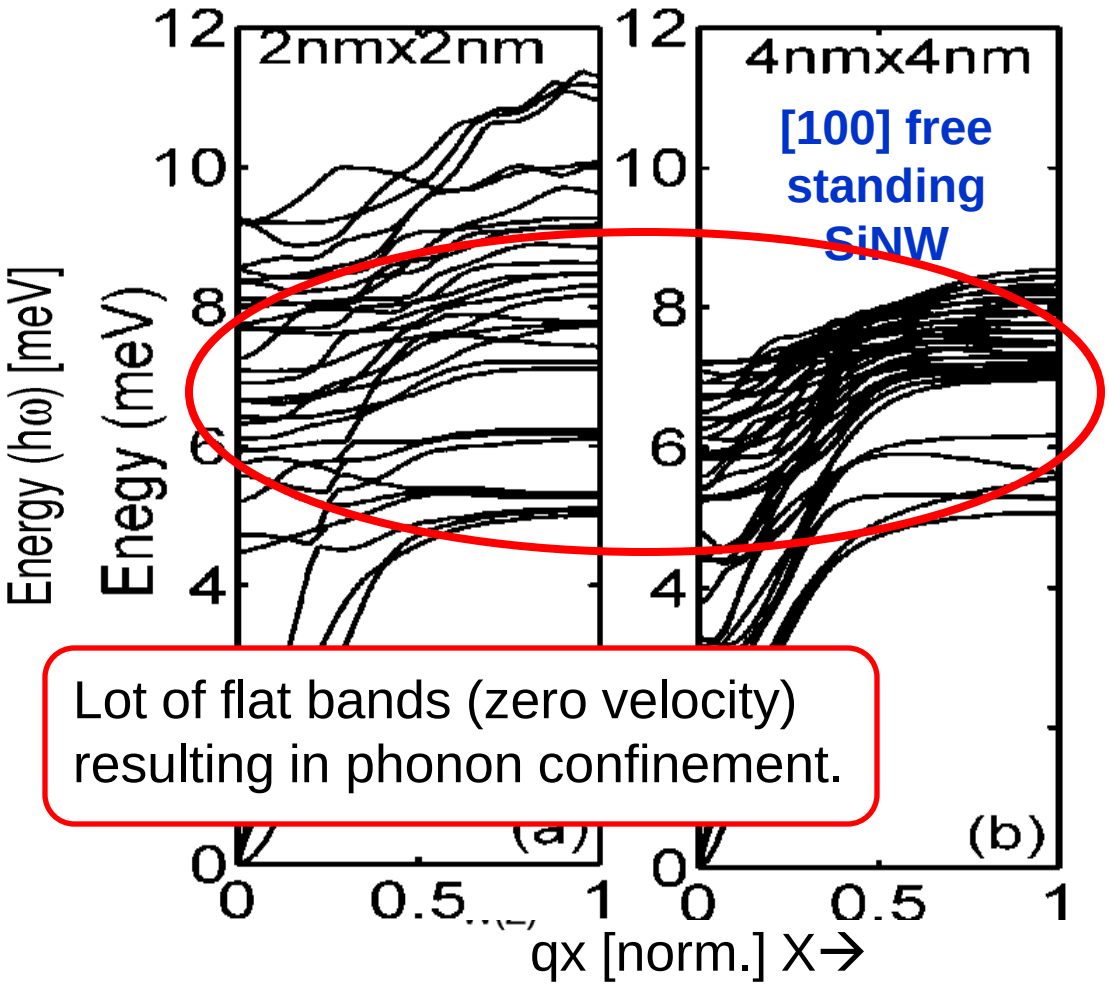
Accurate phonon model crucial for correct calculation of phonon dispersion in nanostructures.

PURDUE UNIVERSITY Abhijeet Paul

[1] Nelsin et. al, PRB, 6, 3777, 1972.

Phonon dispersion in free-standing nanowires

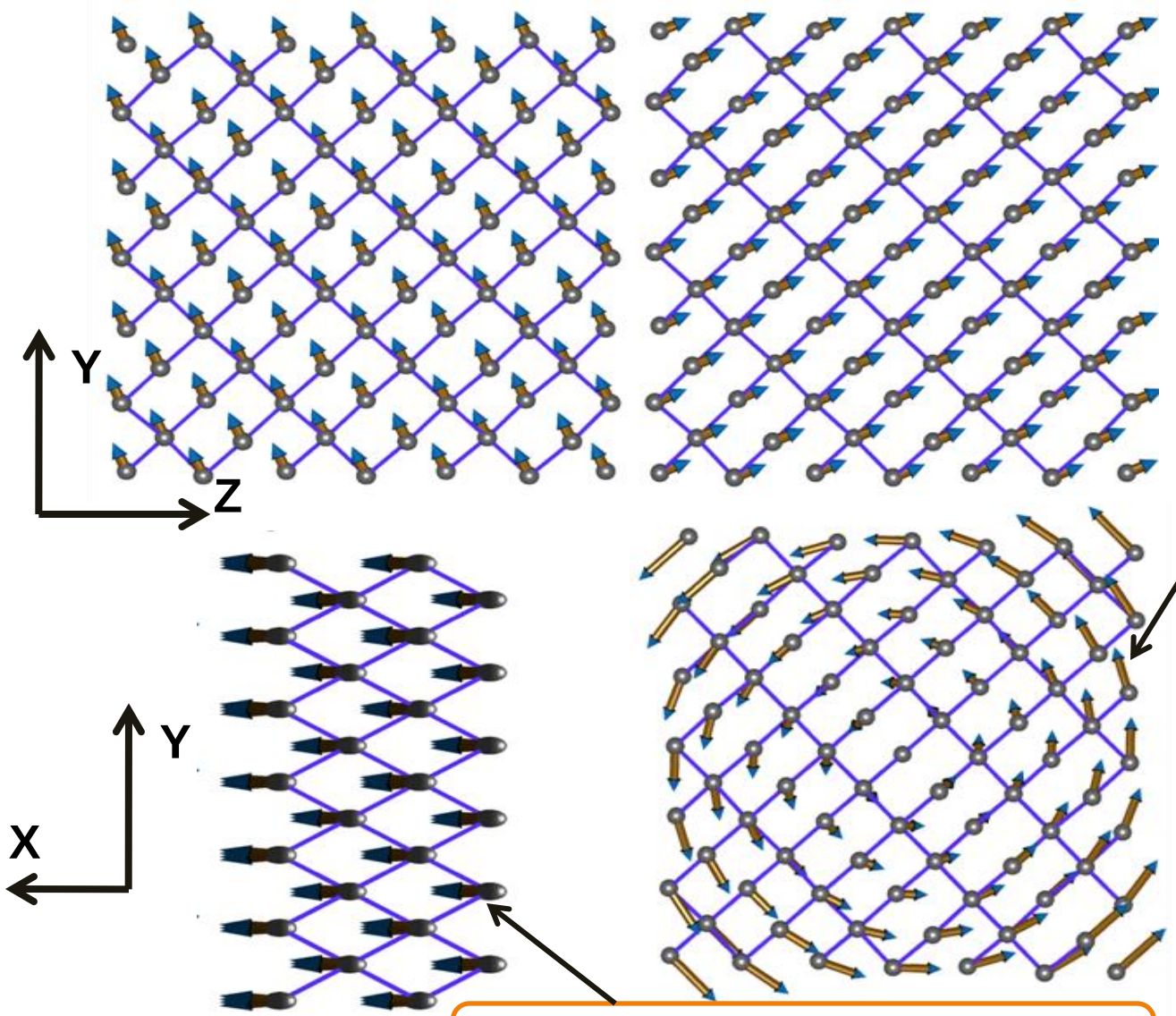




Lot of flat bands (zero velocity) resulting in phonon confinement.

Strong phonon confinement responsible for different lattice properties in SiNWs compared to bulk.

Vibrational modes of free-standing [100] SiNWs



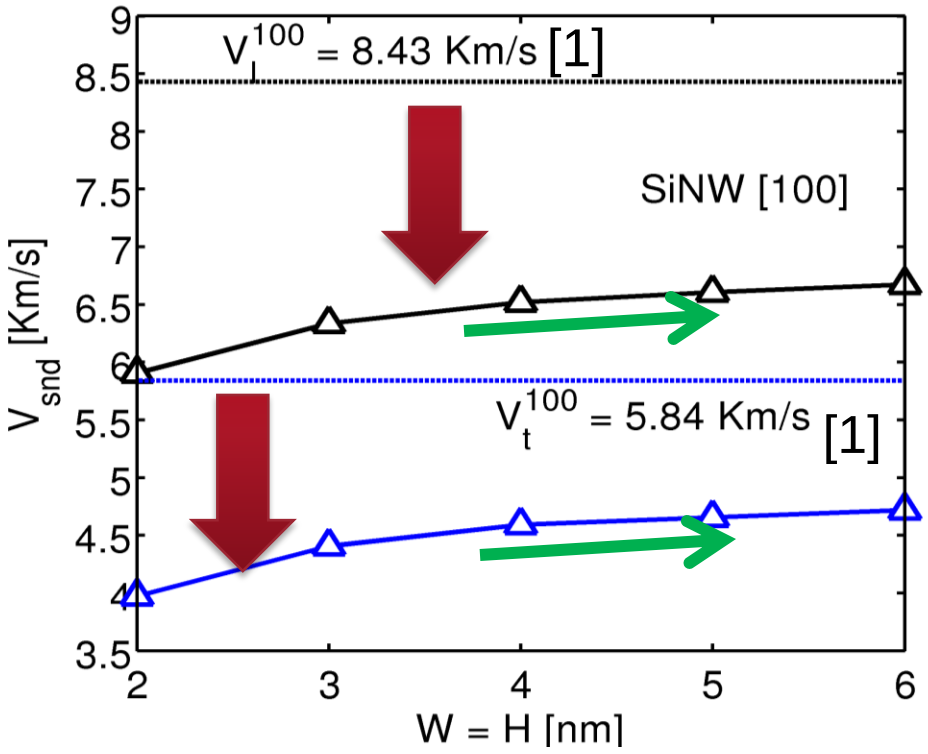
Flexural modes (1,2)
Bends the wire along the axis.

Torsional modes (4)
Rotates the wire along the axis.

New vibrational modes appear in free-standing nanowires.

Longitudinal modes (3)

Sound velocity in [100] free standing SiNWs



$$V_{snd} = V_{grp} = \left.\frac{\partial \omega}{\partial q}\right|_{q \to 0}$$

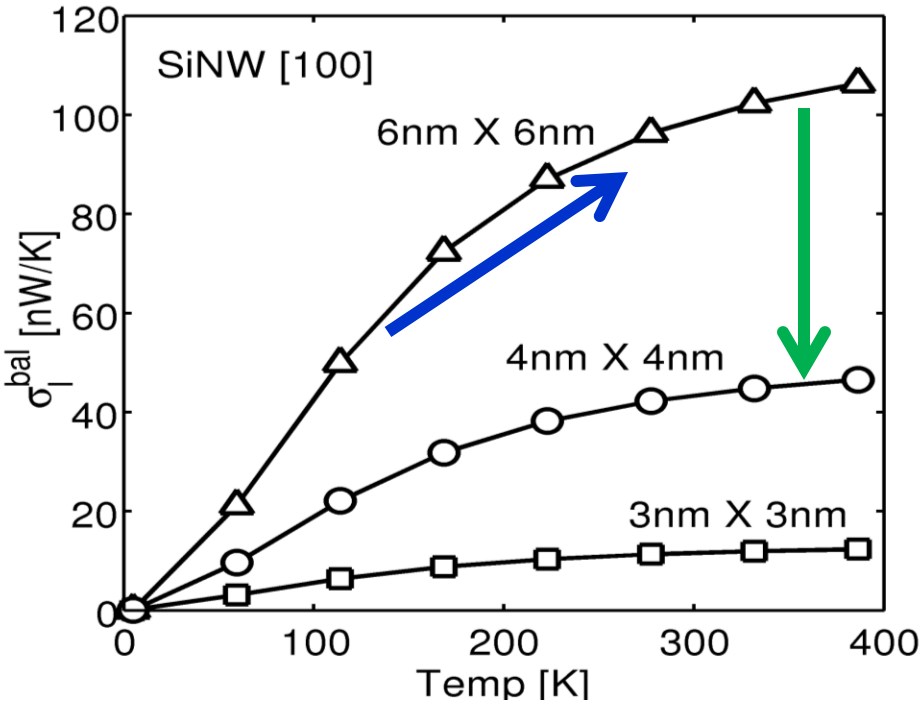
- Both longitudinal and transverse sound velocity is less in SiNW.
- Phonon confinement results in flatter dispersions and hence smaller sound velocity.
- With increasing W/H Vsnd move towards bulk values.

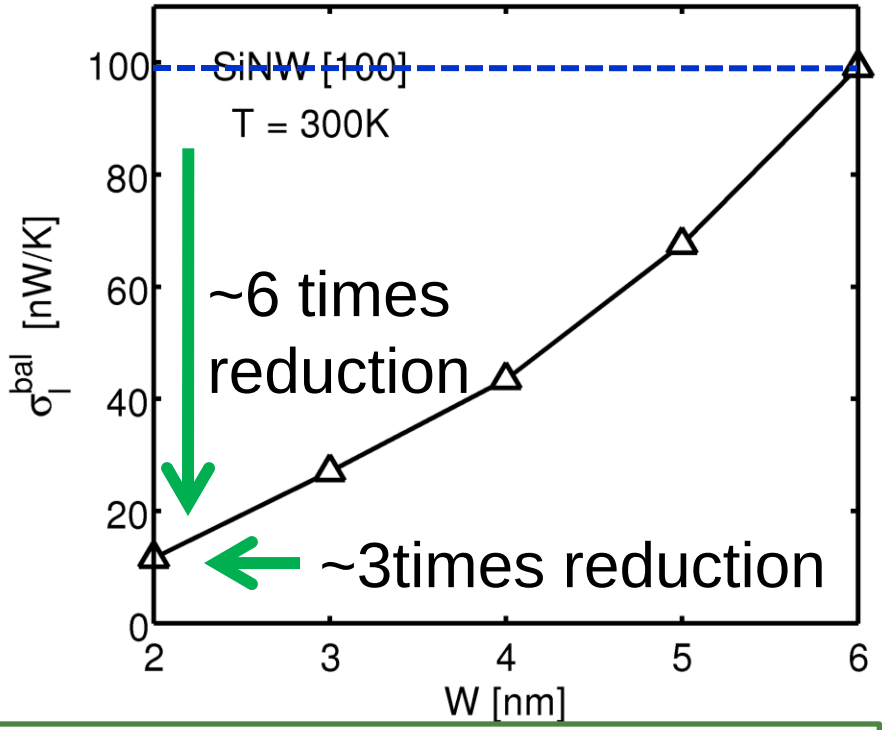
Reduced sound velocity results in lesser dissipation of heat.

A result of phonon confinement.

[1] www.ioffe.ru/SVA/NSM/Semicond/Si/mechanic.html#Acoustic

Ballistic lattice thermal conductance(σ^{bal}_{l}) in [100] SiNW





- Higher temperature → more phonon population → inc. in thermal conductance.
- Thermal conductance drops with decreasing cross-section size.
- ~6 fold reduction in thermal conductance for ~3fold increase in width (from 6nm to 2nm).

Reduction in ballistic σ_l due to decreasing modes with cross-section size reduction.

New things learnt from the work

- ✓ A new generalized model for phonon dispersion in zinc-blende semiconductors.
- ✓ Model benchmarked with expt. data.
- ✓ Free standing SiNW show:
  - ➢ Very different phonon dispersion compared to bulk Si.
  - ➢ New flexural and torsional modes
  - ➢ Strong phonon confinement.
- ✓ Phonon confinement results in:
  - ➢ Reduction of both longitudinal and transverse sound velocity.
  - ➢ Reduction of thermal conductance in small SiNWs.

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  - Basics
  - Material Development
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- Future Proposal
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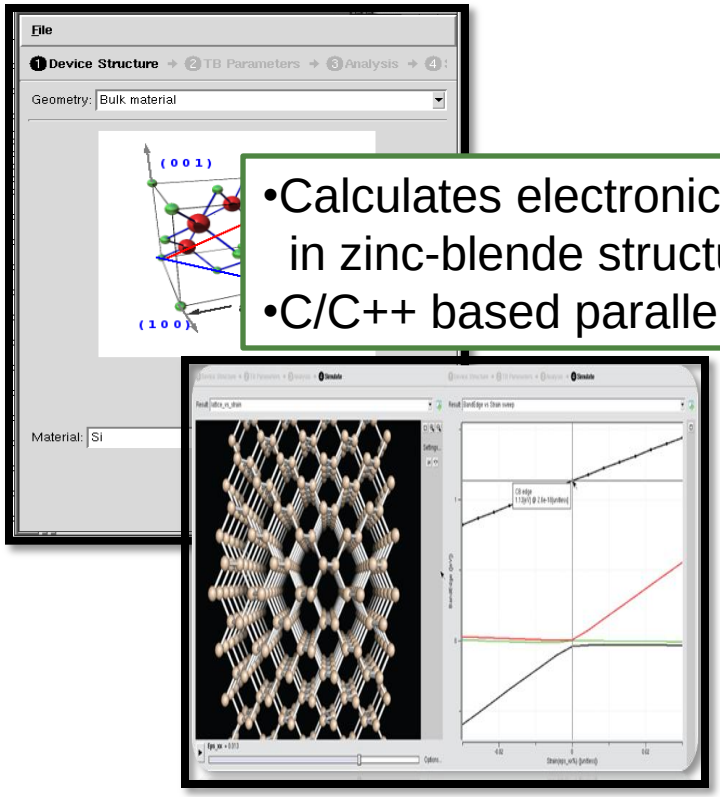
Global scientific outreach using nanoHUB.org

BandStructure Lab (Research Tool)

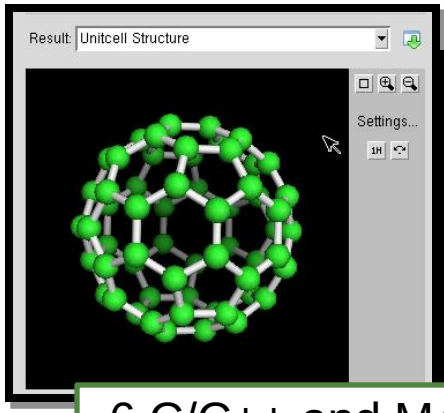


- Calculates electronic bands in zinc-blende structures.
- C/C++ based parallel code.

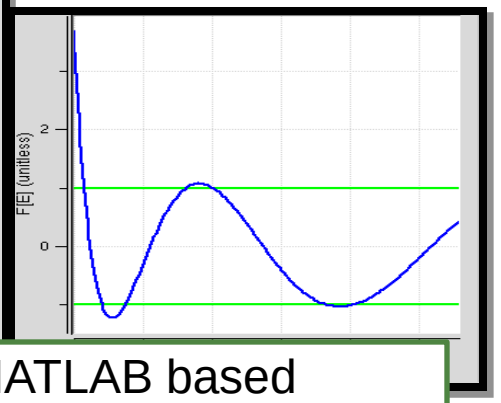
- Most popular tool on nanoHUB.
- Over 3K users.
- Till now ran 34503 simulations.
- Has been cited 28 times in research.

Semiconductor Educational Tools

Crystal Viewer Tool



Periodic Potential lab



6 C/C++ and MATLAB based semiconductor physics tools developed.

- Used in EE305 (Semicond. Introduction) at Purdue University

- Users (last 12 months) = 887
- Simulations (last 12 months) ~3K

Enabled dissemination of device physics knowledge globally.

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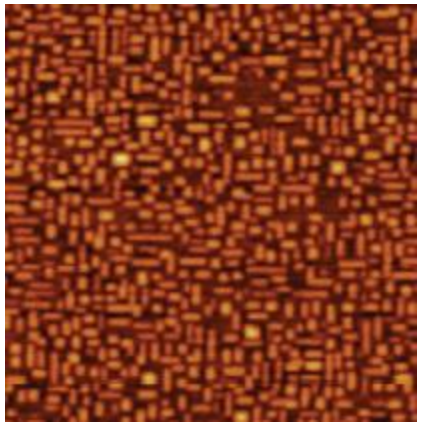
Why to study Si-Ge superlattices ??

Ge/Si(001) nanodots

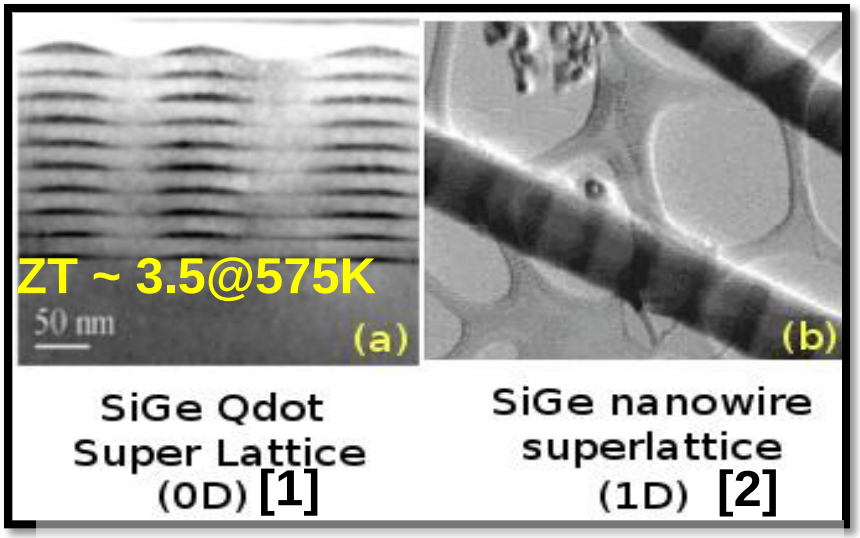


Allows precise thermal conductivity (κ) control.

κ→0.9W/m-K

(>100 fold reduction!!!)

Nature mat.,2010, doi:10.1038/NMAT2752



SiGe structures provide high ZT.

Advantages of using SiGe:

- ✓Advanced CMOS fabrication → high quality SiGe structure.
- ✓Easy integration with Si → better heat recovery at chip level.
- ✓ Monolithic growth on Si → higher energy conversion by thermal resistance reduction.
- ✓In/cross plane tailoring → optimize TE properties.

Nanoscale SiGe structures will need atomic level understanding!!!

[1] Harman et. al, Science, 80, 2002
[2]Wu et. al, Nano. Lett.,2, 2002.

First steps towards future work…

TE and thermal analysis SiGe nano-structures

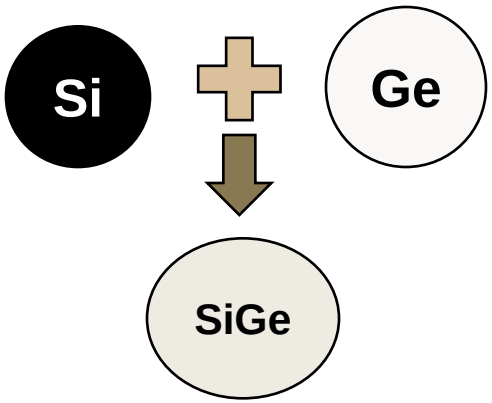
2011

- Calculation of E(k) in SiGe alloys.
- Transmission calculation in SiGe nanowires.
- Lattice property calculations in Si-Ge structures.
- Thermal transport in SiGe superlattices (1D).

Sept 2010

Some initial results are presented for the future directions

Bandstructure Calculation in SiGe alloys: Virtual Crystal Approximation in TB



"Virtual Atom"

[1] Bond-length modification.

$$a_{SiGe} = x a_{Si} + (1-x) a_{Ge}$$

[2] On-site TB parameter modification.

$$E_{A,B}^{strain} = x(E_A + \Delta_A) + (1-x)(E_B + \Delta_B)$$

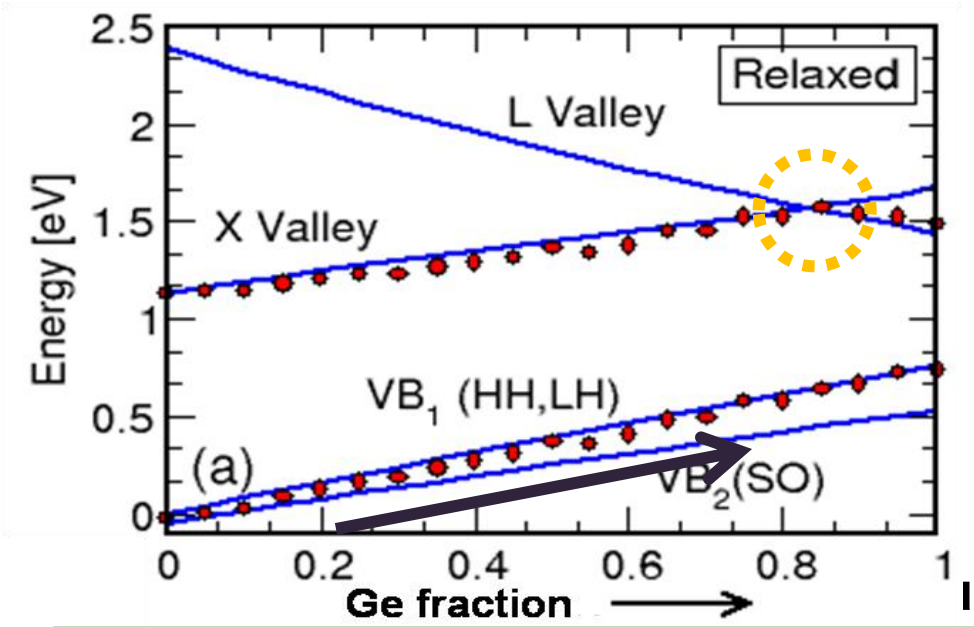
[3] Modification of coupling parameters

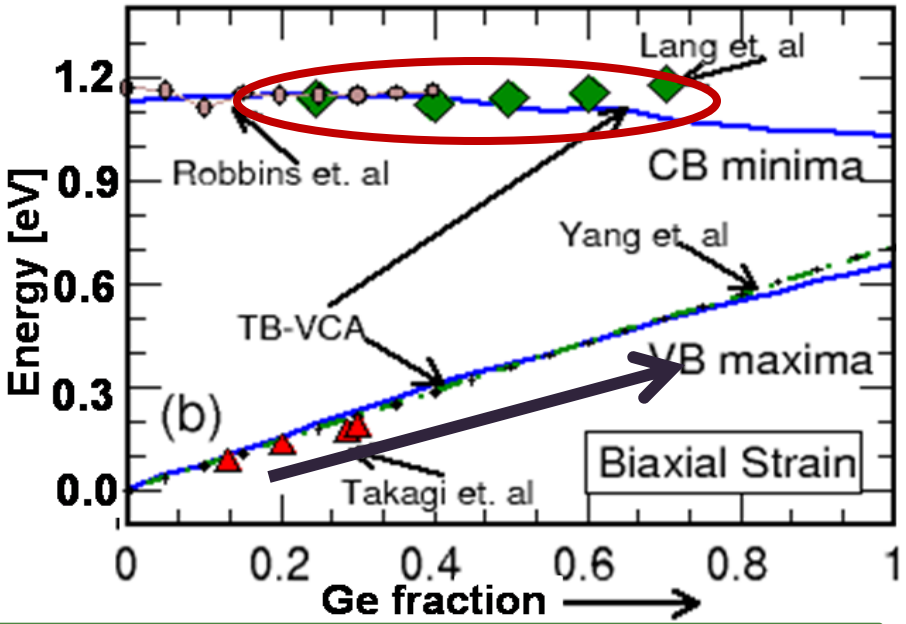
$$V_{\sigma_1\sigma_2}^{SiGe,strain} = x(V^{Si}{}_{\sigma_1\sigma_2}\left[\frac{a_{Si}}{a_{SiGe}}\right]^{\eta_{Si}}) + (1-x)(V^{Ge}{}_{\sigma_1\sigma_2}\left[\frac{a_{Ge}}{a_{SiGe}}\right]^{\eta_{Ge}})$$

Tight-Binding based Virtual Crystal Approximation ➡ **TB-VCA**

PURDUE UNIVERSITY Abhijeet Paul

Benchmarking Bulk Band-structure

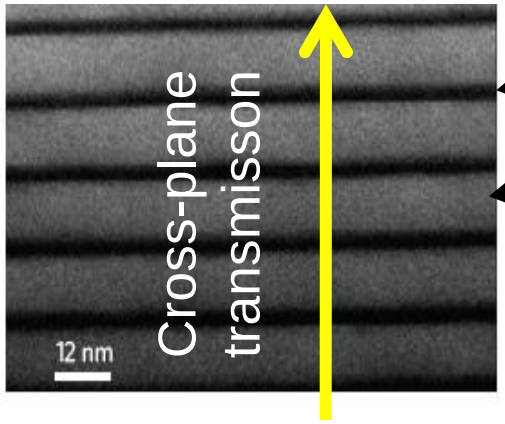


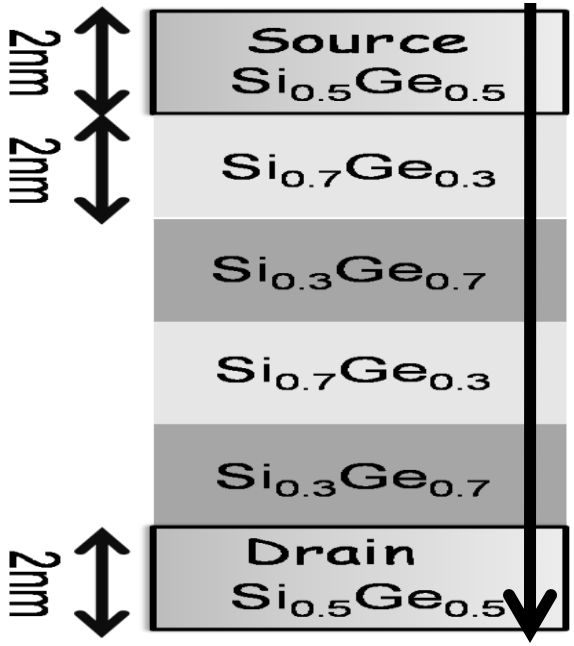


- Cross-over at 85% Ge for relaxed SiGe Conduction band (CB) captured.
- Valance Band Edge → equal amount of change in relaxed and strained SiGe.
- CB edge is almost constant for all Ge% for strained SiGe Bulk.

First benchmark of experimental SiGe bandedges using TB-VCA.
Work Published in IEEE EDL , 31, 2010. doi: 10.1109/LED.2010.2040577

Transport in SiGe superlattice: Transmission results*

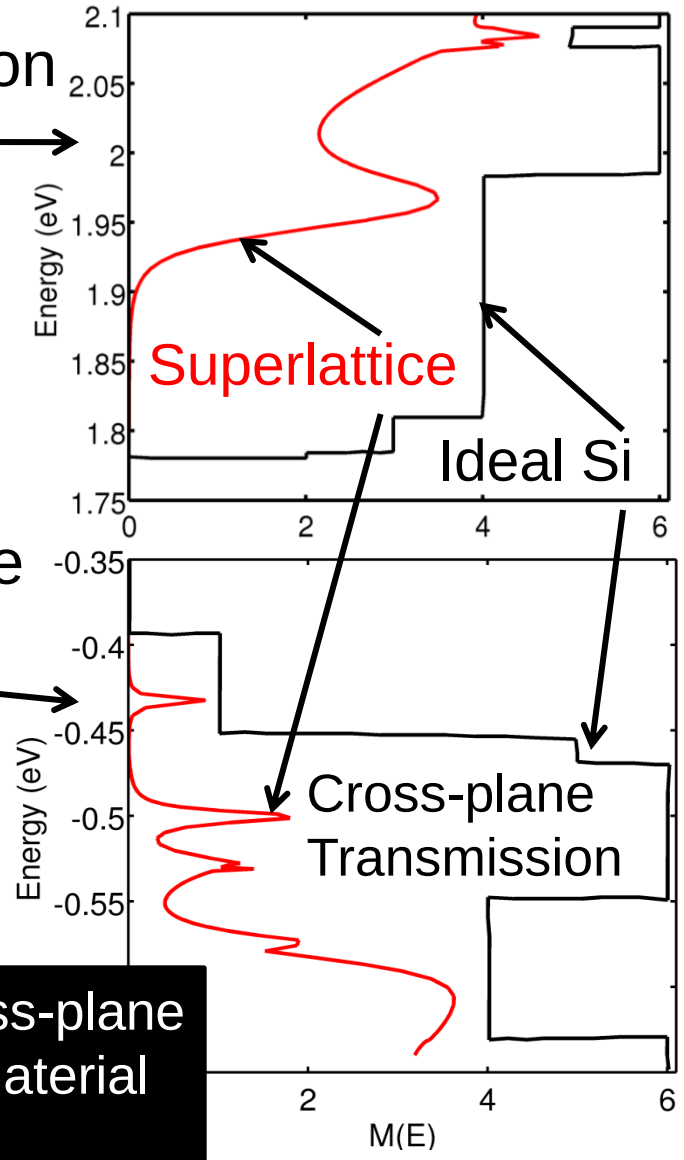




Simulated SiGe Nanowire Superlattice
Radius = 3nm

Conduction Band →

Valence Band →



Strong reduction in cross-plane transmission due to material mismatch.

*This work in progress with Lang Zheng

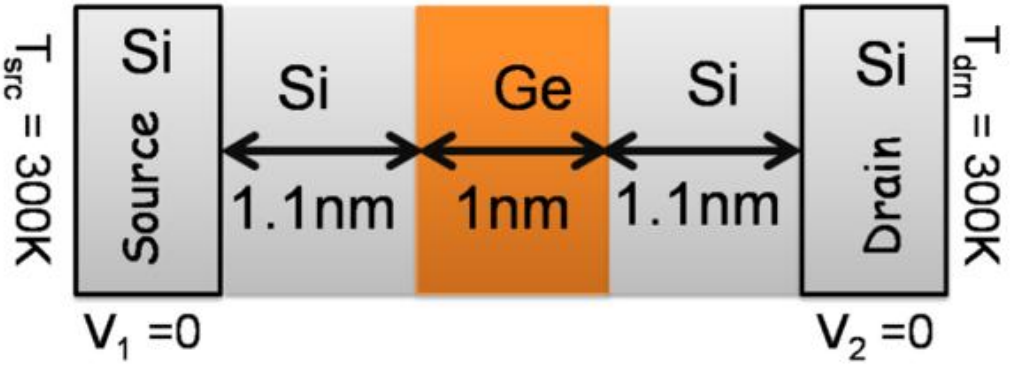
Thermal transport in SiGe superlattices: Phonon NEGF*

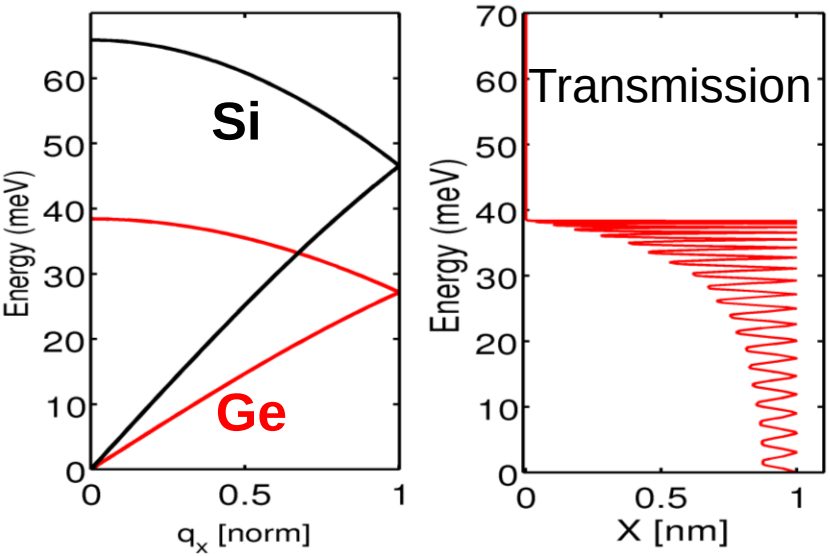
How does heat flow in nano-structures ?

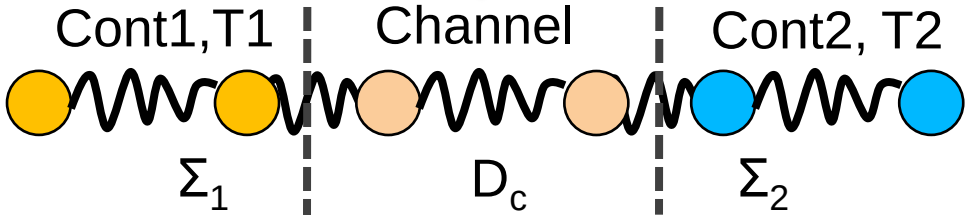
APPROACH
Coherent phonon picture within NEGF* approach.

Simulated Nano-scale Si-Ge-Si device

$\lambda_{ph} = 2-3\text{nm}$







1D Spring Model representation of the device

D_c = channel dynamical matrix

- Ge blocks the phonons.
- Resonant states appear.

Work in progress for calculating energy density, phonon local temperature, etc.

Some open questions and probable solutions

- **How to handle alloy scattering in VCA for nanostructures?**
  - Use of bulk scattering potential not adequate in nanostructures.
  - Use of random alloy method can provide solution.
  - Work going on in this direction with Saumitra Mehrotra.
- **Transmisison in SiGe super lattices:**
  - What happens to inplane transmission?
  - What happens at other composition and widths ?
  - Work in progress with Lang Zeng.
- **Nanoscale thermal transport:**
  - Is boundary condition (BC) with temperatures correct?
  - What is **'temperature'** in non eqb. nanoscale systems?
  - Need BCs in terms of energy fluxes.
  - Work in progress with Dr. Tillmann Kubis and Dr. Mathieu Luisier.

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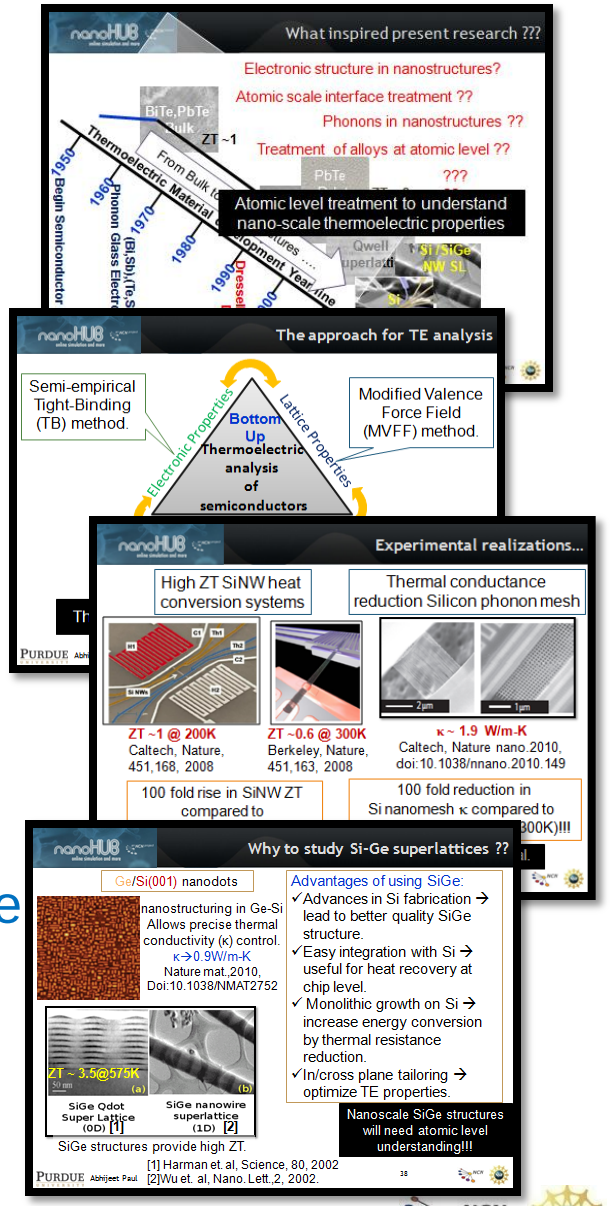
Summary

- The current developments, challenges and opportunities in thermoelectricity introduced.
- Thermoelectric analysis in semiconductor nanostructures:
  - Electronic structure and **new** lattice dynamics model with transport.
- Electronic and lattice effects on SiNWs TE properties:
  - Tuning Seebeck coefficient by geometry confinement.
  - Uniaxial strain improves n-type ballistic PF.
  - Reduction in ballistic thermal conductance due to phonon confinement.
- Future research direction:
  - Analysis of thermoelectric and thermal effects in SiGe nanowire superlattices.



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- **Overall guidance and direction**
  - Prof. Gerhard Klimeck and Prof. Mark Lundstrom, Purdue University, USA.
  - Prof. Leonid Rokhinson, Purdue University, USA (PhD committee member).
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  - Dr. Mathieu Luisier, Purdue University, USA (OMEN/OMEN-BSLAB development).
  - Prof. Timothy Boykin, University of Alabama Huntsville, USA (PhD committee member, TB and solid state phys. theory)
  - Dr. Neophytos Neophytou, TU Wien, Austria (Initial MATLAB codes)
- **Discussions and work**
  - Saumitra Mehrotra, Parijat Sengupta, Sunhee Lee, Lang Zeng, Dr. Tillmann Kubis, Raseong Kim and Changwook Jeong, Purdue University, USA
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  - Junzhe Geng, Victoria Savikhin and Mohammad Zulkifli, Purdue University, USA
- **Funding and Computational Resources**
  - MSD-FCRP, SRC, NSF and MIND for funding.
  - NCN and nanoHUB.org for computational resources.

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