Progress from DOE EFRC: Solid-State Solar-Thermal Energy Conversion Center (S^{3}TEC Center)

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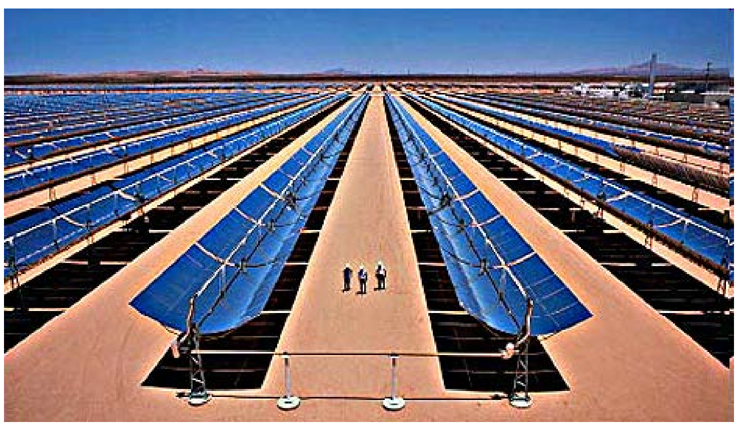
Seeds: D. Broido (BC), P. Jarillo-Herrera (MIT)

Electricity from Sunlight

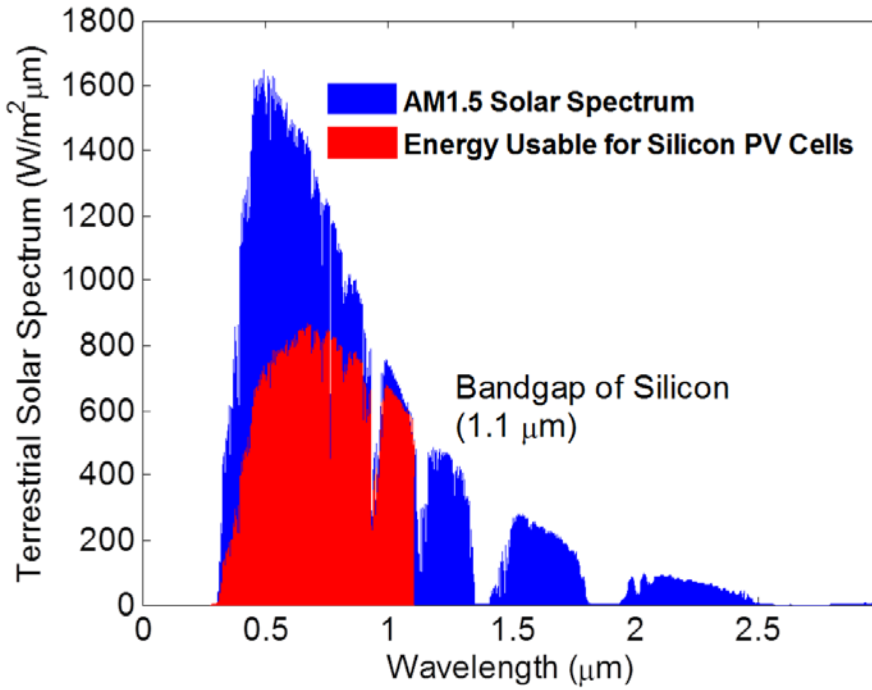
Photovoltaic

homesolarpvpanels.com

Thermal-Mechanical

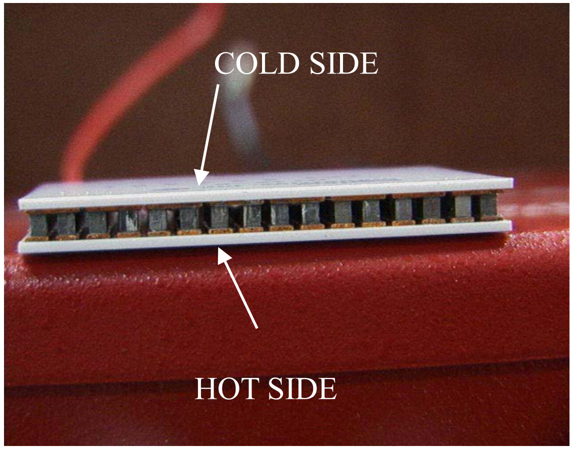


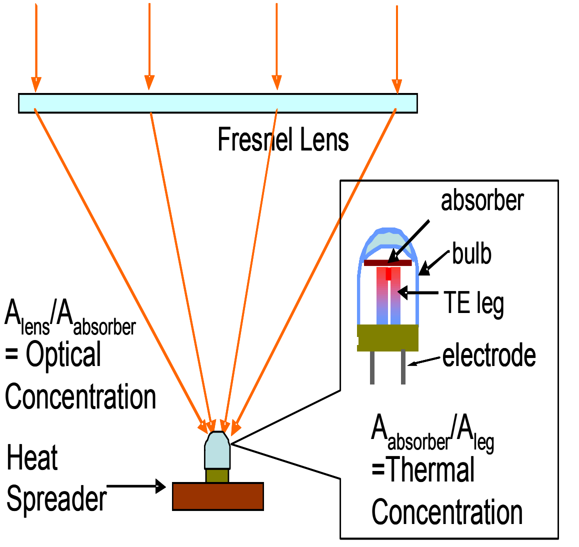
http://www.treehugger.com/Solar-Thermal-Plant-photo.jpg



Our Goal:
Full-Spectral
Solar Thermal and
Yet Solid-State!

Solar Thermoelectric Devices





Solar Thermoelectrics

Nondimensional Figure of Merit

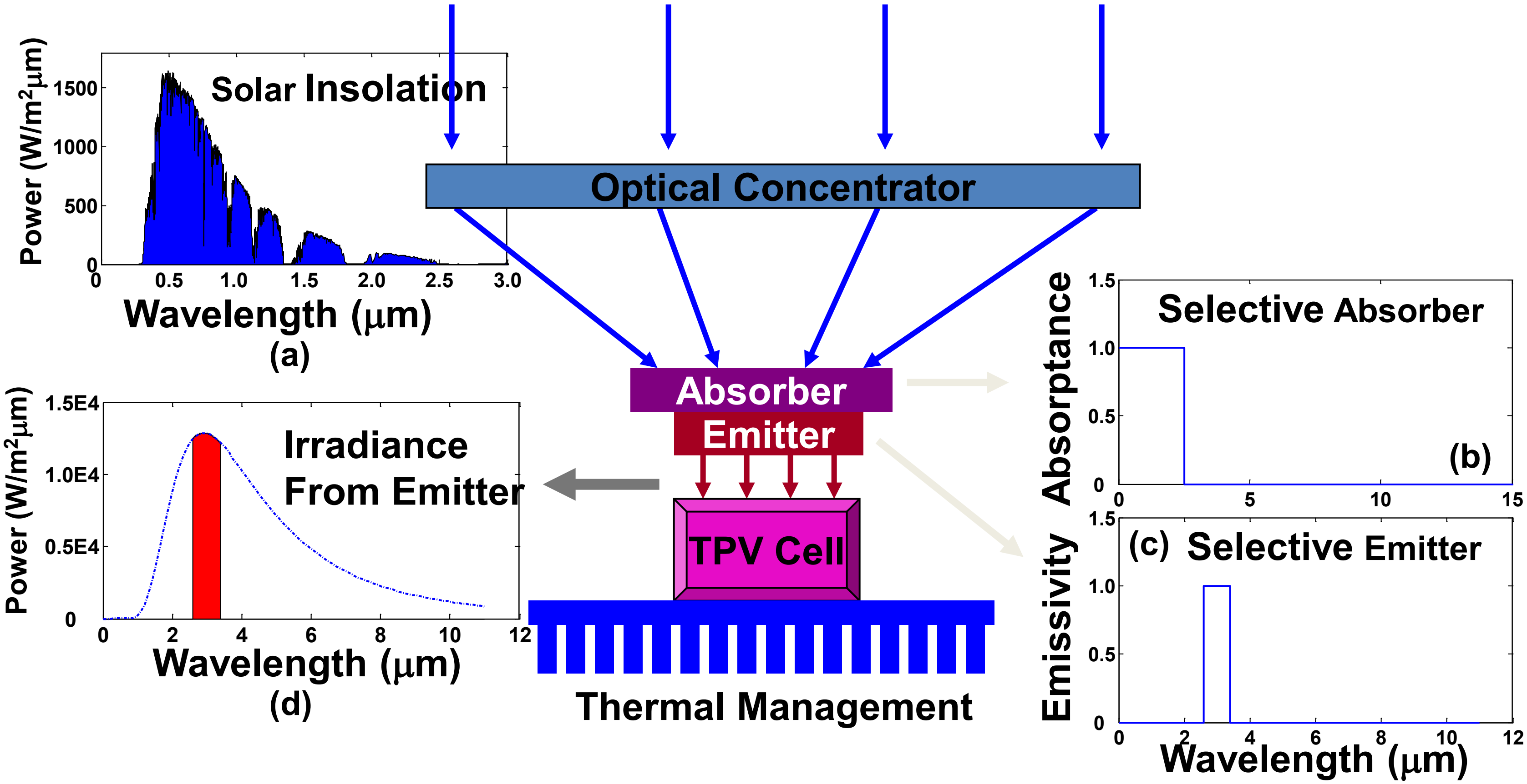
Joule Heating

Seebeck Coeff. Electron Cooling

$$ZT = \frac{\sigma S^2 T}{k}$$

Reverse Heat Leakage Through Heat Conduction

Solar Thermophotovoltaics

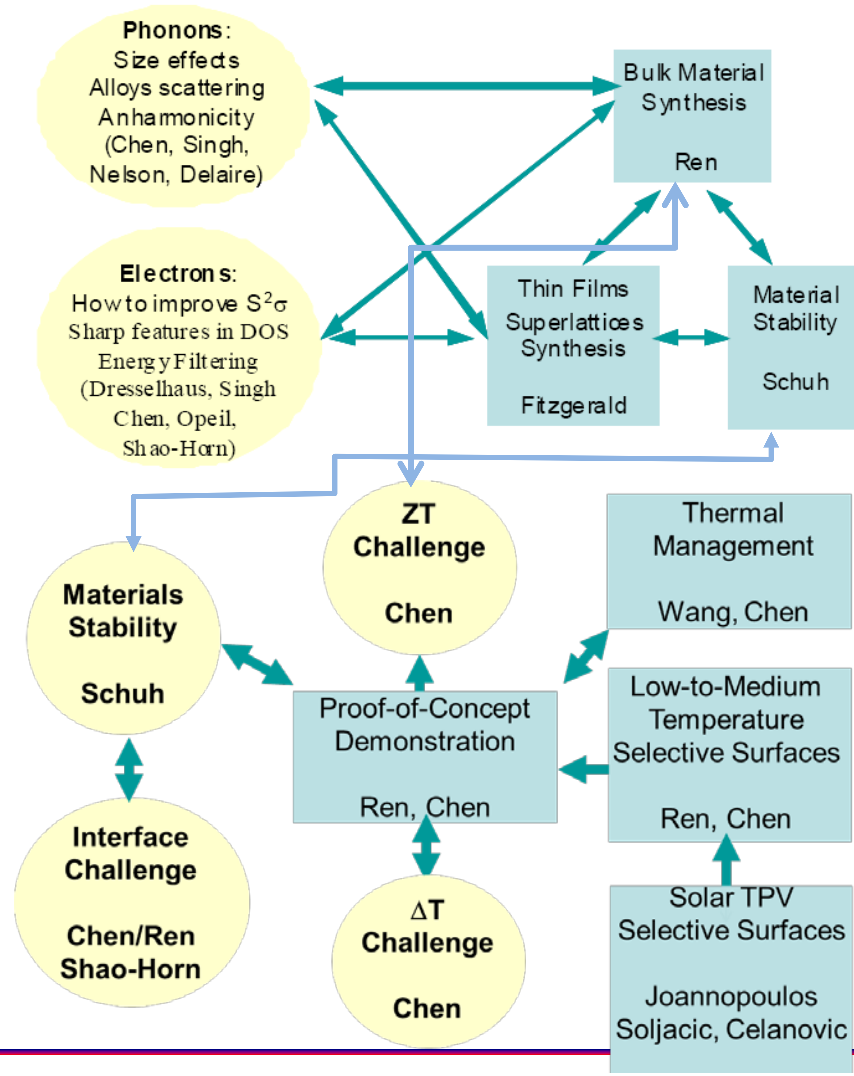


- **Theoretical maximum efficiency: 85.4%; comparable to that of infinite number of multi-junction cells, but with only a single junction PV cell.**
- **Key Challenges: Selective surfaces absorbing solar radiation but re-emitting only in a narrow spectrum near the bandgap of photovoltaic cells, working at high temperatures.**

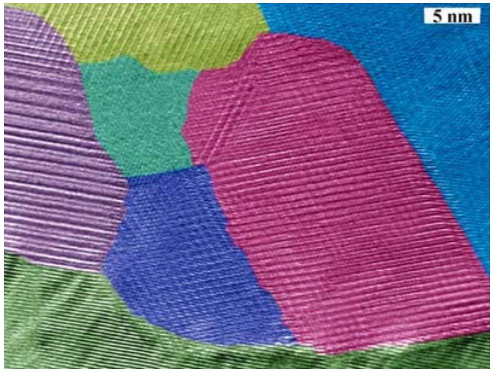
Solar Thermoelectrics: Approach

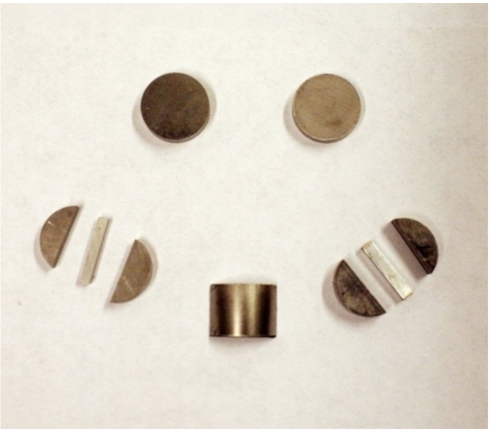
Fundamental Science:

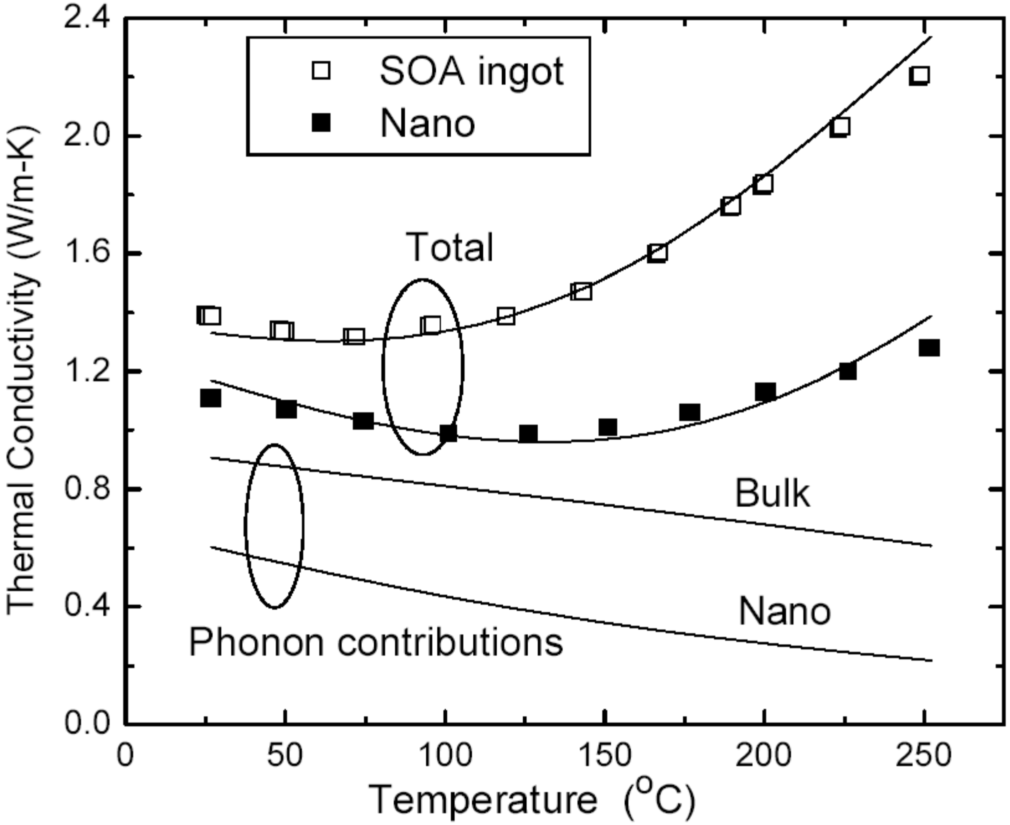
- Fundamental understanding of electron and phonon transport in thin films and bulk nanostructures.
- Engineering electron transport.
- Engineering phonon transport.
- Thin film fabrication.
- Bulk nanostructure synthesis.
- Nanostructure stability.
- Proof-of-principle demonstration.
    - ZT challenge
    - Interface challenge
    - DT challenge



Nanostructured Thermoelectric Materials

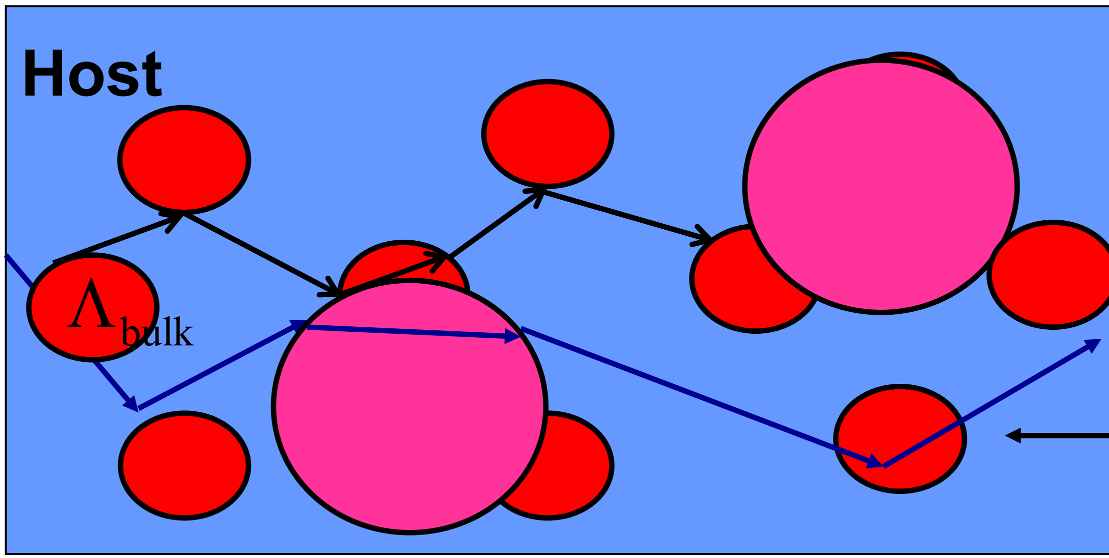






Poudel et al. Science, v. 320, p. 634, 2008

Importance of Understanding Phonon Mean Free Path



$$\Lambda_{nano} < \Lambda_{bulk}$$

Nanoparticles

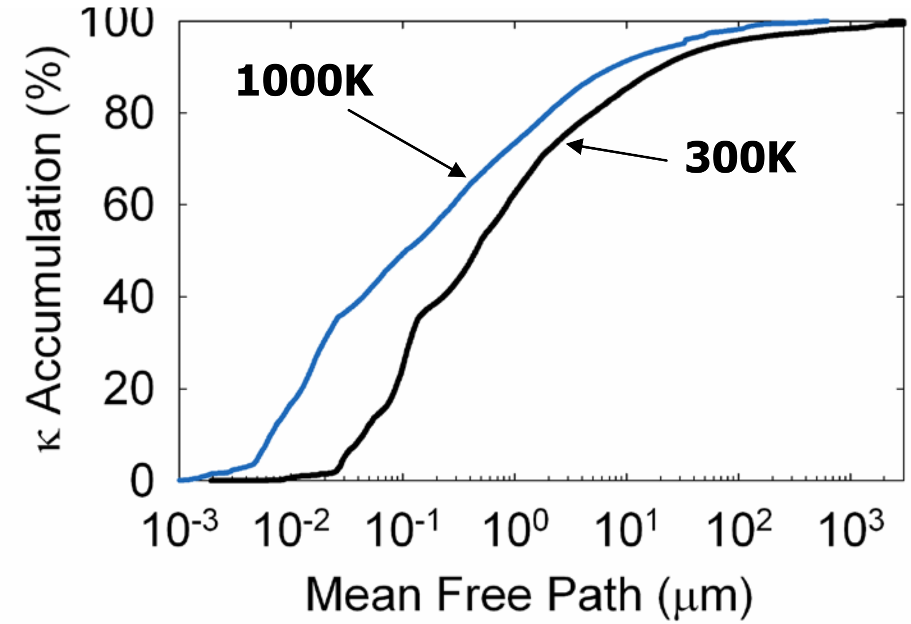
Phonon Mean Free Path in Si
Classical Molecular Dynamics Simulations

$$k = \frac{1}{3}\int C\,\mathrm{v}\,\Lambda\, d\omega$$

$$k = \frac{1}{3}\int \underbrace{C\,\mathrm{v}\,\Lambda}_{k_\Lambda}\, d\Lambda$$

Change Variables

$\Lambda(\omega)$ ⟷ $\omega(\Lambda)$

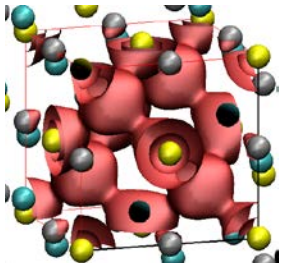


Dames and Chen, CRC Handbook, M. Rowe, 42-1, 2006.
Henry and Chen, J. Comp. & Theo. Nanosciences, 5, 141, 2008.

First Principle Simulation

First Principle (DFT)calculations

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$



→ e-band, e-DOS → Seebeck, e-conductivity

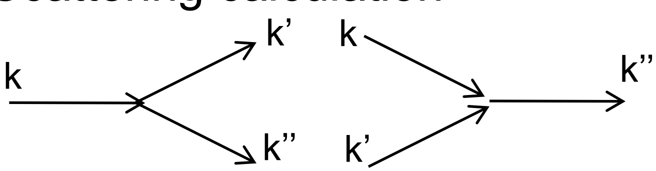
→ ph-band, ph-DOS

- Density functional perturbation theory
- **Real space approach**

Anharmonic Interatomic force

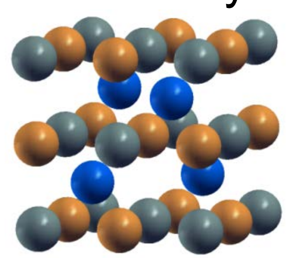
$$V = V_0 + \sum_i \Pi_i u_i + \frac{1}{2!}\sum_{ij} \Phi_{ij} u_i u_j + \frac{1}{3!}\sum_{ijk} \Psi_{ijk} u_i u_j u_k + \frac{1}{4!}\sum_{ijkl} X_{ijkl} u_i u_j u_k u_l$$

Scattering calculation



$$W_{i \to f} = \frac{2\pi}{\hbar} \left| \langle f | V | i \rangle \right|^2 \rho$$

Molecular dynamics simulations

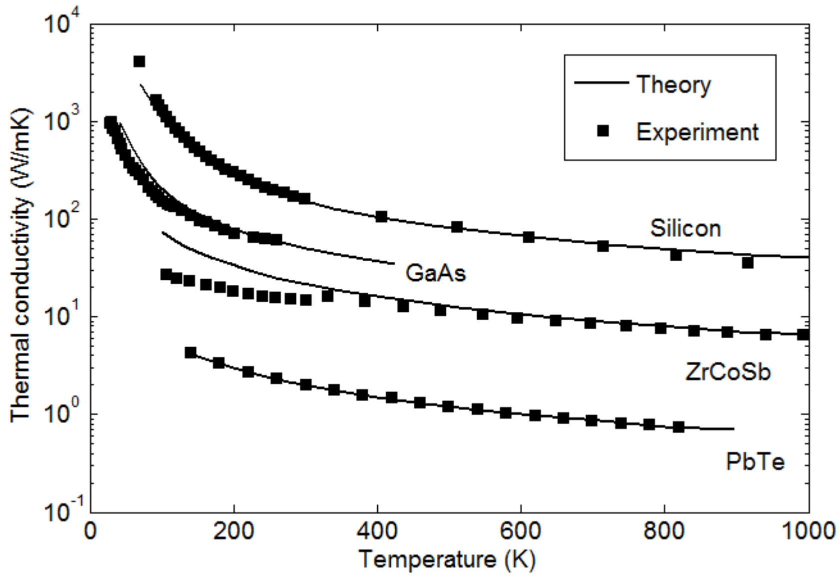


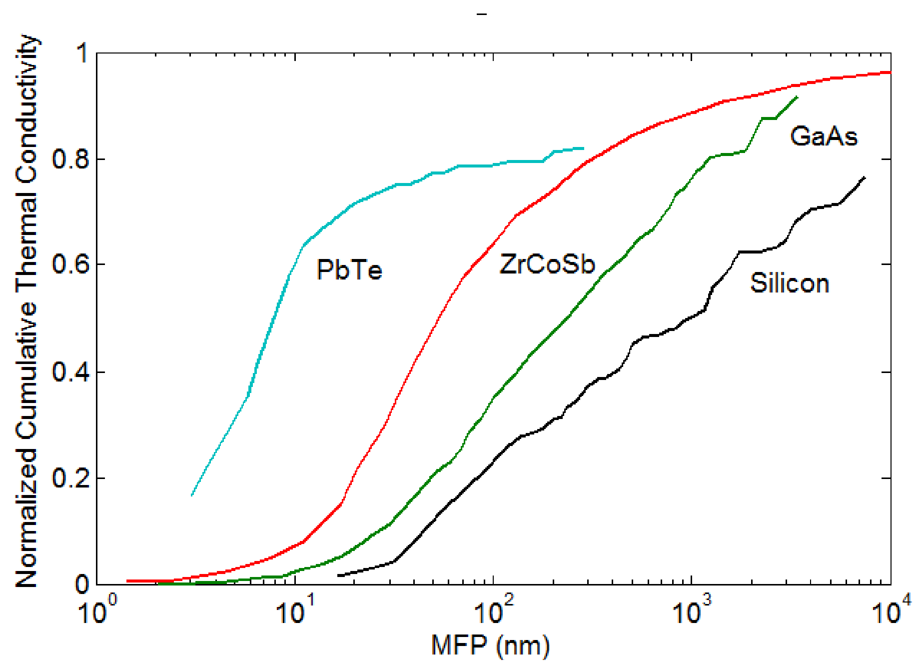
$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\nabla V$$

Alloy effects

Thermal conductivity + mean free path (mode-dependent)

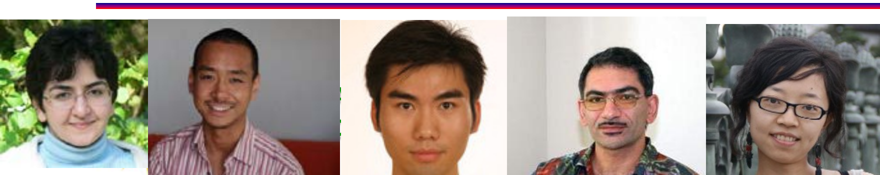
Extracting Mean Free Path of TE Materials



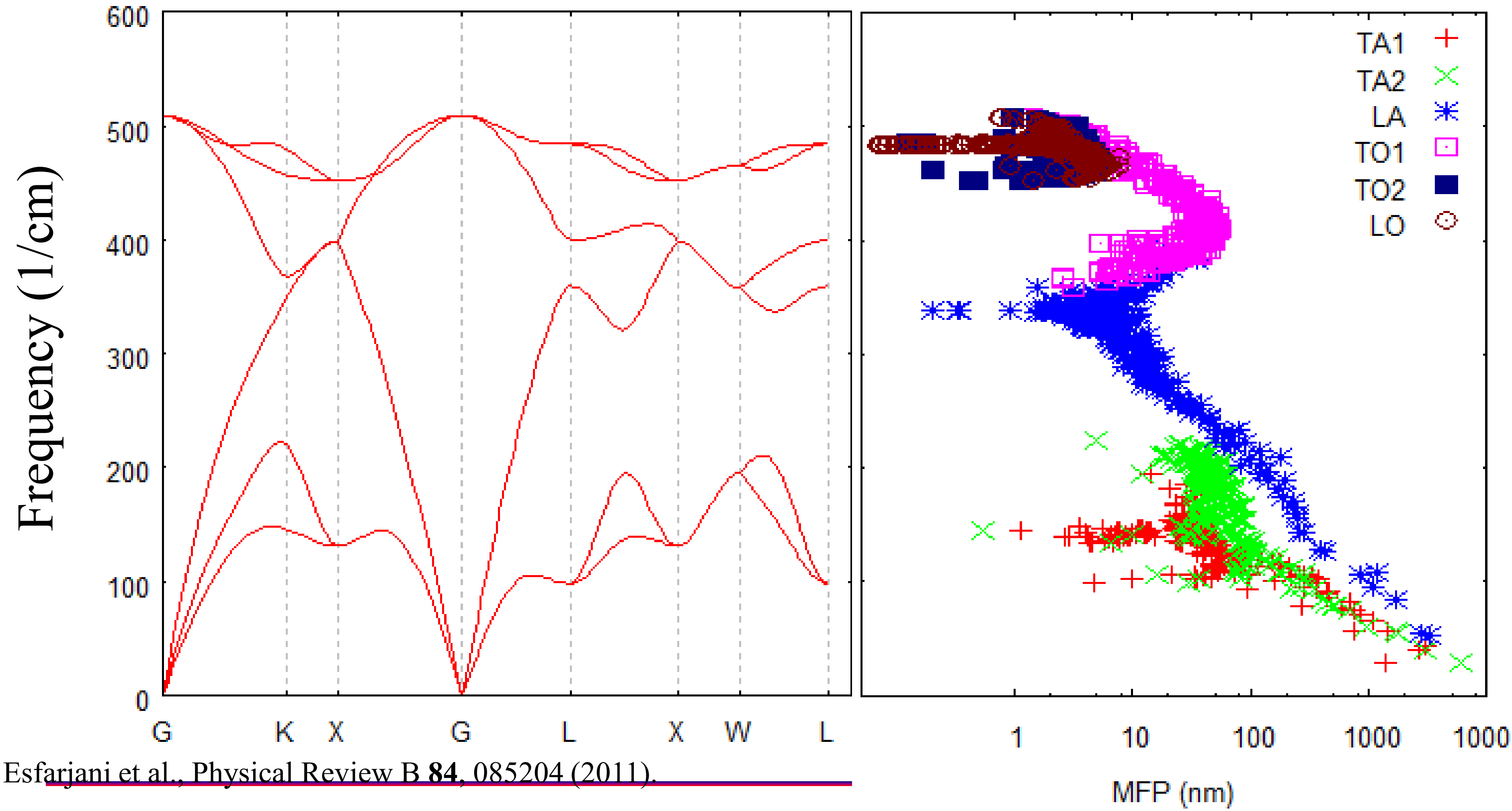


Apply to other materials!

Zebarjadi et al., Energy & Env. Sci, 2012

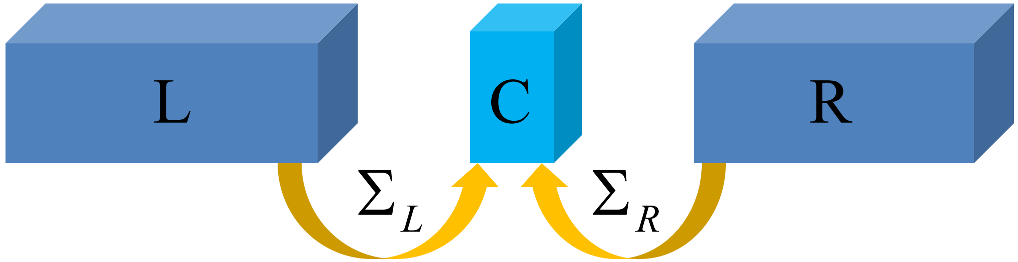


Phonon Mean Free Path in Si at 300 K



Esfarjani et al., Physical Review B **84**, 085204 (2011).

Interfaces: Atomistic Green's Function (AGF)



Green's Function

$$G = [\omega^2 I - \phi_C - \Sigma_L - \Sigma_R]^{-1}$$

$$\Sigma_\alpha = \phi_{C\alpha} g_\alpha \phi_{C\alpha}^{+} \qquad g_\alpha = [\omega^2 I - \phi_\alpha - \phi_{\alpha\alpha} g_\alpha \phi_{\alpha\alpha}^{+}]^{-1}$$

Stillinger-Weber (SW) or Density Functional Theory (DFT)

Semi-empirical Potential First-Principles Calculations

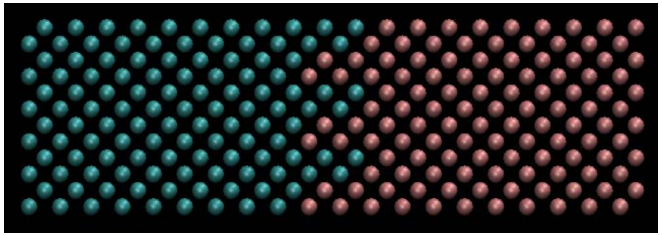
Transmission Function

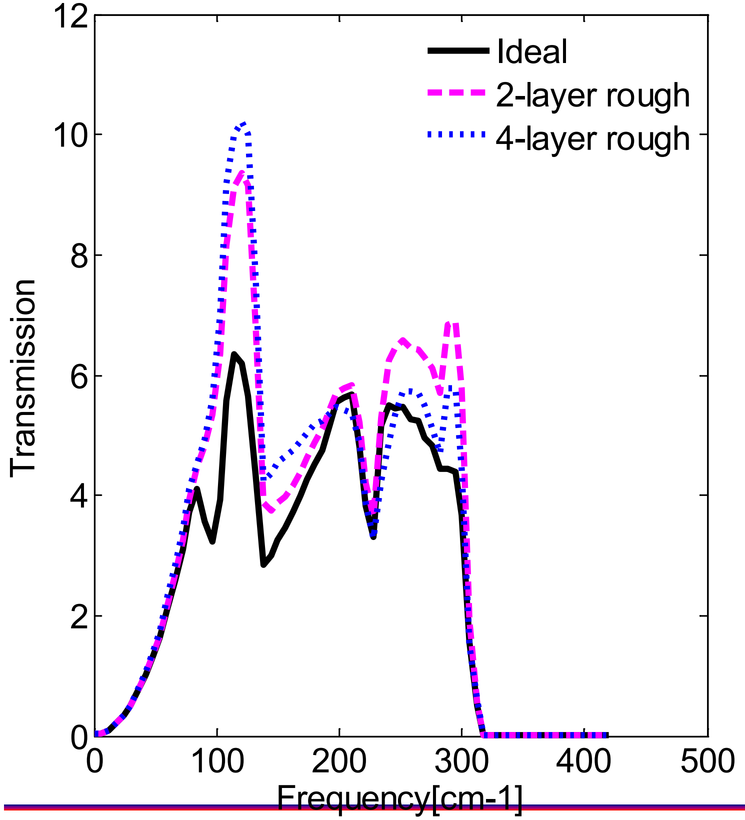
$$\Xi(\omega, \vec{k}_t) = Tr[\Gamma_L G \Gamma_R G^{+}] \qquad \Gamma_\alpha = -2\,\mathrm{Im}[\Sigma_\alpha]$$

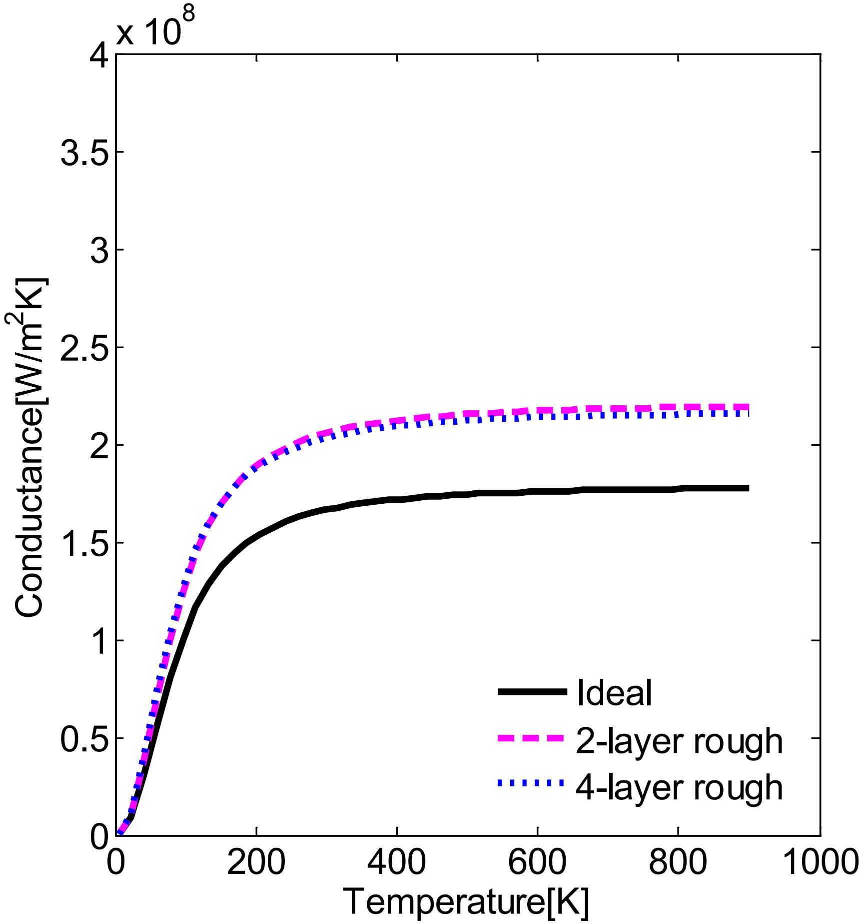
Thermal Conductance (Landauer form)

$$\sigma = \frac{1}{s}\int_0^\infty \frac{\hbar\omega}{2\pi}\frac{\partial f}{\partial T}\Xi(\omega)d\omega$$

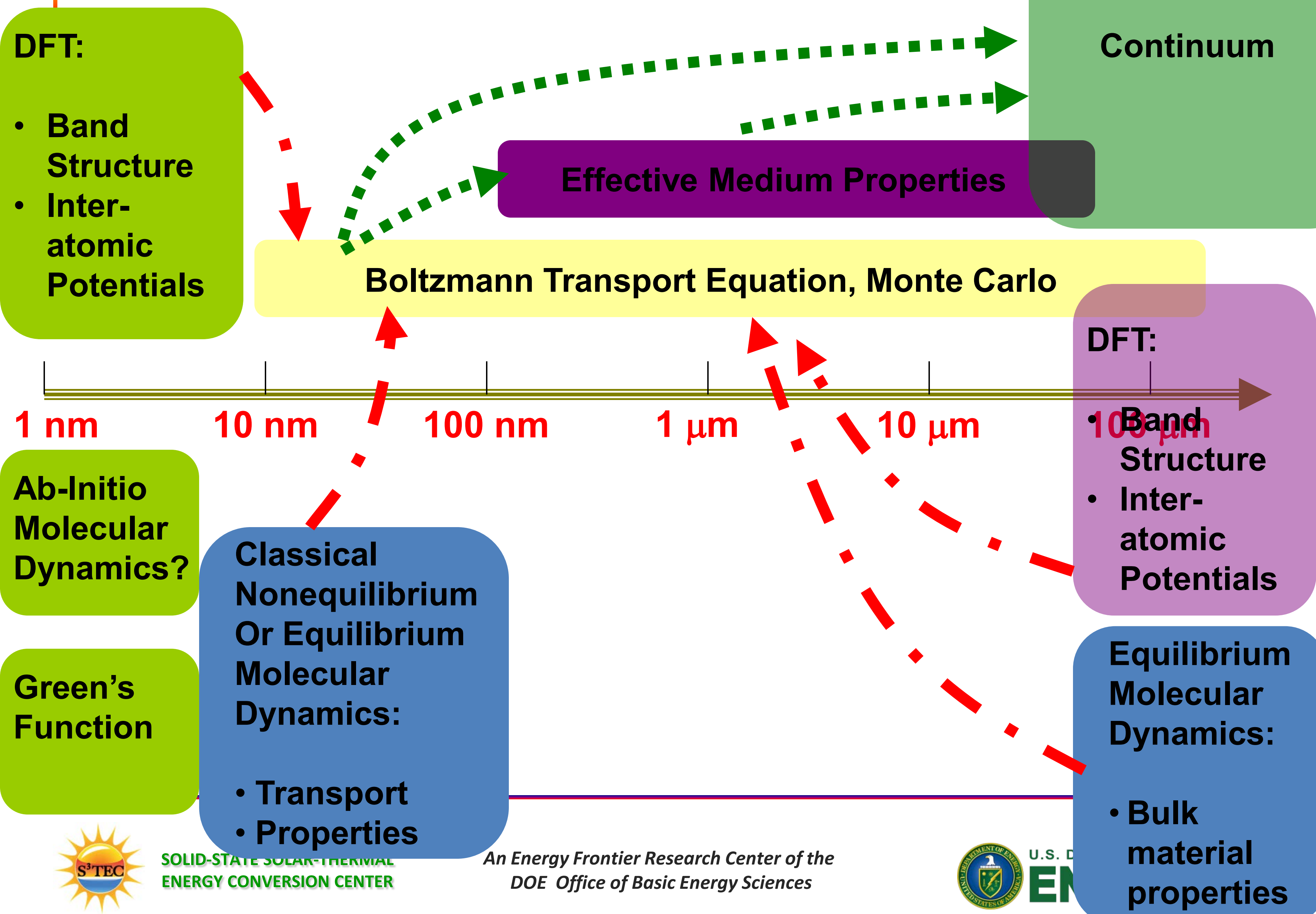
Interface Phonon Transmission



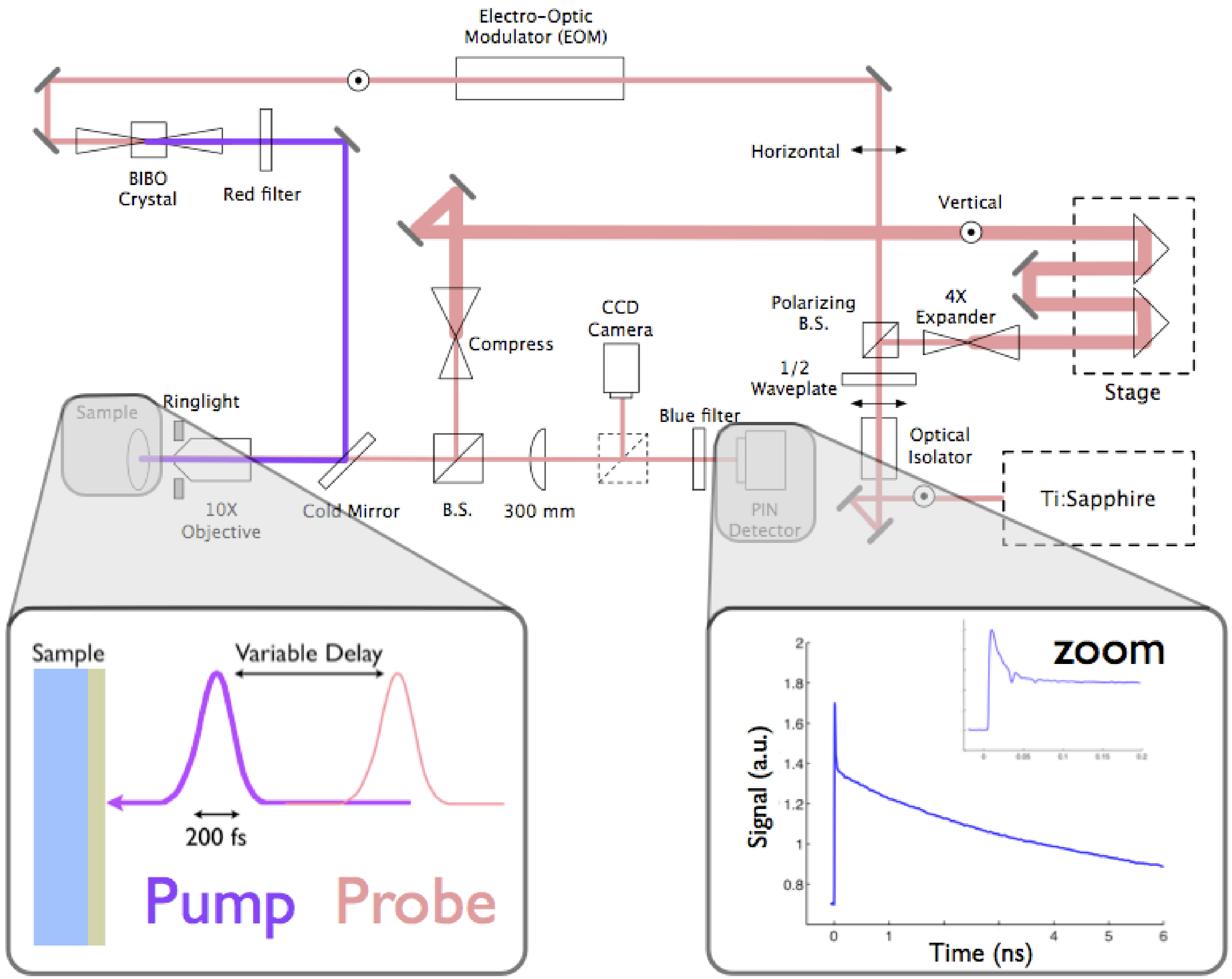




Multiscale Phonon Simulation

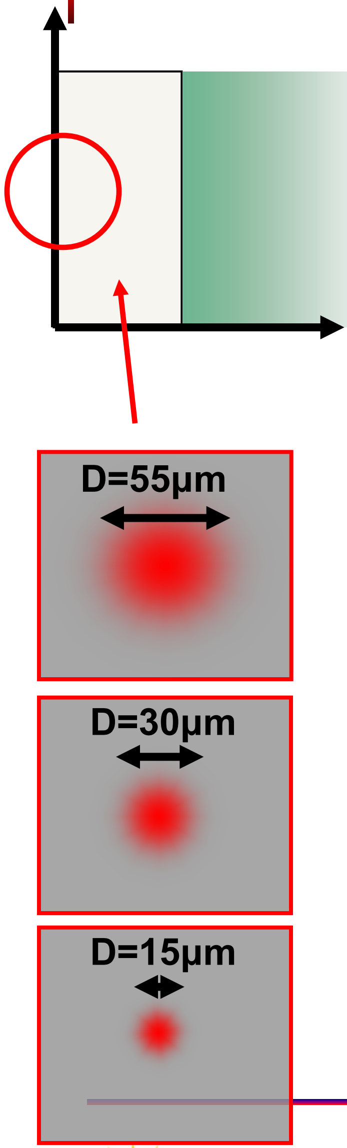


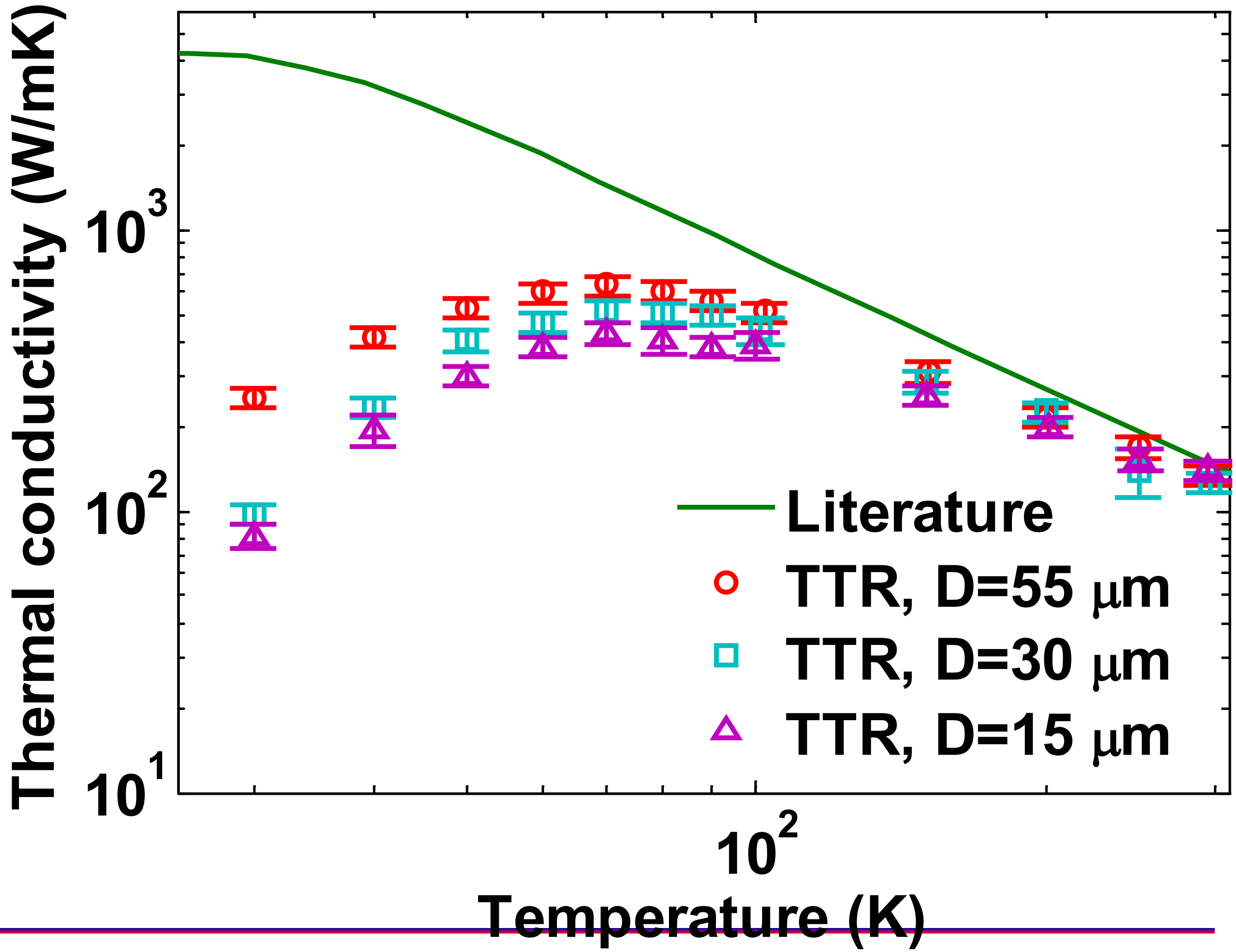
Pump-probe System for Thermal Conductivity Measurement



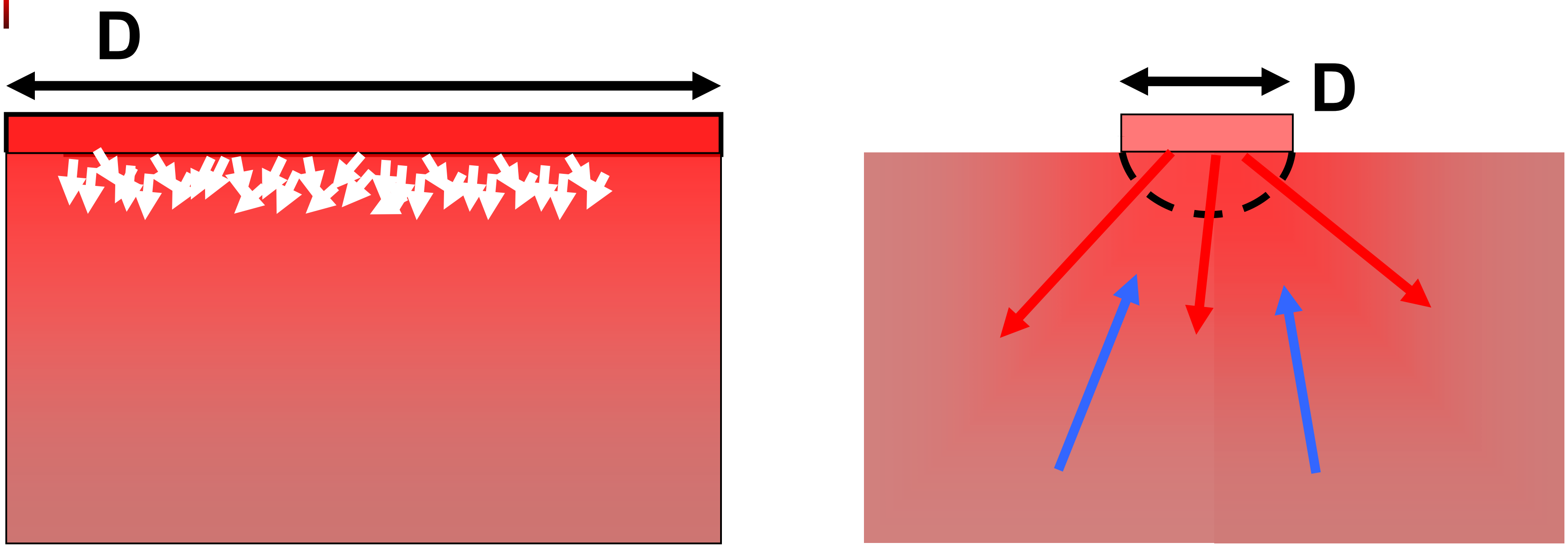
Schmidt et al. Review of Scientific Instruments, 79, 114902, 2008.

Experimental Results on Si





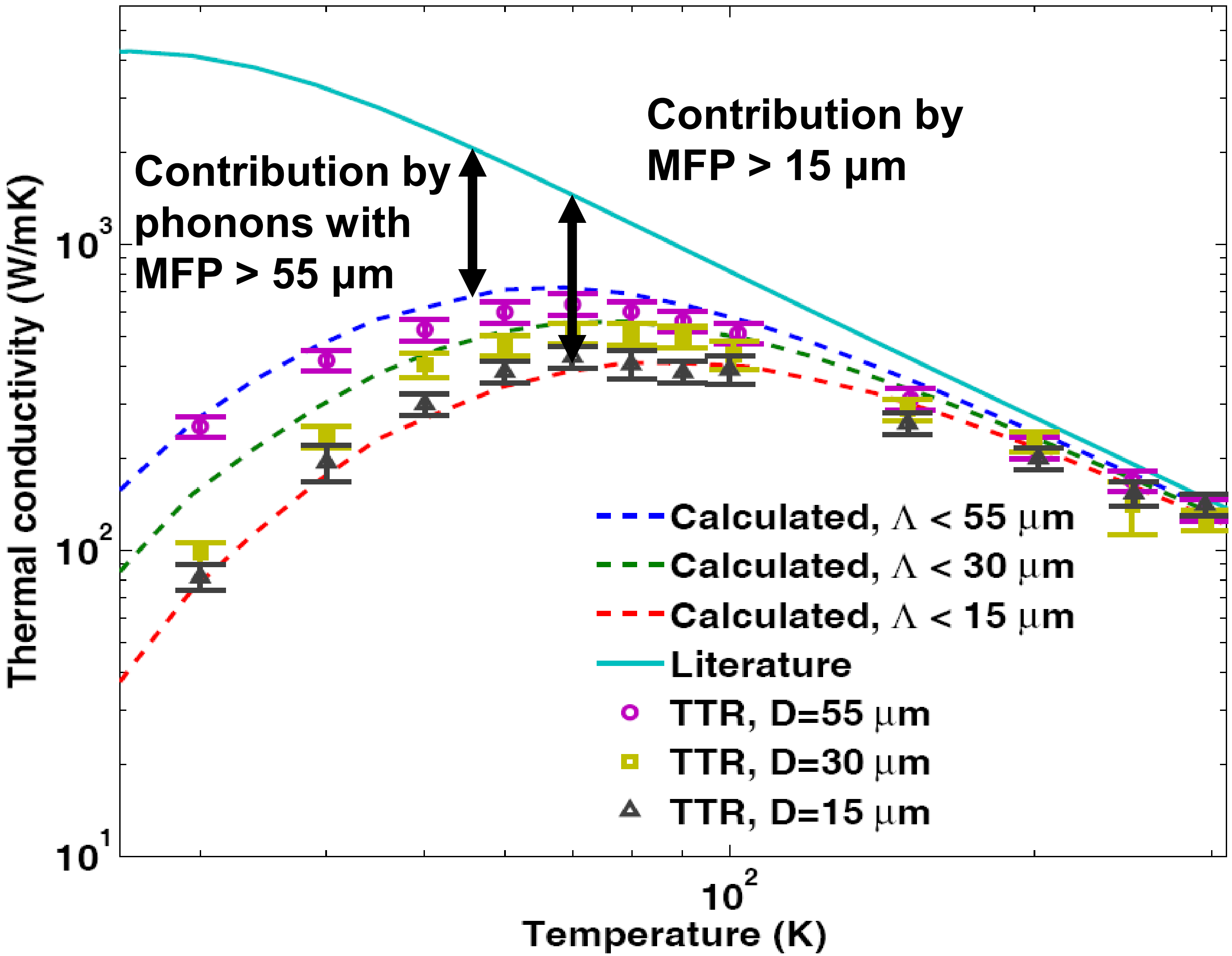
Effect of Quasi-ballistic Transport



$$\frac{q_{B\omega}}{q_{D\omega}} \sim \frac{D}{\Lambda_\omega}$$

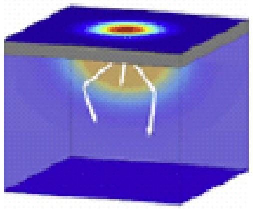
Chen, J. Heat Transf., 118, 539, 1996.

Comparison with Experiments

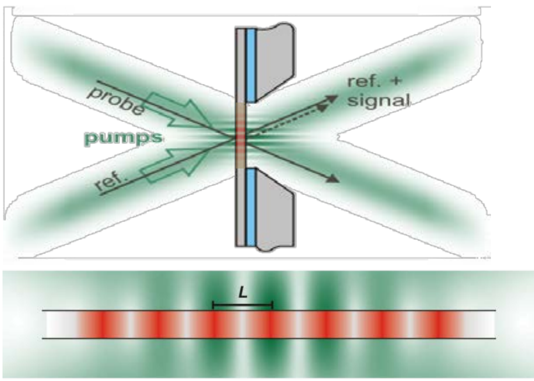


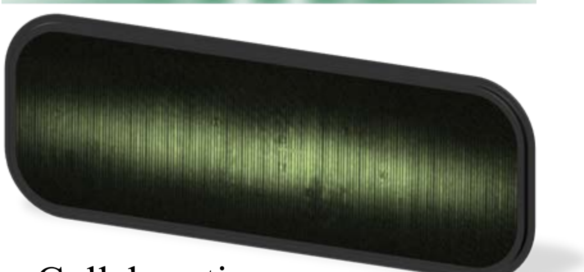
Physics: Measuring how far vibrations travel

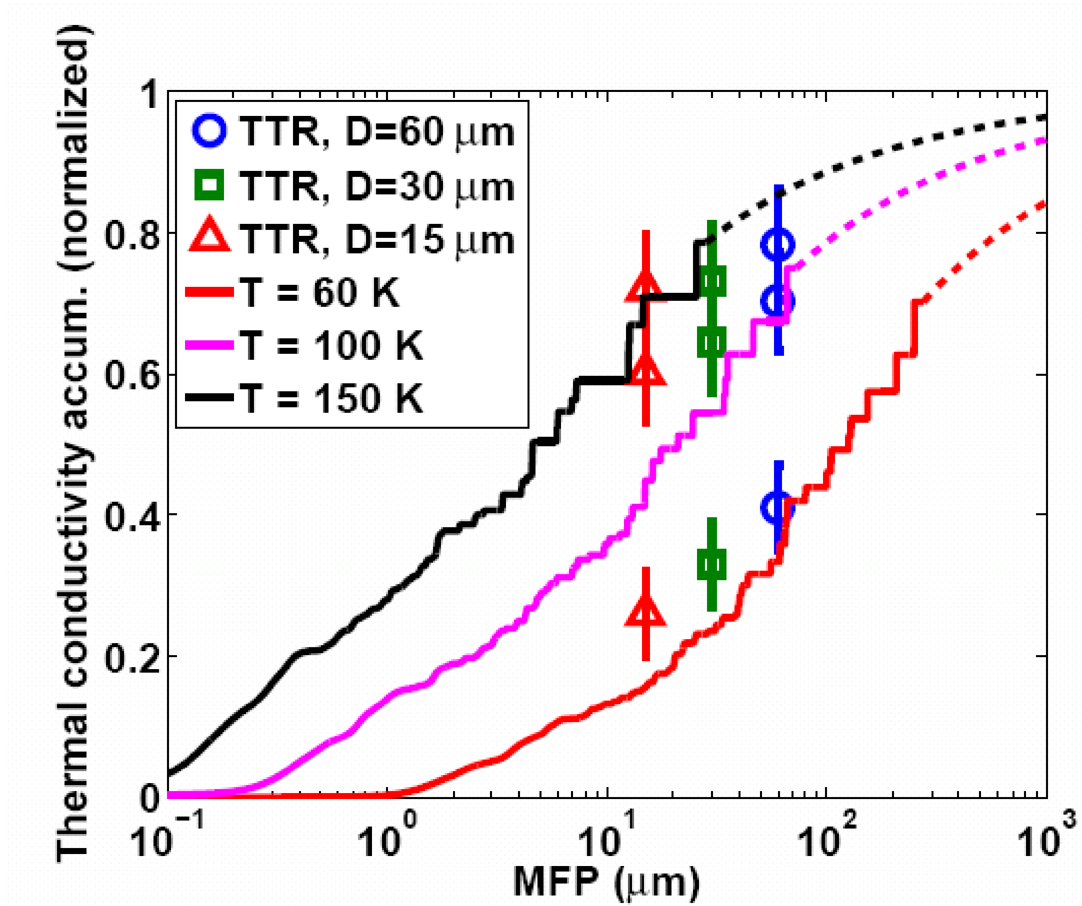
August 25, 2011



Optical Techniques to Measurement Phonon Mean Free Path Distribution





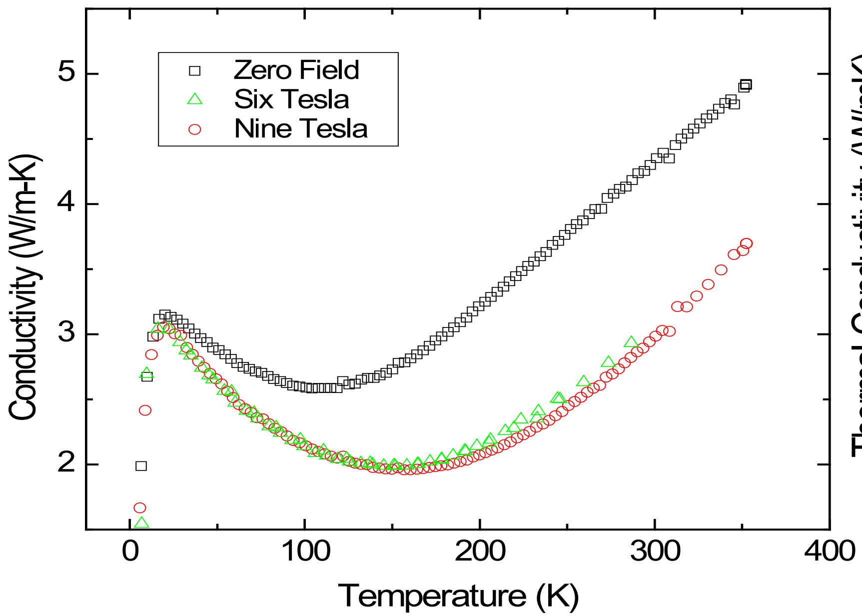


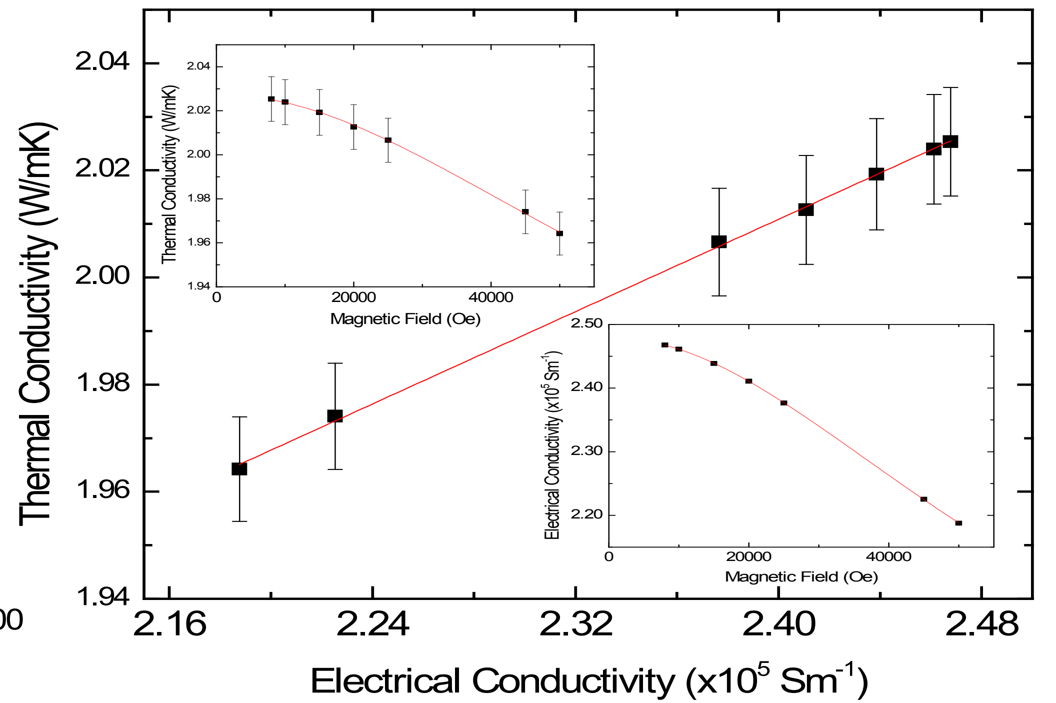
Collaborations:
G. Chen/K. Nelson/M.S. Dresselhaus

Minnich et al., PRL, 107, 095901, 2011

Direct Measurement
Electronic Thermal Conductivity

$k = k_p + k_e$

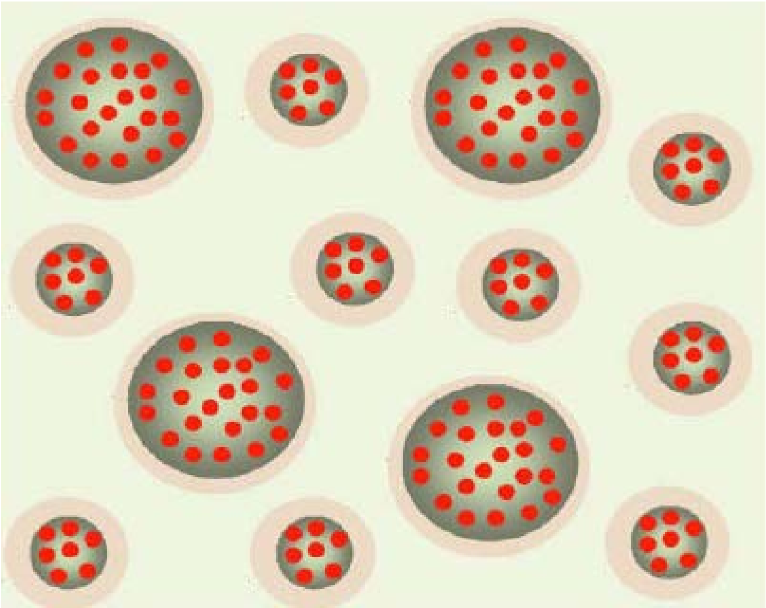


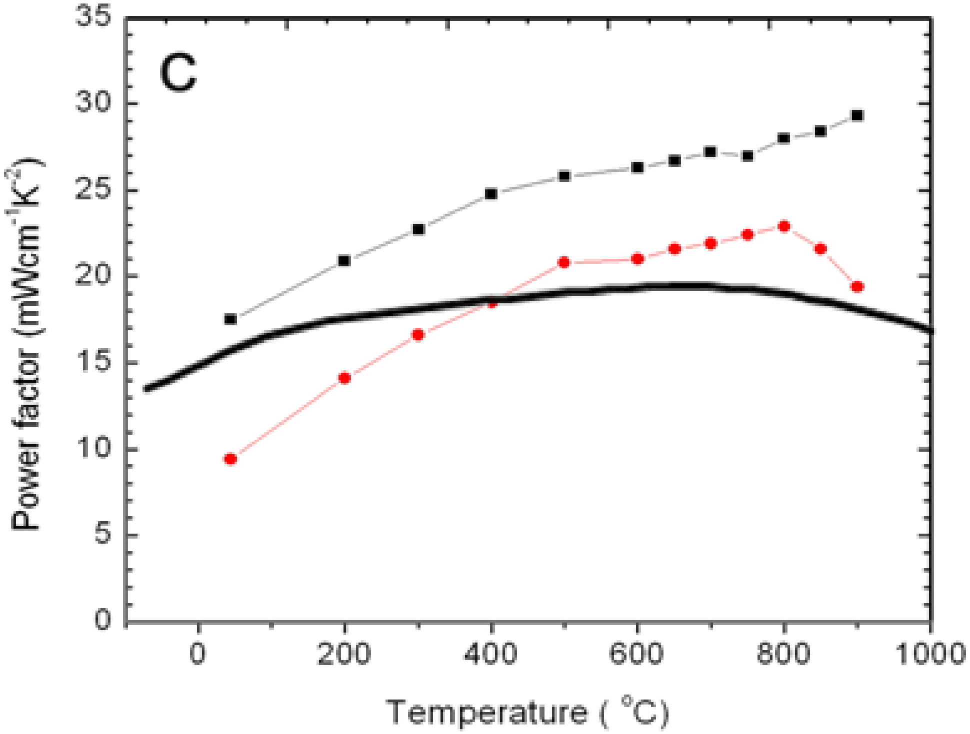


- In semiconductors, Lorenz Number depends on carrier concentration
- Measurements of thermal conductivity under magnetic field determine electronic contribution and Lorenz number

Opeil/Ren/Dresselhaus/Chen

Modulation Doping

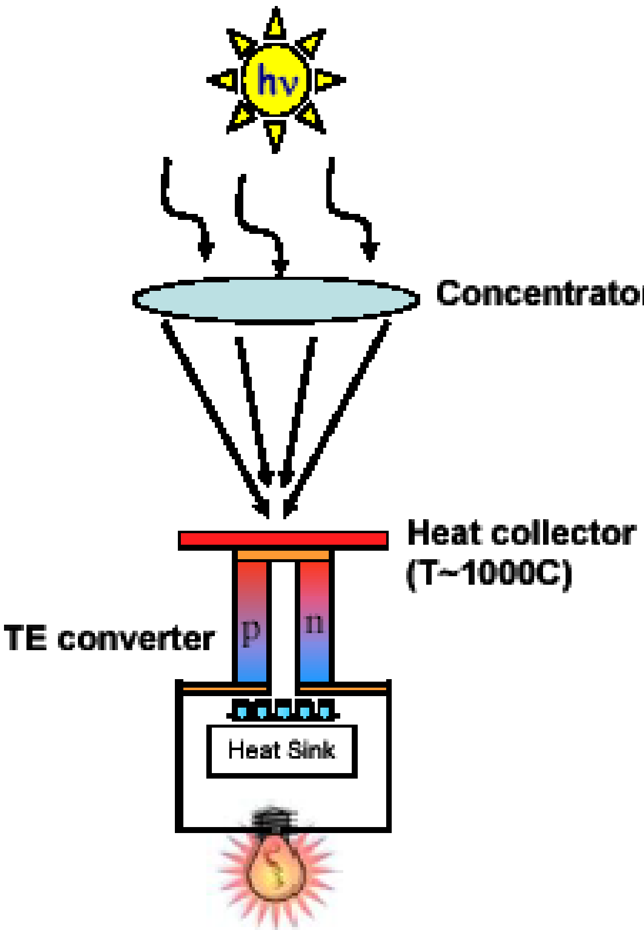




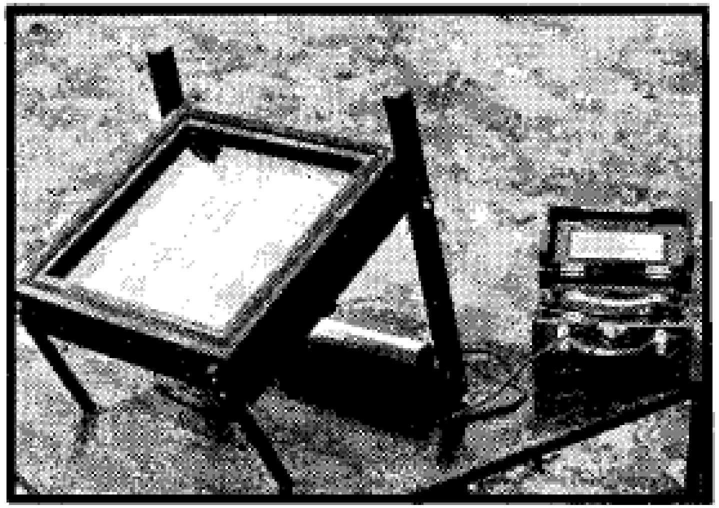
Chen/Ren/Dresselhaus

Zebarjadi et al., Nano Letters, 11, 2225, 2011.

Prototype Generators



- US Patent No. 389124:
  E. Weston in 1888
- M. Telkes, JAP, 765, 1954



Efficiency: 0.63%

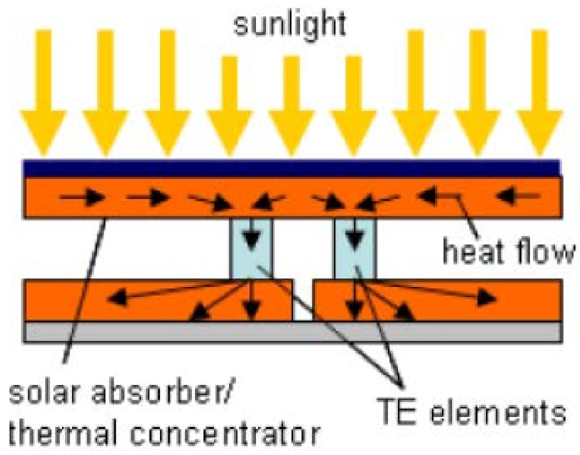
Heat Flux Consideration

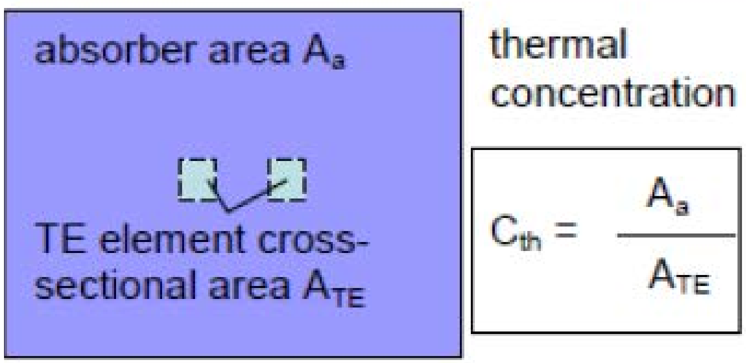
$$q = k\frac{\Delta T}{L} \approx 1\frac{\mathrm{W}}{\mathrm{m} * \mathrm{K}}\frac{100\,\mathrm{K}}{\mathrm{L}}$$

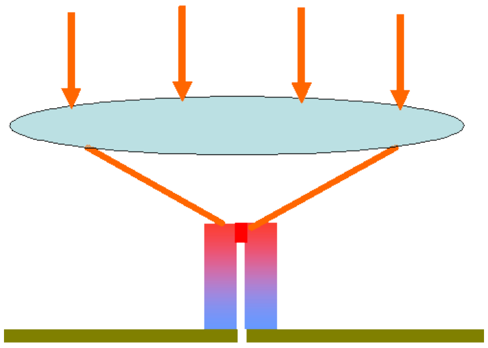
q=1000 W/m^2 (1 Sun); L=100 mm

q=100,000 W/m^2 (100 Sun); L=1 mm

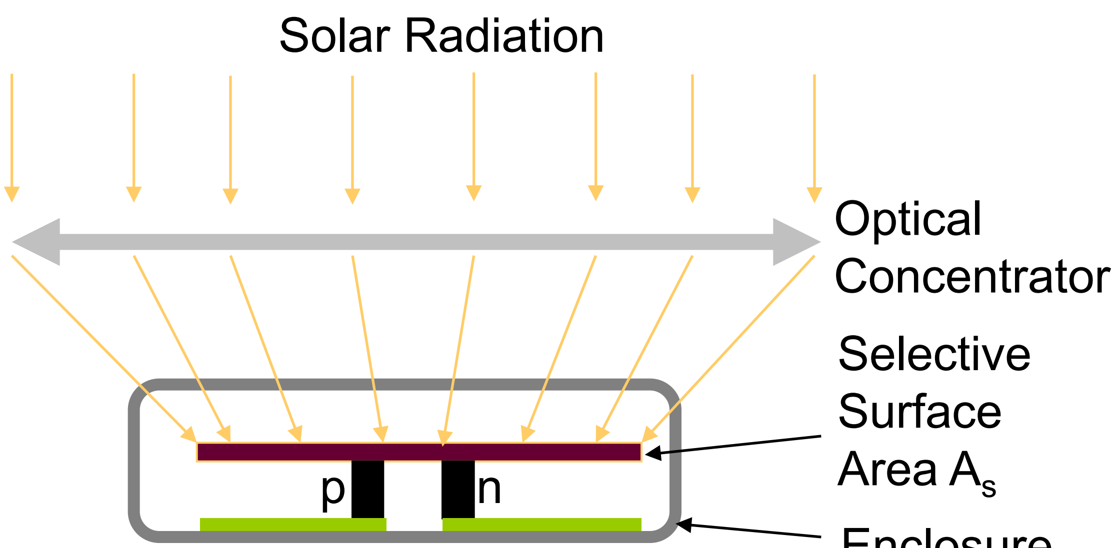
Possible Configurations



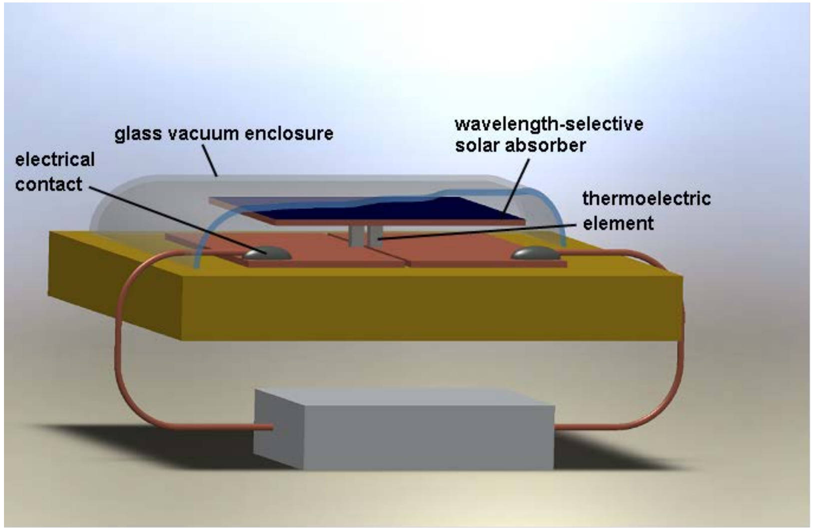


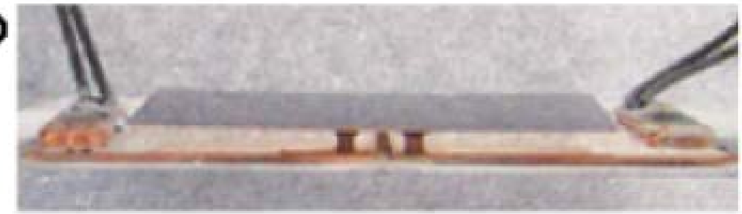


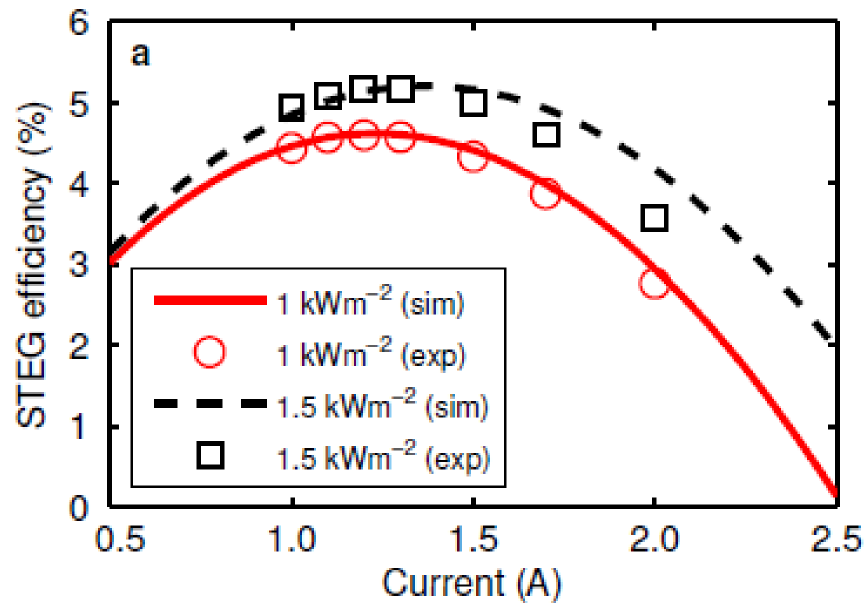
Optical Concentration



Solar Thermoelectric Power Conversion



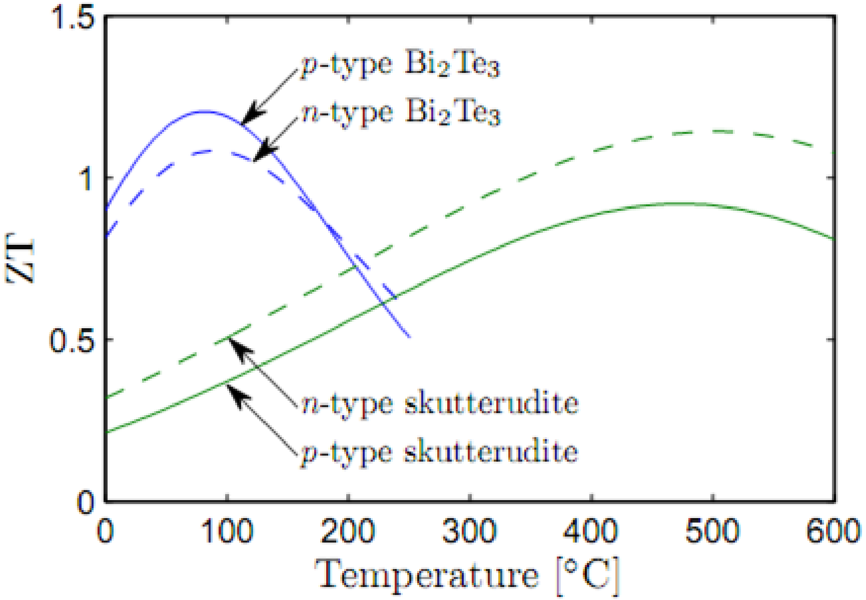
b


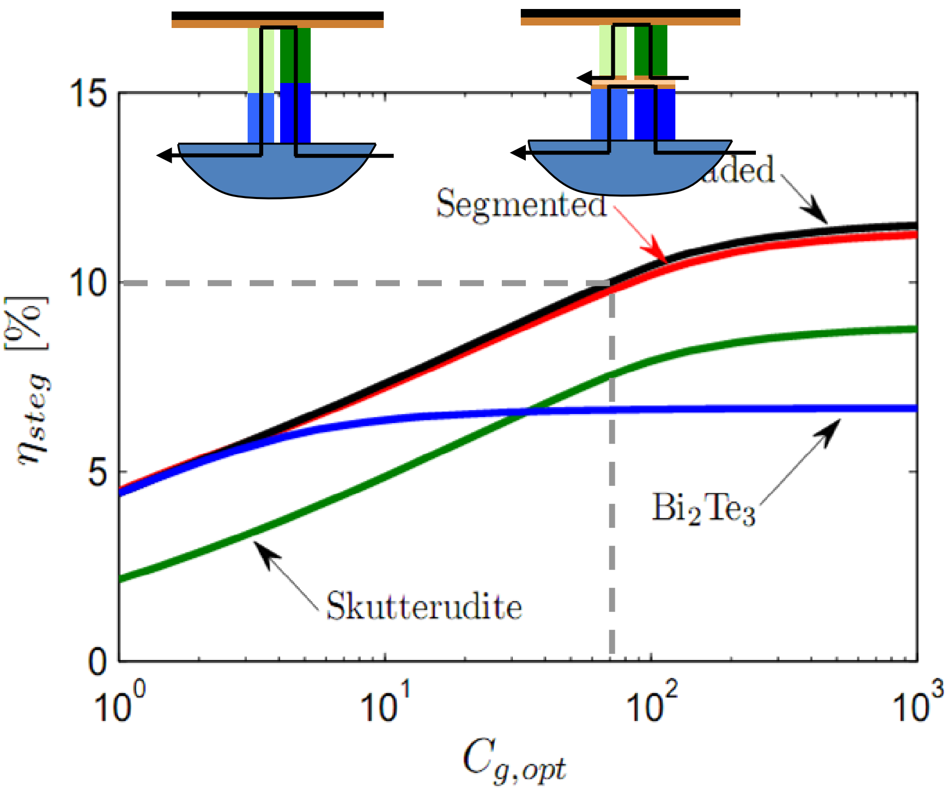


c


Kraemer et al., Nature Materials, May, 2011

Cascaded/Segmented STEGs





- STEG efficiency of >10% with current materials
- Small difference between segmented and cascaded system

D. Kraemer et al., Nature Mat., 2011.

K. McEnaney et al., J. Appl. Phys., 2011.

Summary

- Phonon thermal conductivity from first principle.
- Interface transmittance from Green's function.
- Optical spectroscopy on thermal conductivity and phonon mean free path.
- Modulation doping to improve electron performance.
- Demonstration of STEG with promising efficiency.