ME 697R: Computational Methods for Nanoscale Energy Transport

Chapter 1: Introduction

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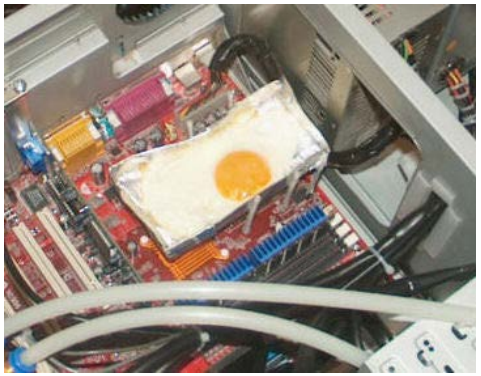
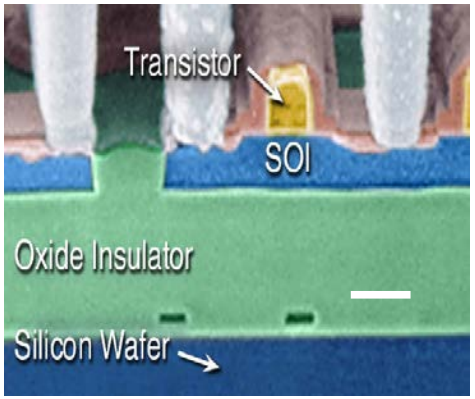
Applications of Nanoscale Energy Transport

- Thermal management of electronics

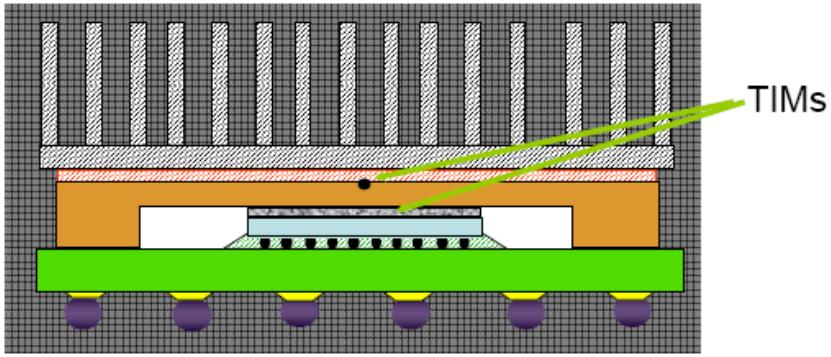


http://warrenkwok.blogspot.com/2007_03_01_archive.html

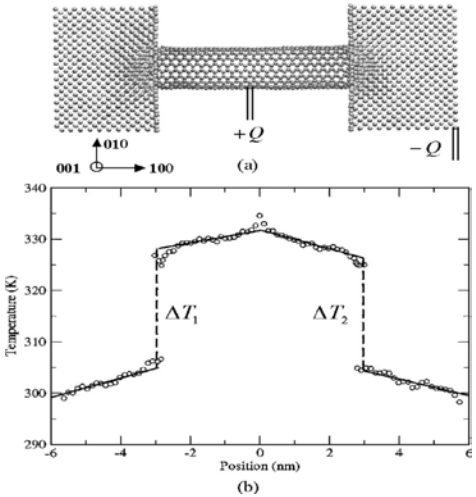


transistor

- Thermal interface materials for packaging



Courtesy Ravi Mahajan

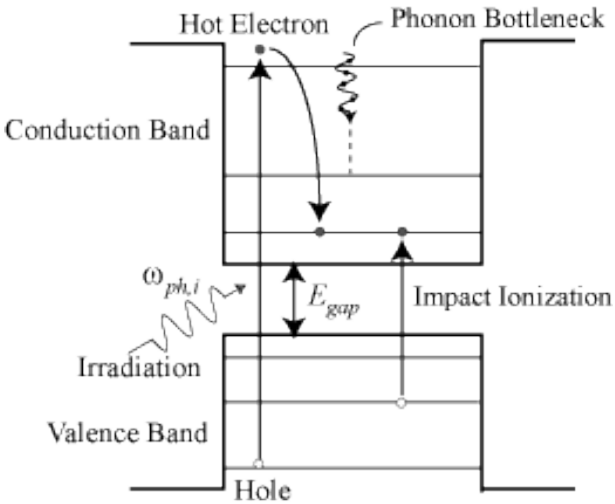


CNT-silicon interface

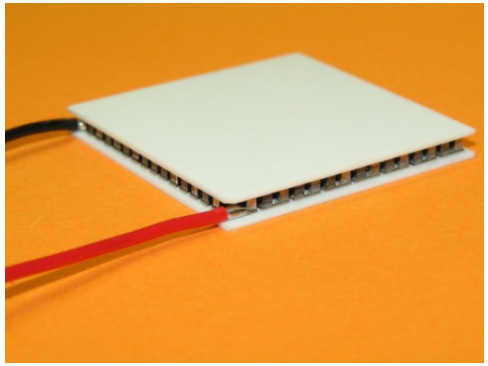
Applications of Nanoscale Energy Transport

- Energy conversion

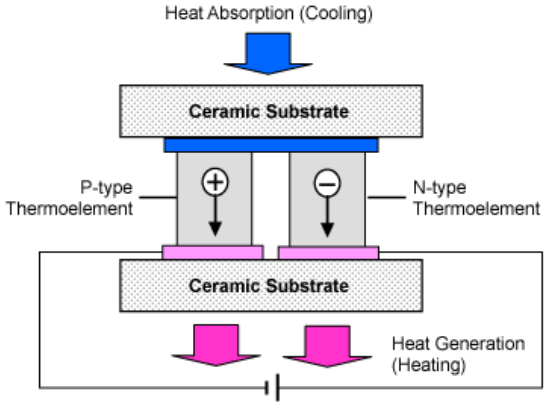
http://deviceace.com/science/266/more-efficient-solar-cells-thanks-to-cnt-films-that-transmit-infrared-light.html



photovoltaics



http://www.thermoelectric.com/2005/pr/tem/

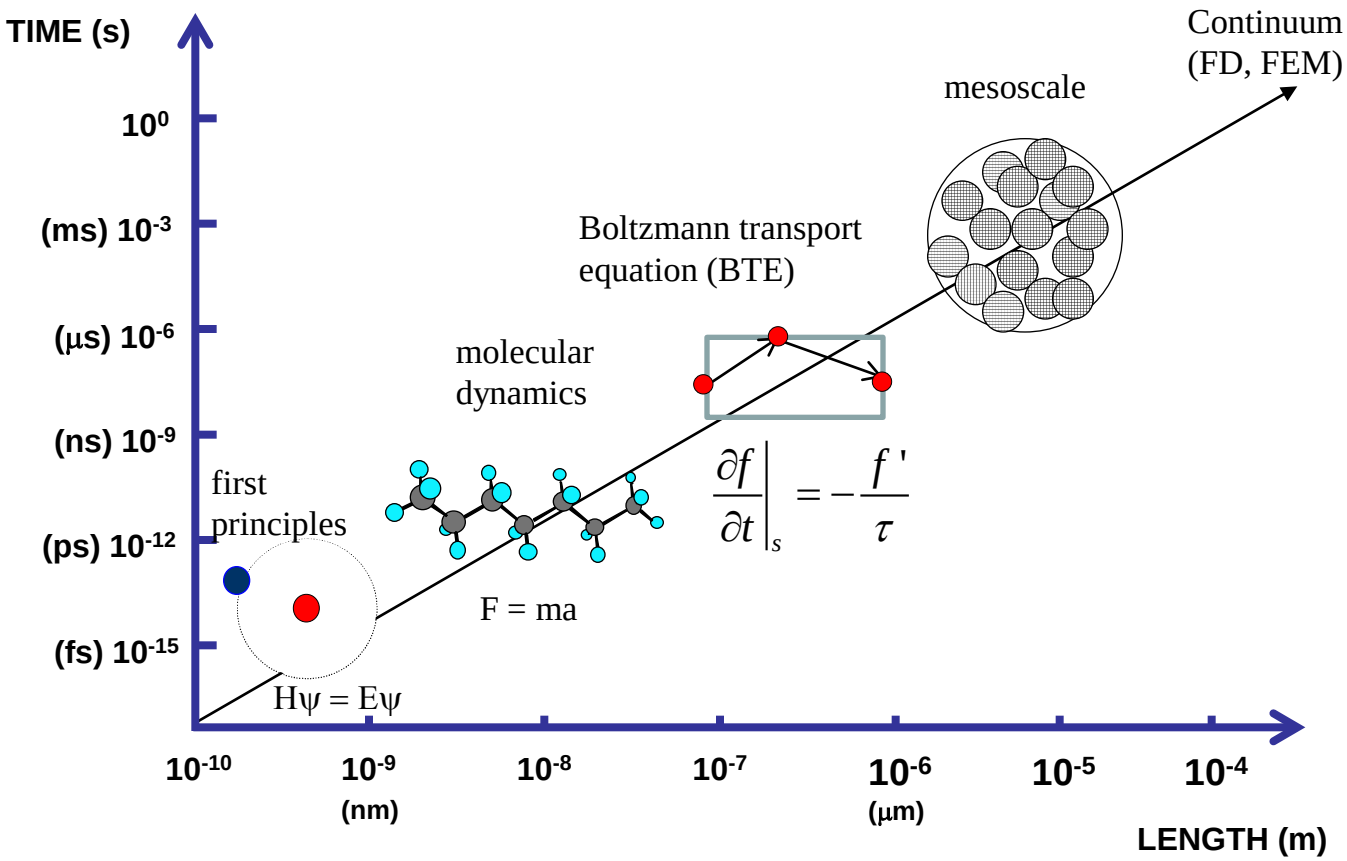


thermoelectrics

http://winking-falcon.com/engineering%20web/2manufacturing/manufacturing.htm

laser manufacturing

Length and Time Scales of Simulation Methods



- Parameters obtained in a smaller scale simulation can inform larger scale simulations.

The Nobel Prize in Chemistry 2013

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Martin Karplus

Photo: Keilana via Wikimedia Commons

Michael Levitt

Photo: Wikimedia Commons

Arieh Warshel

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

http://www.nobelprize.org

THE U.S. MATERIALS GENOME INITIATIVE

"...to discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative"
– President Obama, 2011

Meeting Societal Needs

Advanced materials are at the heart of innovation, economic opportunities, and global competitiveness. They are the foundation for new capabilities, tools, and technologies that meet urgent societal needs including clean energy, human welfare, and national security.

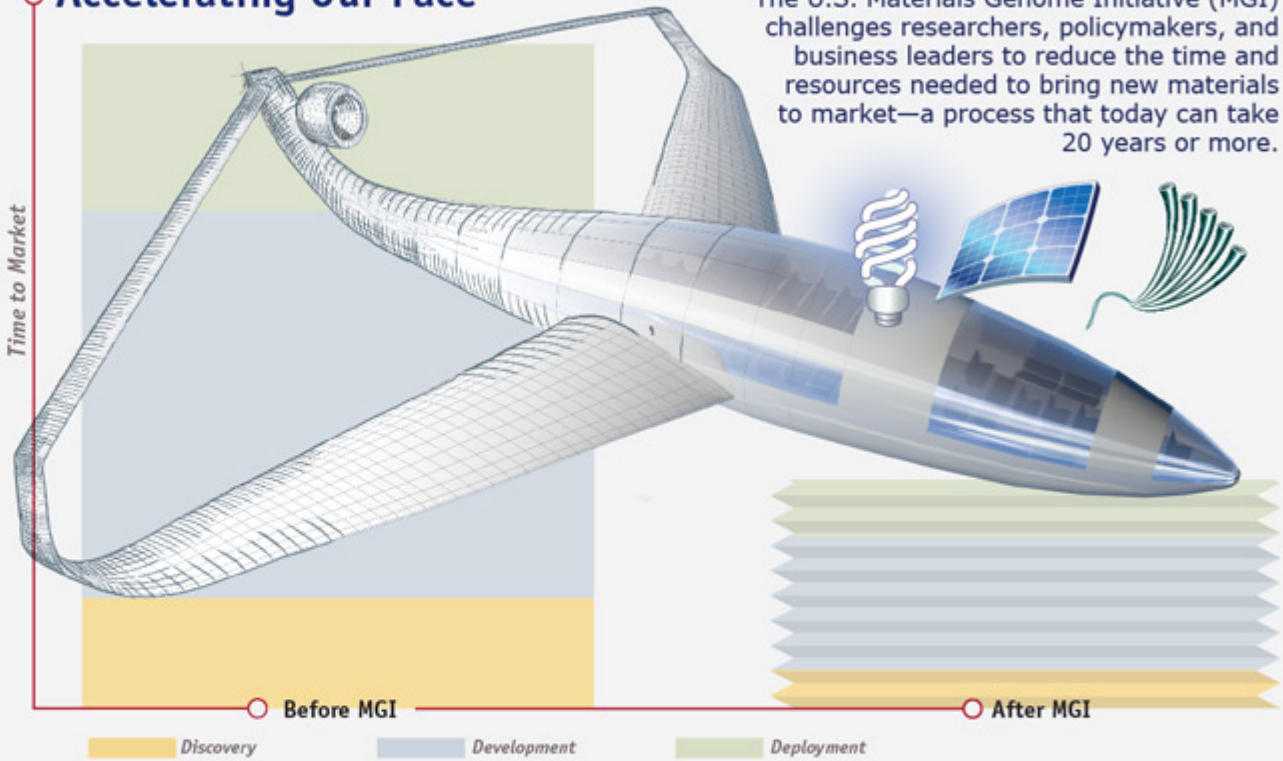
Clean Energy

Human Welfare

National Security

Accelerating Our Pace

The U.S. Materials Genome Initiative (MGI) challenges researchers, policymakers, and business leaders to reduce the time and resources needed to bring new materials to market—a process that today can take 20 years or more.



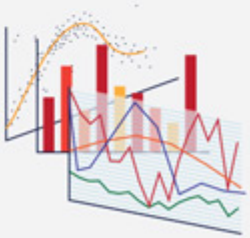
Building Infrastructure for Success

The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.

Computational tools

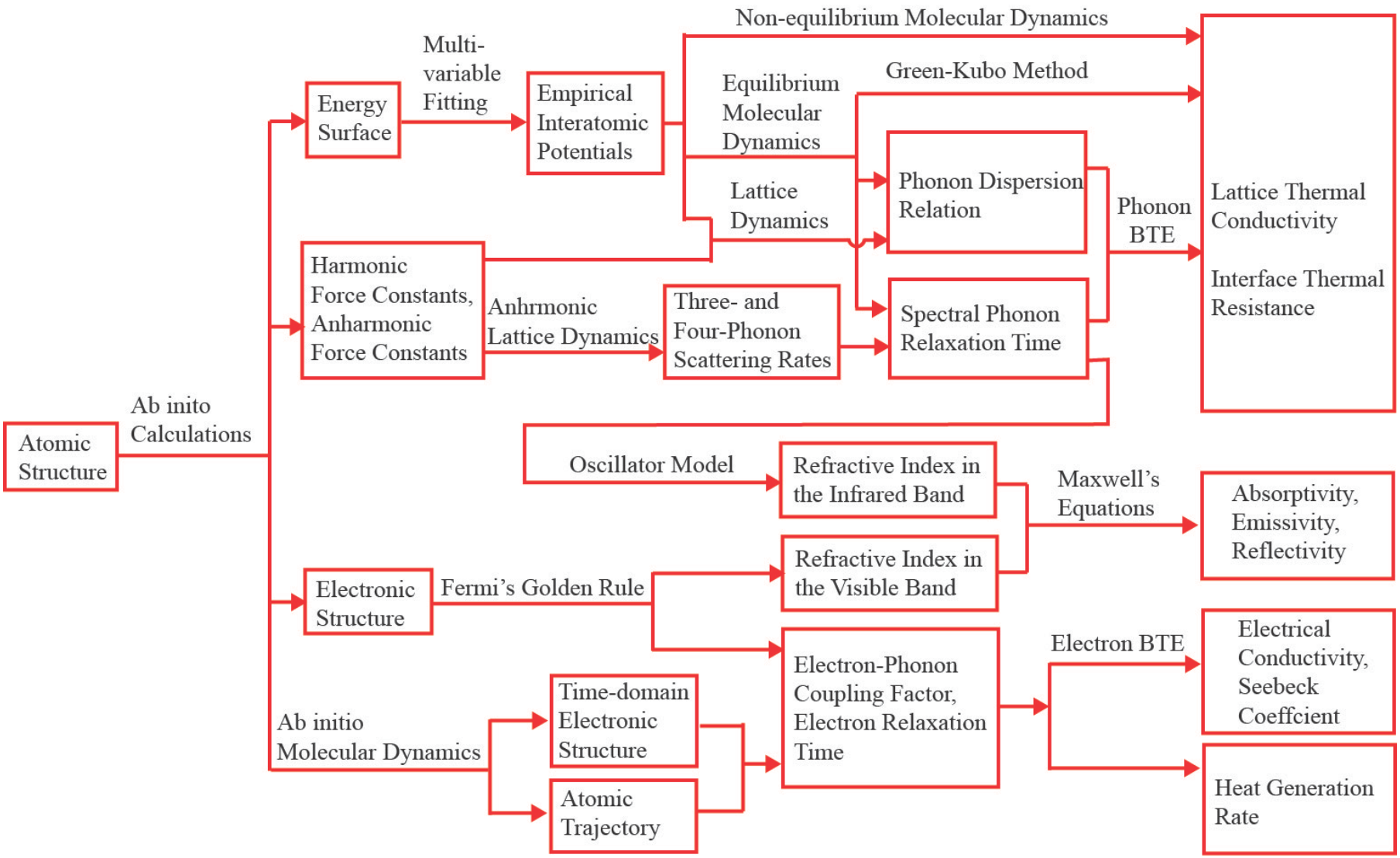
Experimental tools

Collaborative networks

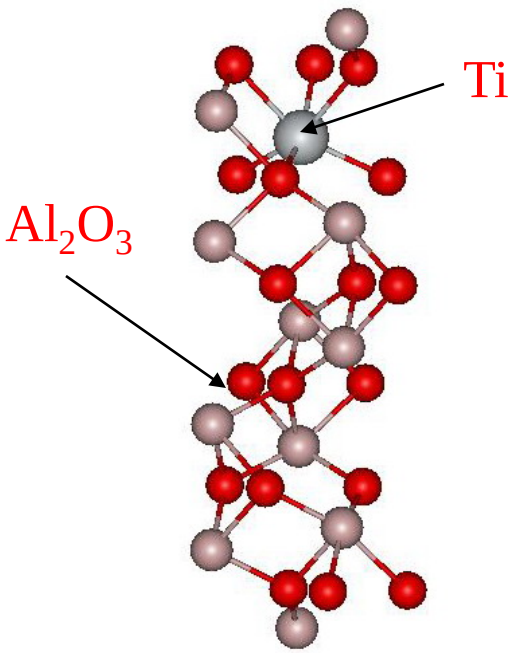


Digital data

Example Multiscale Multiphysics Approaches

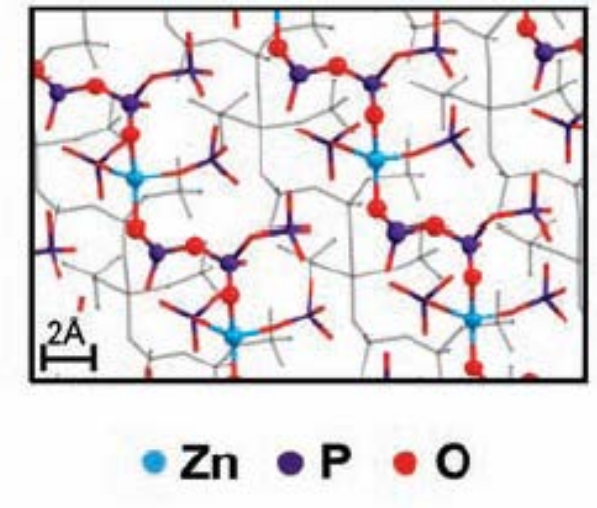


First Principles Calculations: Geometry Optimization



Laser material: Ti doped Al_2O_3

Bao and Ruan, J. Heat Transfer 138, 042702 (2016).

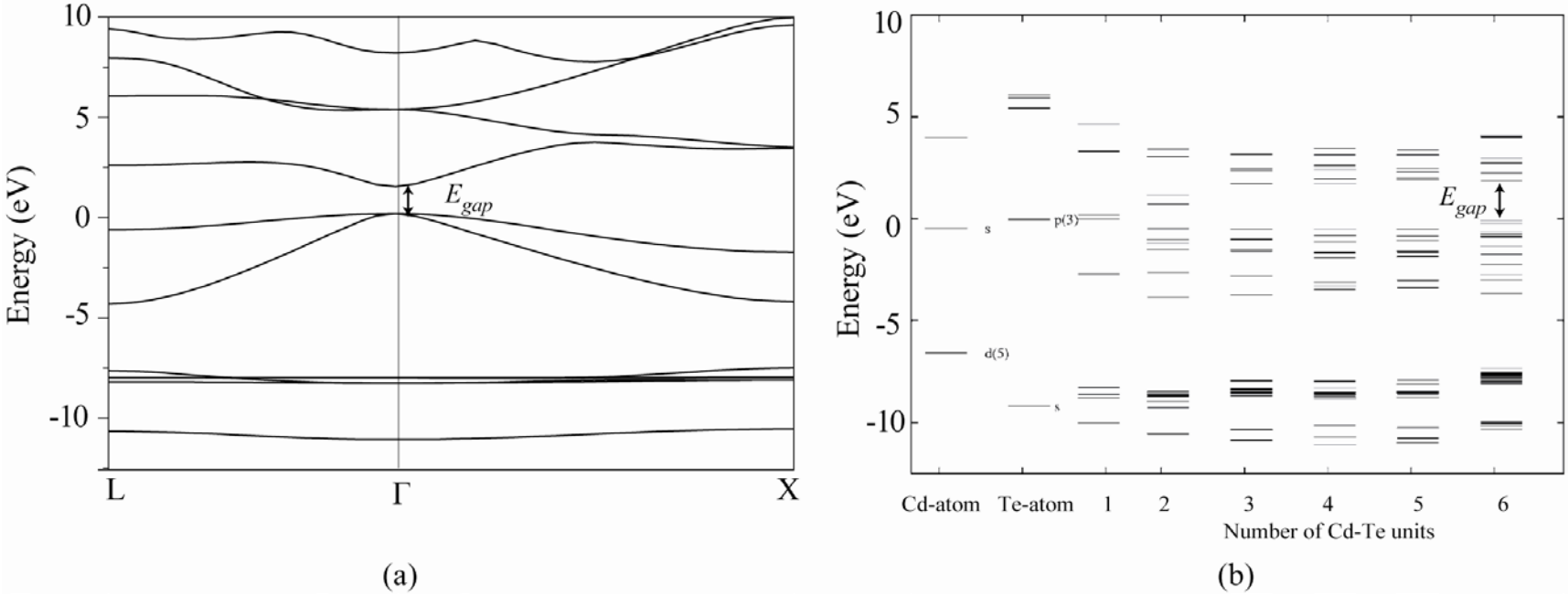


lubricant additives

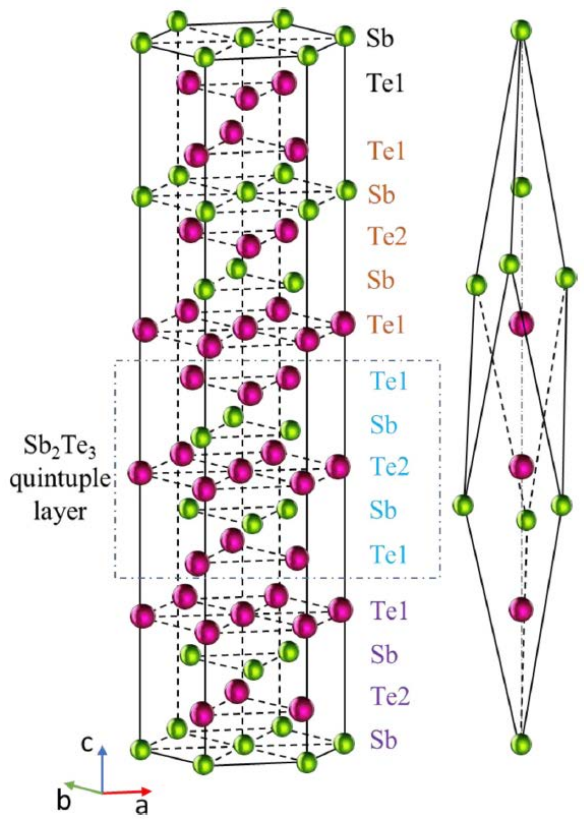
N.J. Mosey, et al, Science 307, 1612-1615 (2005).

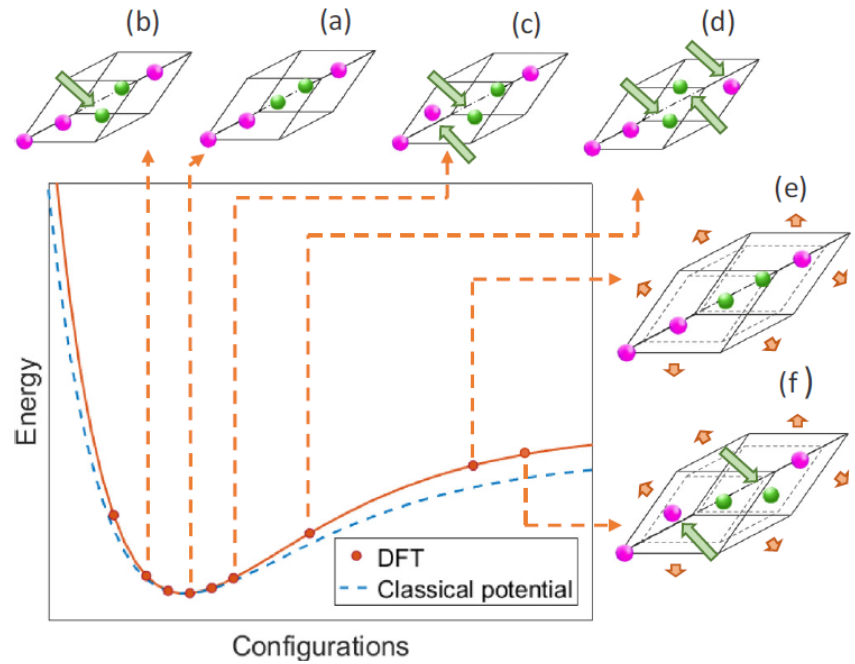
First Principles Calculations: Band Structure

- Band structure of CdTe bulk and nanocrystals



First Principles Calculations: Interatomic Potentials





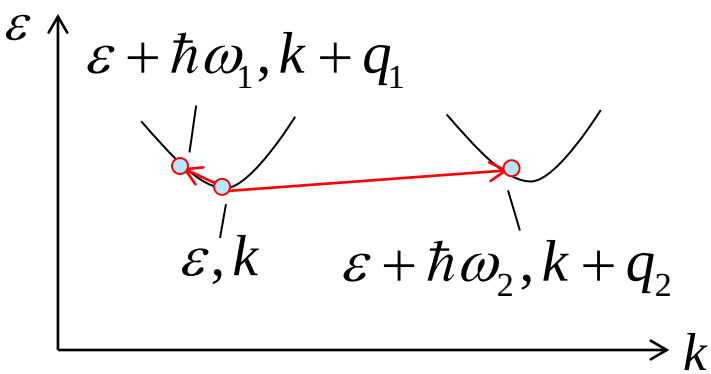
$$V(r) = D_e(1 - e^{-a(r-r_e)})^2$$

$$D_e = ?, \alpha = ?, r_e = ?$$

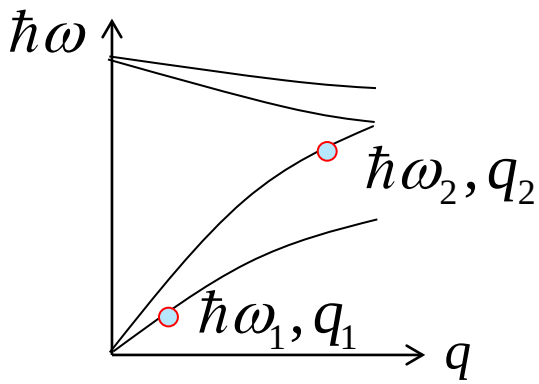
Qiu and Ruan, Phys. Rev. B, **80**, 165203 (2009).
Chowdhury, Feng, and Ruan, Phys. Rev. B, **99**, 155202 (2019).

First Principles Calculations: Electron-Phonon Coupling

Bandstructure



Phonon dispersion



Conservation of energy & momentum

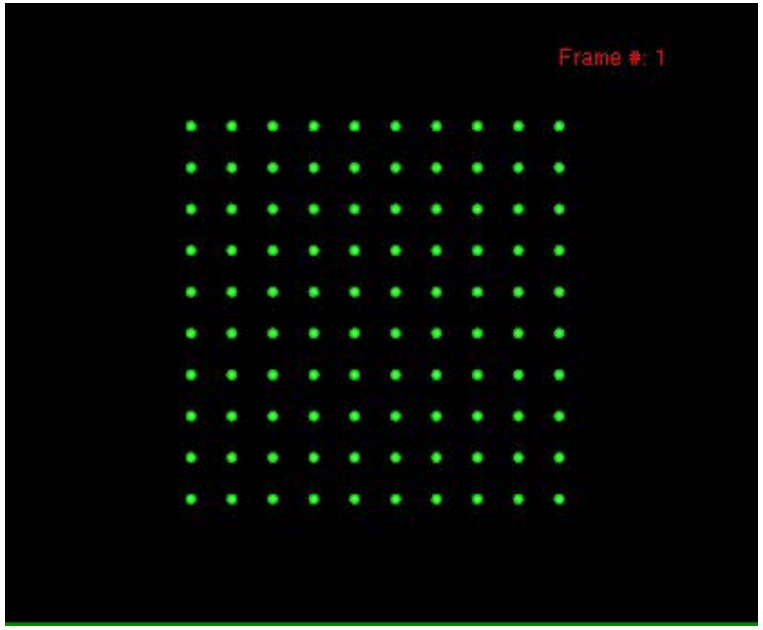
Coupling between electron states through phonon

$$\varepsilon' = \varepsilon \pm \hbar\omega \qquad k' = k \pm q$$

Search phase space of both electron & phonon

Response of charge density to phonon perturbation

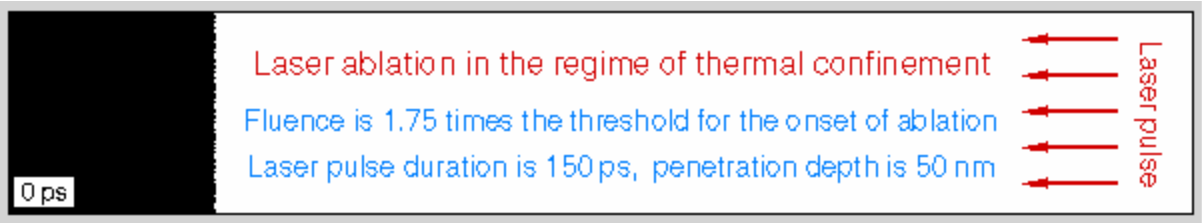
Molecular Dynamics Simulations: Trajectory



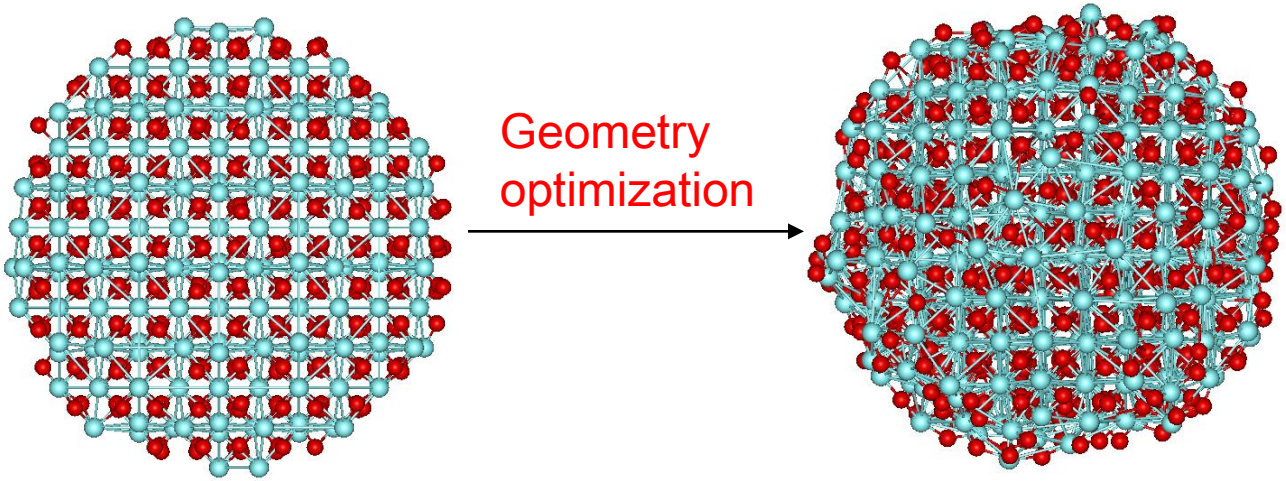
Laser ablation of metals,
Courtesy of Dr. L. V. Zhigilei
at University of Virginia.
J. Appl. Phys., 88, 1281-
1298 (2000).

Trajectory of a BCC crystal,

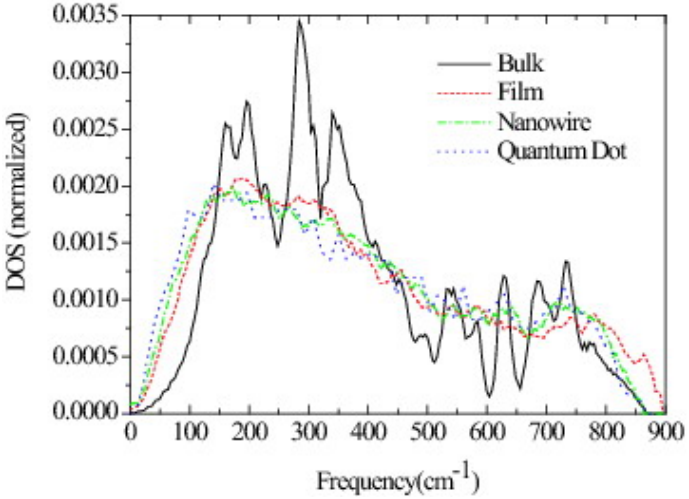
Courtesy of Dr. Sylke Boyd at UMN



Molecular Dynamics: Geometry Optimization

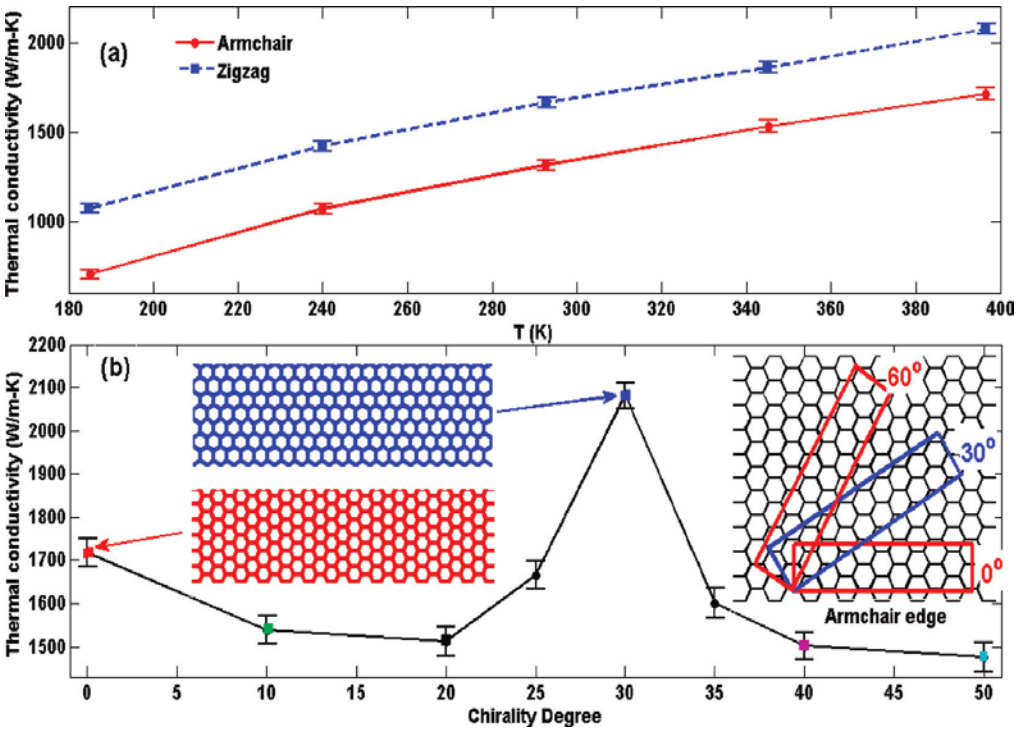


Bao and Ruan, *Phys. Rev. B*, 2008.



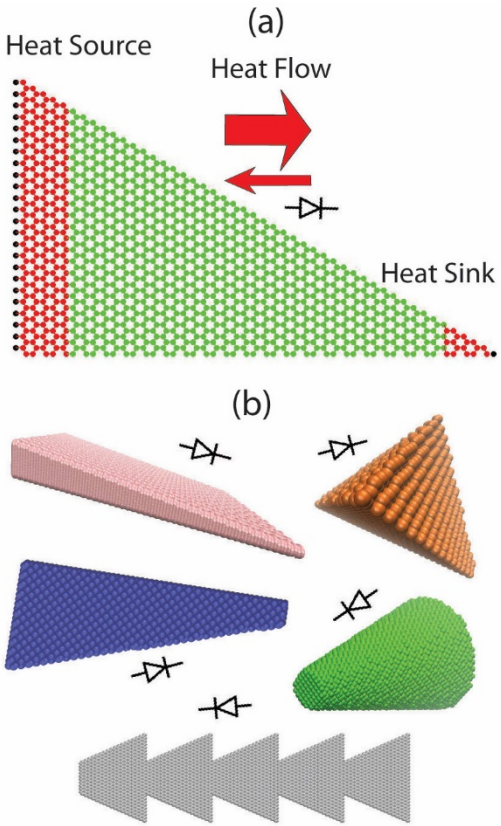
Phonon density of states

Molecular Dynamics: Thermal Conductivity



Thermal conductivity of graphene nanoribbon

Hu, Ruan, and Chen, *Nano Letters*, 2009.



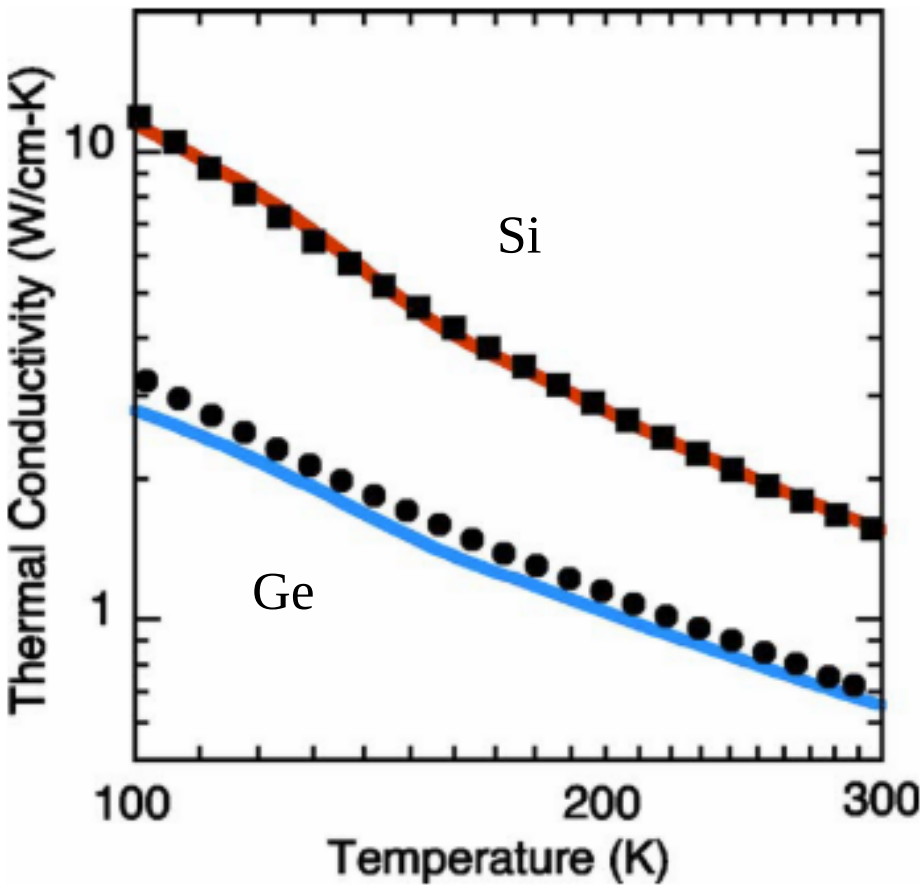
Thermal rectification

Wang, Vallabhaneni, Hu, Qiu, Chen, and Ruan, *Nano Letters*, 2014.

Boltzmann transport equation: *k*

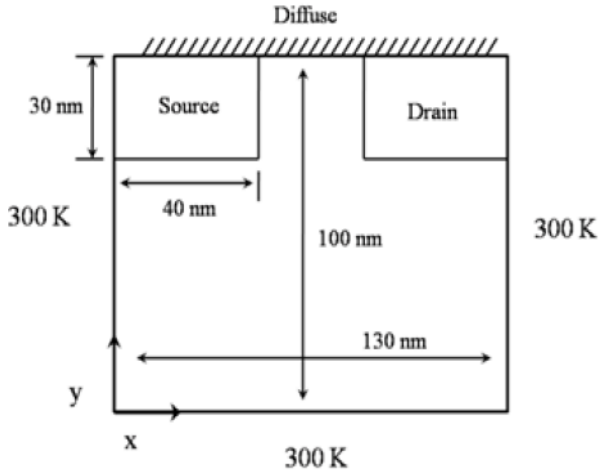
$$k_x = \frac{1}{V}\sum_\lambda c_\lambda v_{\lambda,x}^2 \boxed{\tau_\lambda}$$

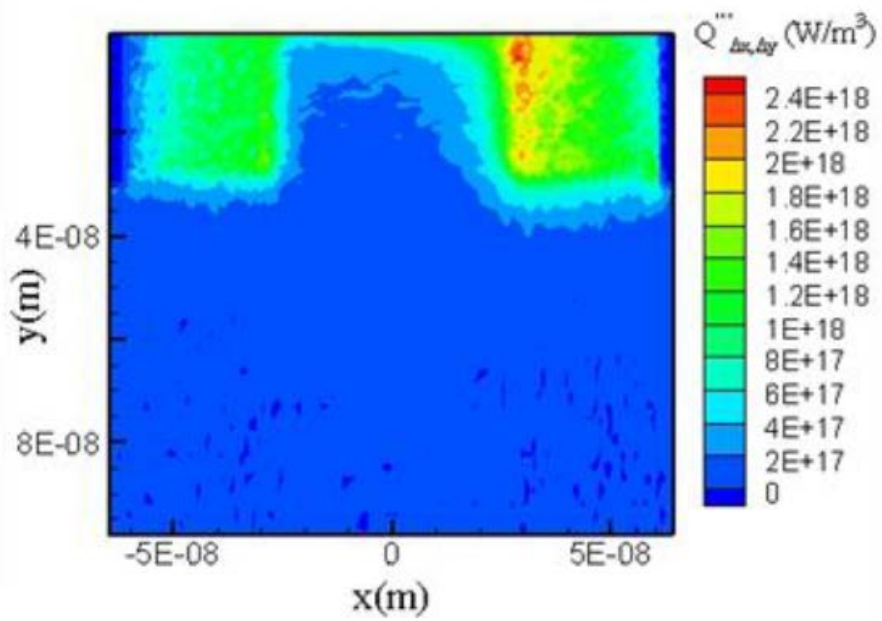
τ can be from MD or first principles

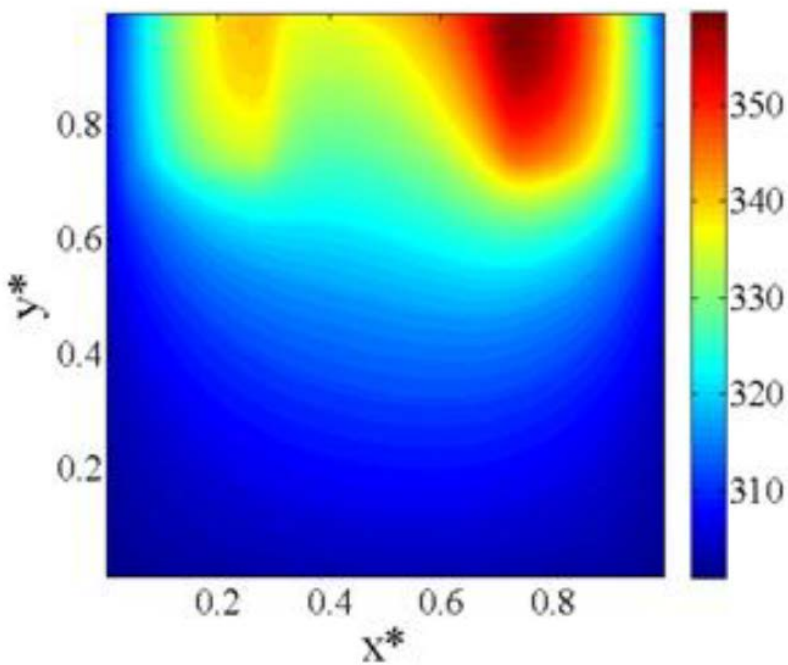


Broido, Malorny, Birner, Mingo, and Stewart, APL (2007).

Boltzmann transport equation: T distribution







J. Loy, D. Singh and J. Murthy, IHTC 2010