Vibrationally Accurate Interatomic Potentials

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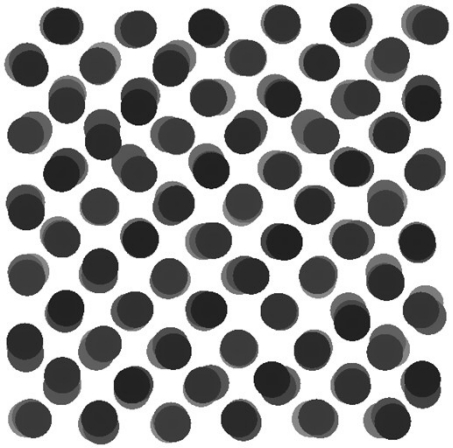
Modes (Phonons) & MD Simulations

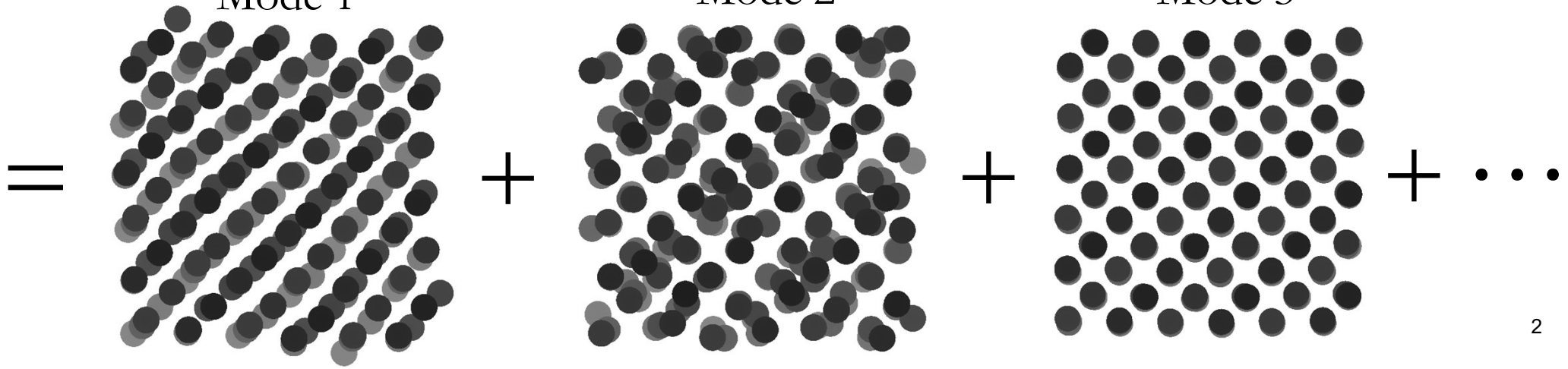


Heat flux Q

Thermal conductivity $\kappa \propto \int_0^\infty \langle Q(0)Q(t)\rangle dt$

$\kappa = \kappa_{mode,1} + \kappa_{mode,2} + \kappa_{mode,3} + \cdots$

Mode 1 Mode 2 Mode 3

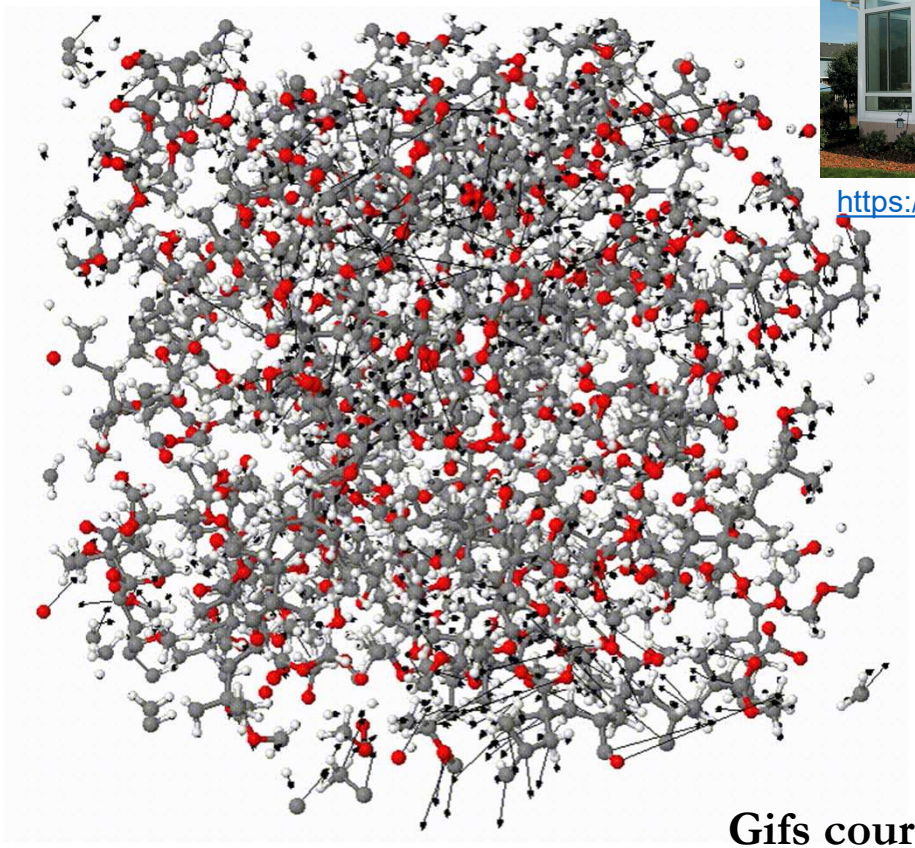


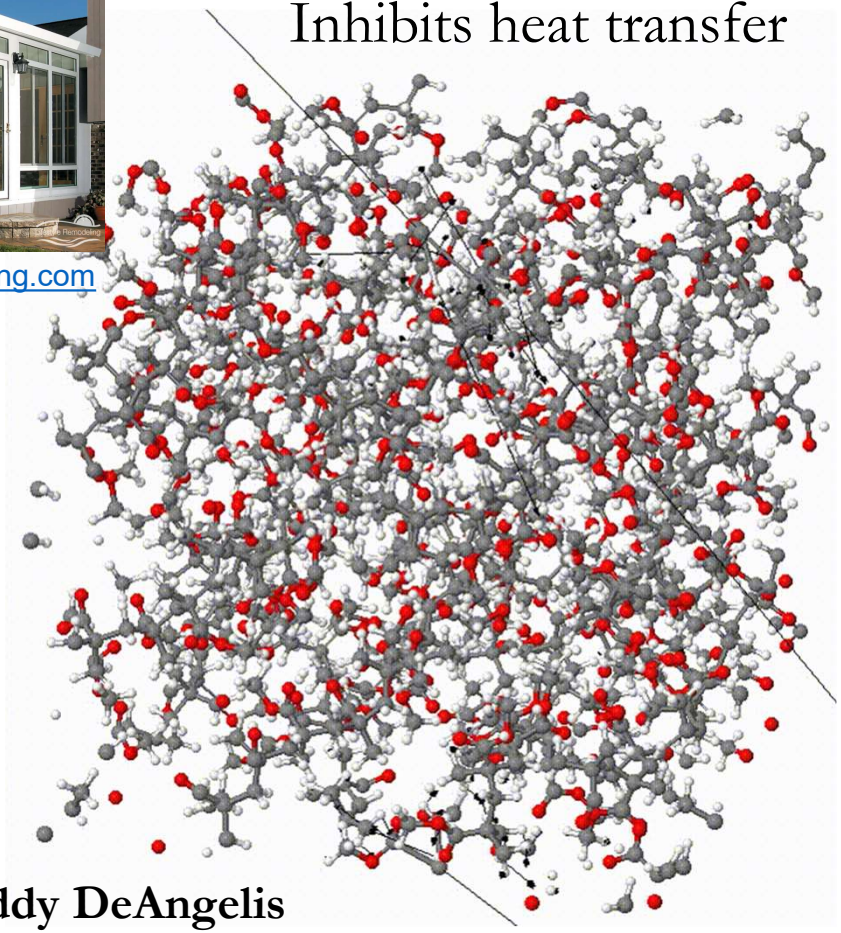
Vibrational Modes & Heat Transfer

Aids heat transfer

https://lifestyleremodeling.com

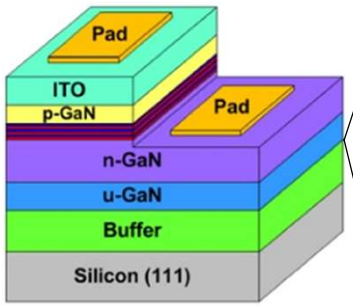
Inhibits heat transfer



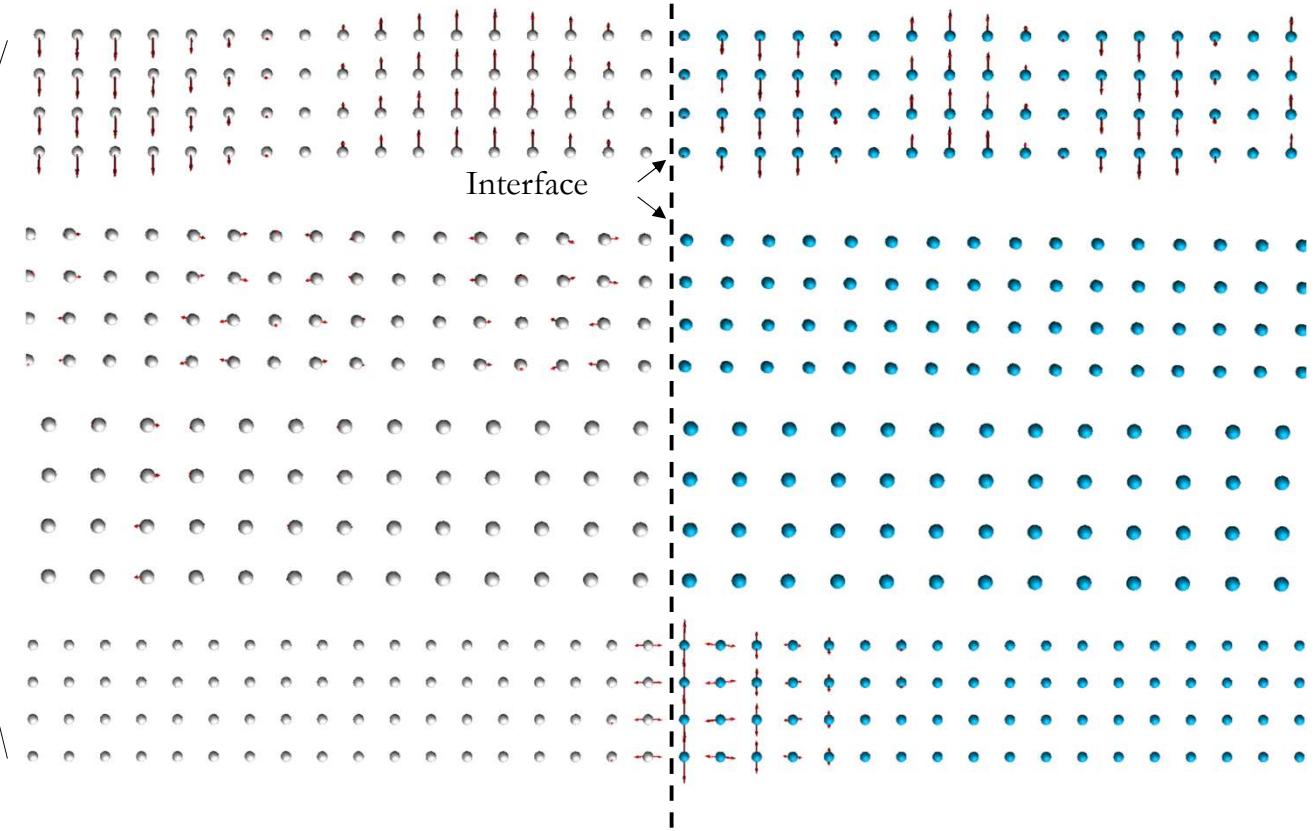


Gifs courtesy of Freddy DeAngelis

Modes at Interfaces



Z. J. Liu, T. et al, Monolithic Integration of Algan/Gan Hemt on Led by Mocvd, IEEE Electron Device Letters, **35**, 330-332 (2014).



Extended Modes

Partially Extended Modes

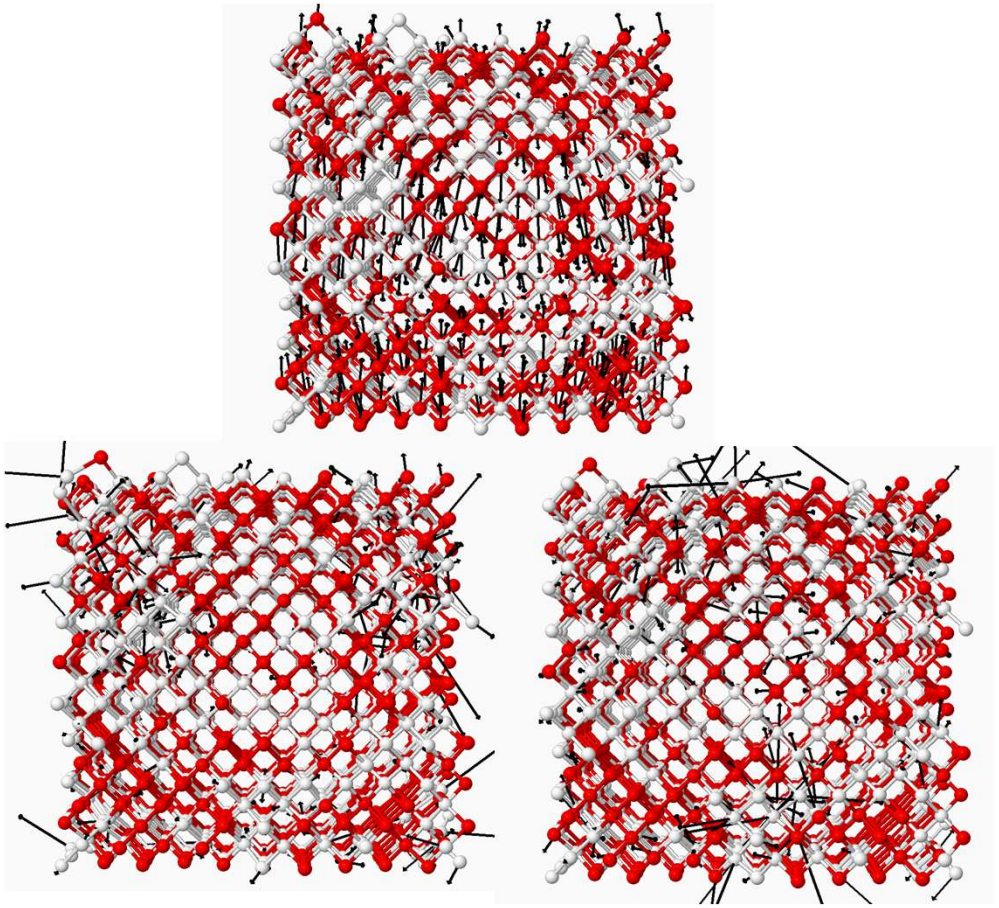
Isolated Modes

Interfacial Modes

Gifs courtesy of Kiarash Gordiz

Modes & Energy Conversion

Thermoelectric generator

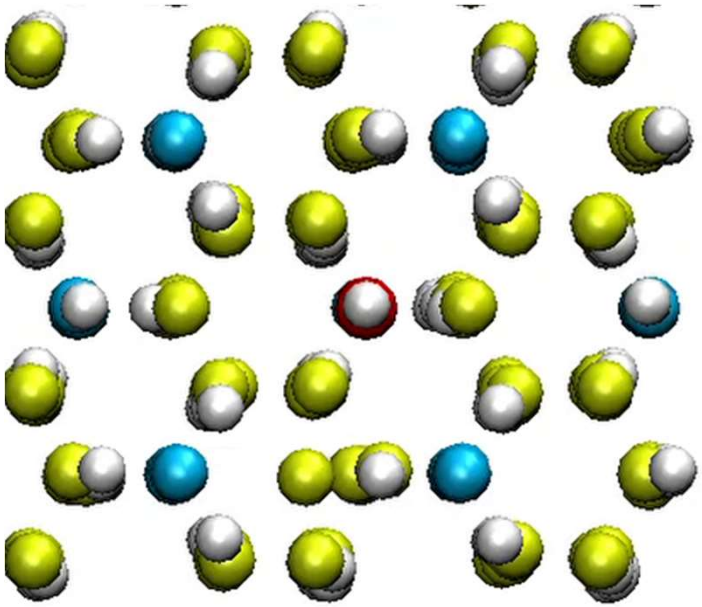


B. Yu et al, Enhancement of Thermoelectric Properties by Modulation-Doping in Silicon Germanium Alloy Nanocomposites, Nano letters, **12**, 2077-2082 (2012).

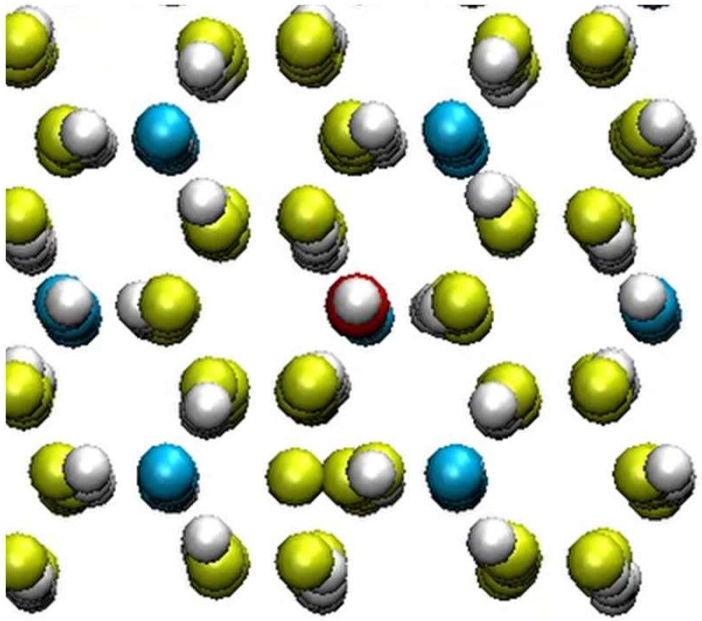
Gifs courtesy of Hamid Seyf

Modes Make Things Happen

MD @ T=300K



MD @ T=300K + energy input to a few selected modes



Li

P

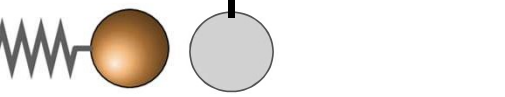
O

Ge

Movies courtesy of Kiarash Gordiz

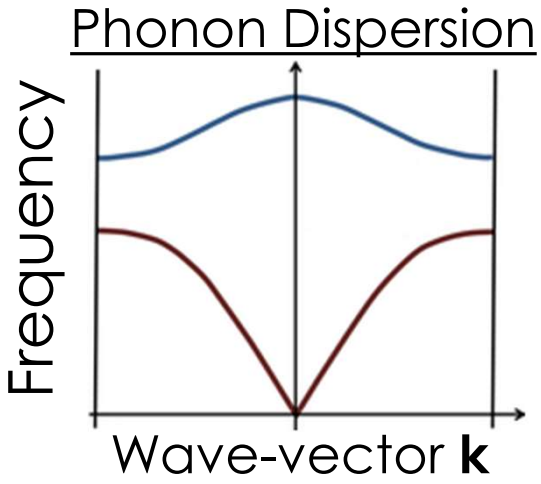
Phonon Theory

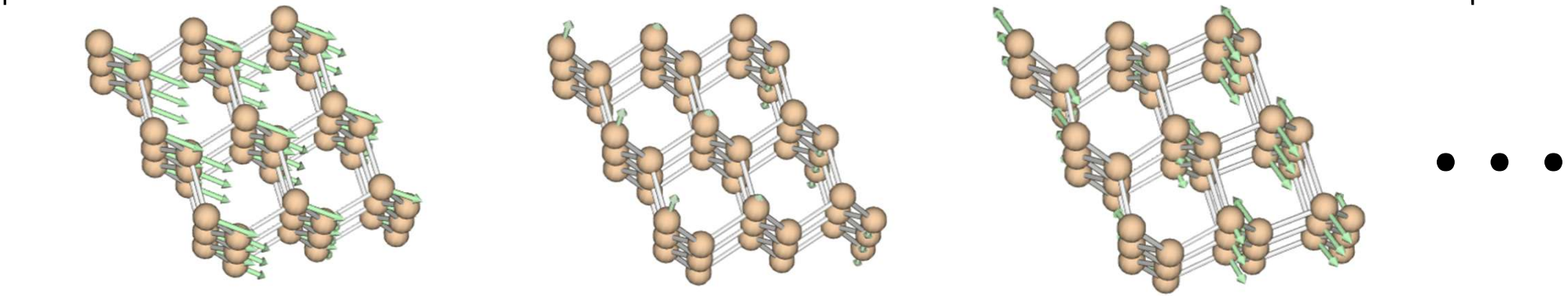
$u_i = x_i - x_i^{equilibrium}$



Mass X Acceleration = Harmonic Force

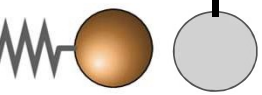
$$m_i \ddot{u}_i = -\sum_j K_{ij} u_j$$





Taylor Expansion Potential

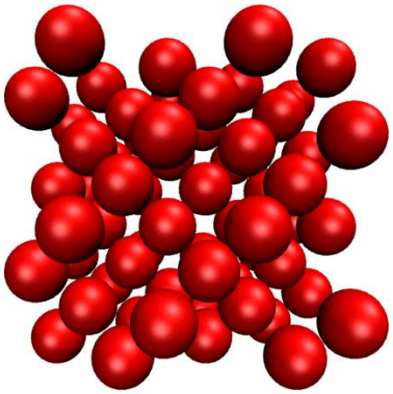
$$u_i = x_i - x_i^{equilibrium}$$



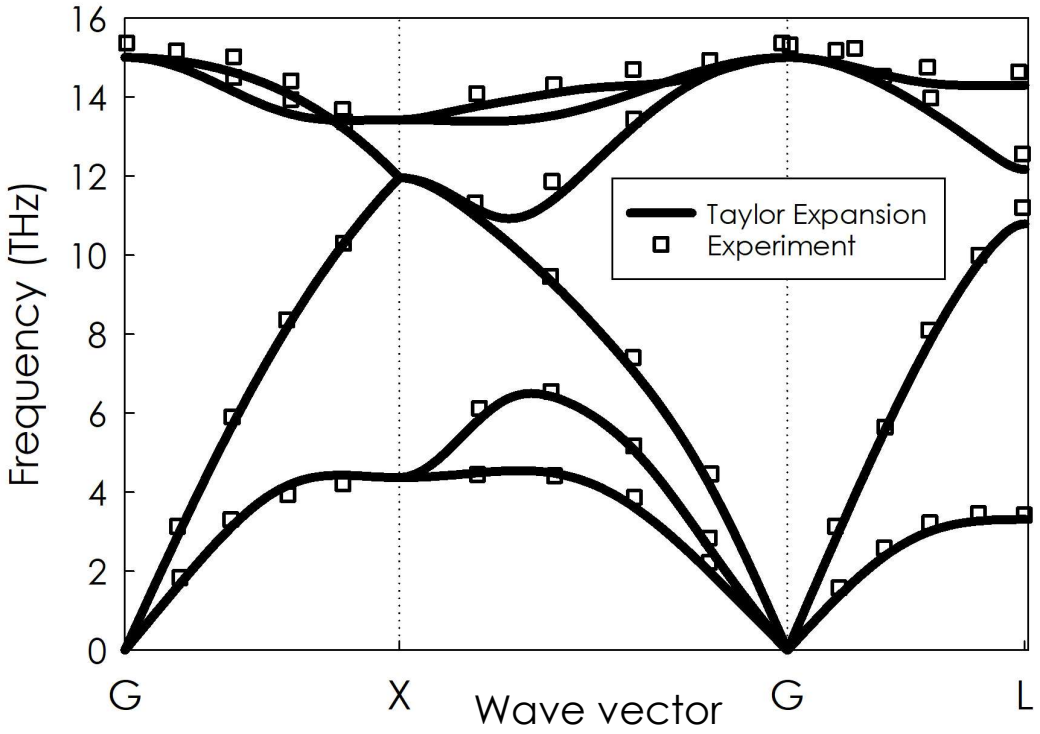
$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + \frac{1}{3!}\sum_{ijk} K_{ijk} u_i u_j u_k + \ldots$$

$$K_{ij} = \frac{\partial^2 E}{\partial u_i \partial u_j}$$

$$K_{ijk} = \frac{\partial^3 E}{\partial u_i \partial u_j \partial u_k}$$



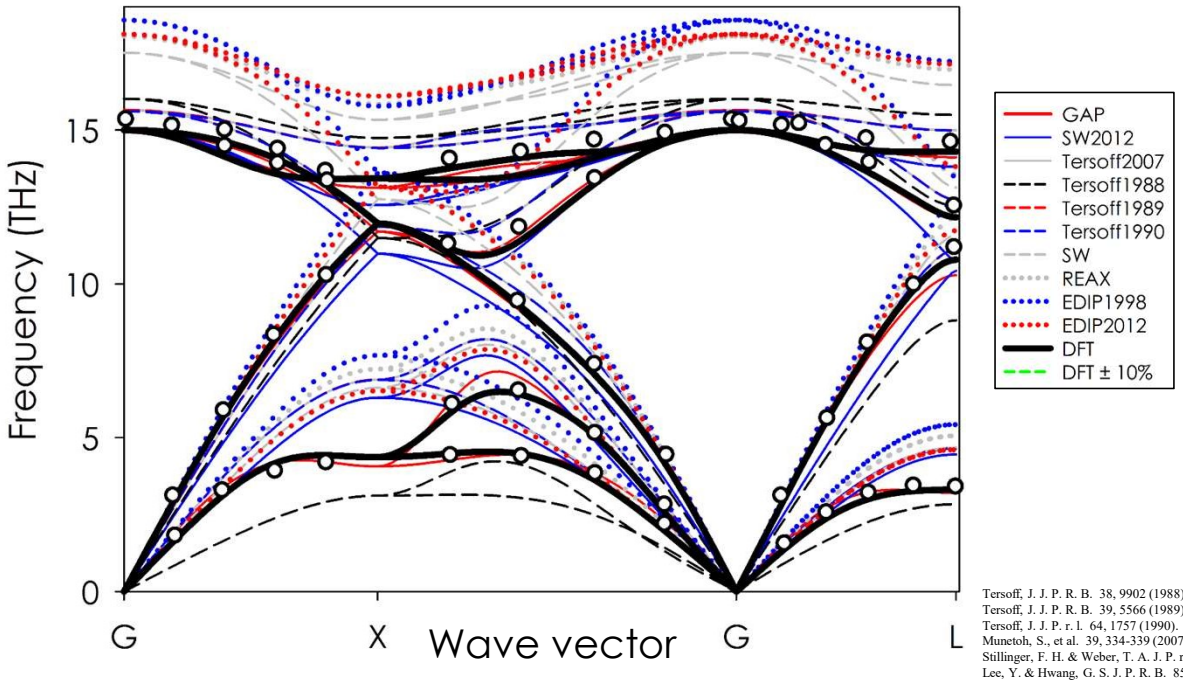
Silicon Phonon Dispersion



W.Weber, Phys. Rev .B 15, 4789 (1977).

Current Potentials

Silicon Phonon Dispersion



Tersoff, J. J. P. R. B. 38, 9902 (1988).
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Munetoh, S., et al. 39, 334-339 (2007).
Stillinger, F. H. & Weber, T. A. J. P. r. B. 31, 5262
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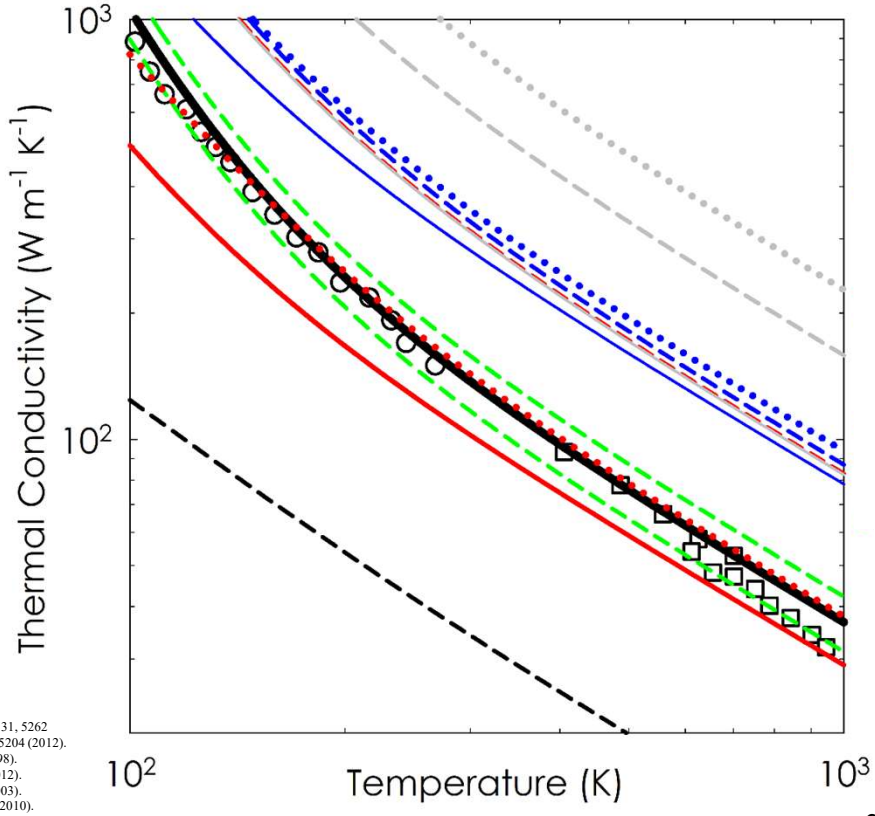
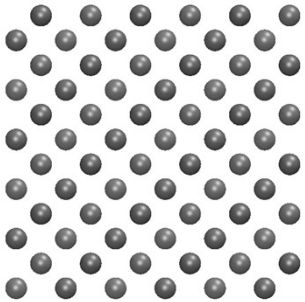
Jiang, C et al. I. J. P. R. B. 86, 144118 (2012).
Van Duin, A. C. et al. 107, 3803-3811 (2003).
Bartók, A. P. et al. J. P. r. l. 104, 136403 (2010).
W.Weber, Phys. Rev .B 15, 4789 (1977).

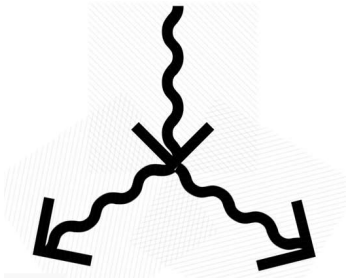
Silicon Thermal Conductivity



The "Phonon Potential"

$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + E_{anharmonic}$$





Morse

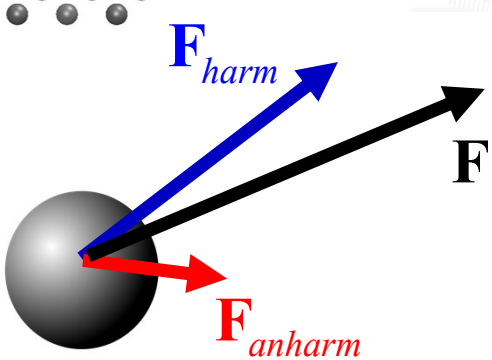
$$E = \lambda_1\left[1-\exp\left(-\lambda_2\left(r-\lambda_3\right)\right)\right]^2$$

3-body

$$E = \lambda_1\left(\theta-\theta_0\right)^2 + \lambda_2\left(\theta-\theta_0\right)^3 + \cdots$$

SNAP

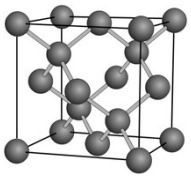
$$E = \beta_0 + \sum_k \beta_k B_k$$



$$\mathbf{F} = \mathbf{F}_{harm} + \mathbf{F}_{anharm}$$

https://github.com/rohskopf

Silicon

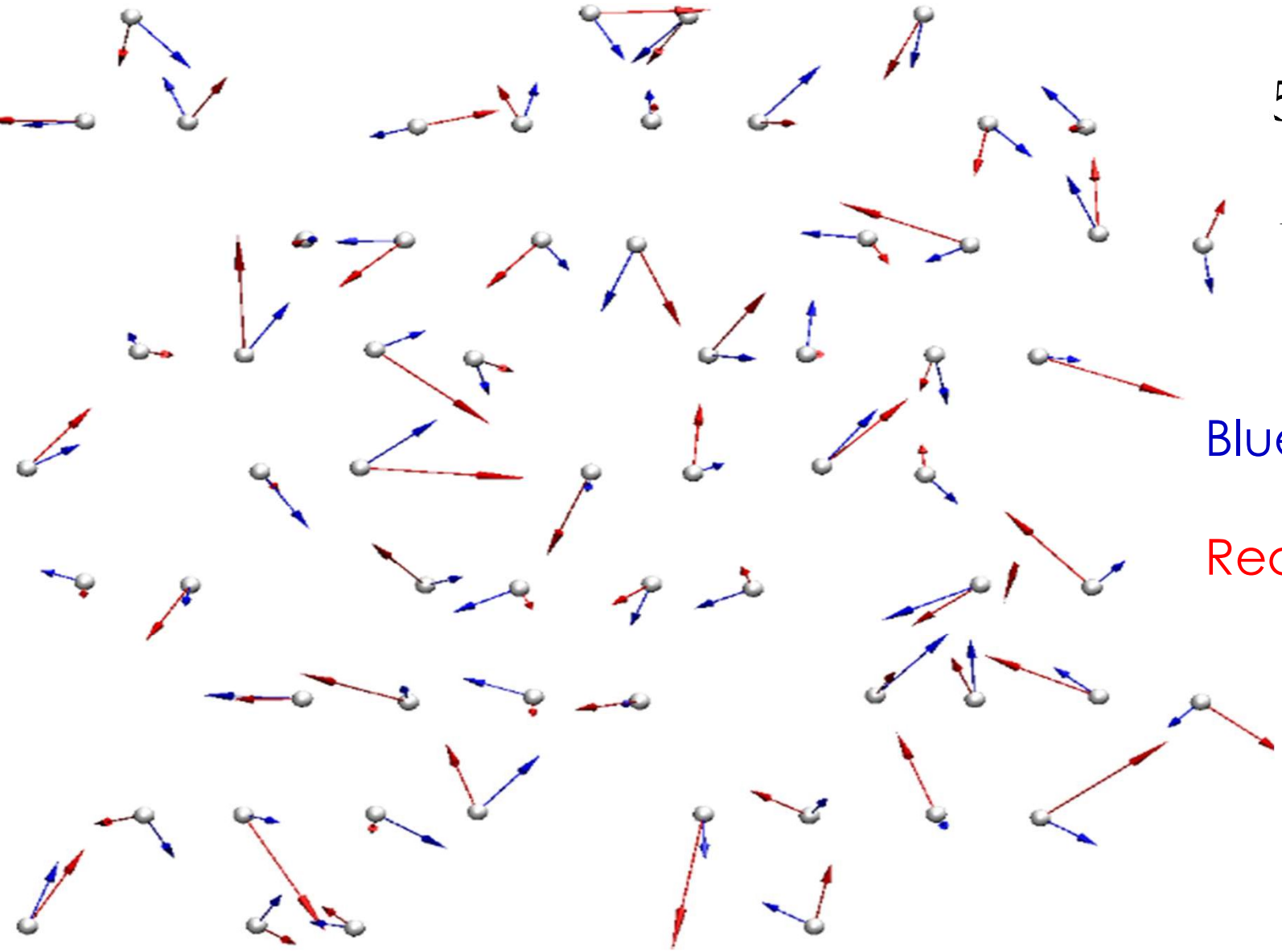


$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + \lambda_1 \left[1 - \exp\left(-\lambda_2 \left(r - \lambda_3\right)\right)\right]^2 + \lambda_4 \left(\theta - \theta_0\right)^2$$

Harmonic part fit with least squares

Anharmonic part fit with genetic algorithm

https://github.com/rohskopf

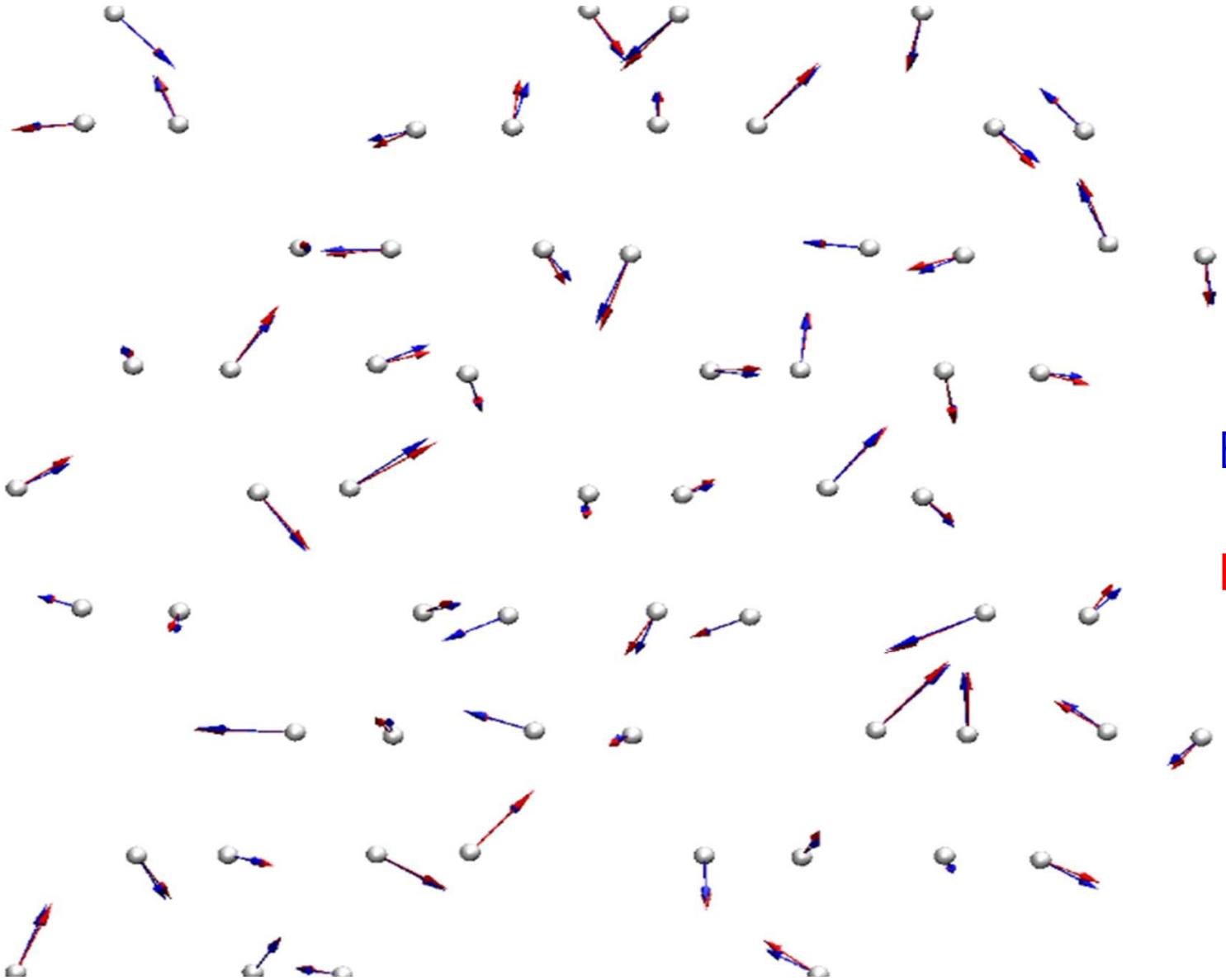


50 % force error

$$Error = \sum \frac{\left|\mathbf{F}_{DFT} - \mathbf{F}_{potential}\right|}{\left|\mathbf{F}_{DFT}\right|}$$

Blue: DFT force

Red: Potential force



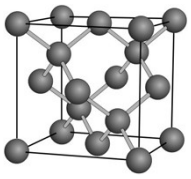
3 % force error

$$Error = \sum \frac{\left|\mathbf{F}_{DFT} - \mathbf{F}_{potential}\right|}{\left|\mathbf{F}_{DFT}\right|}$$

Blue: DFT force

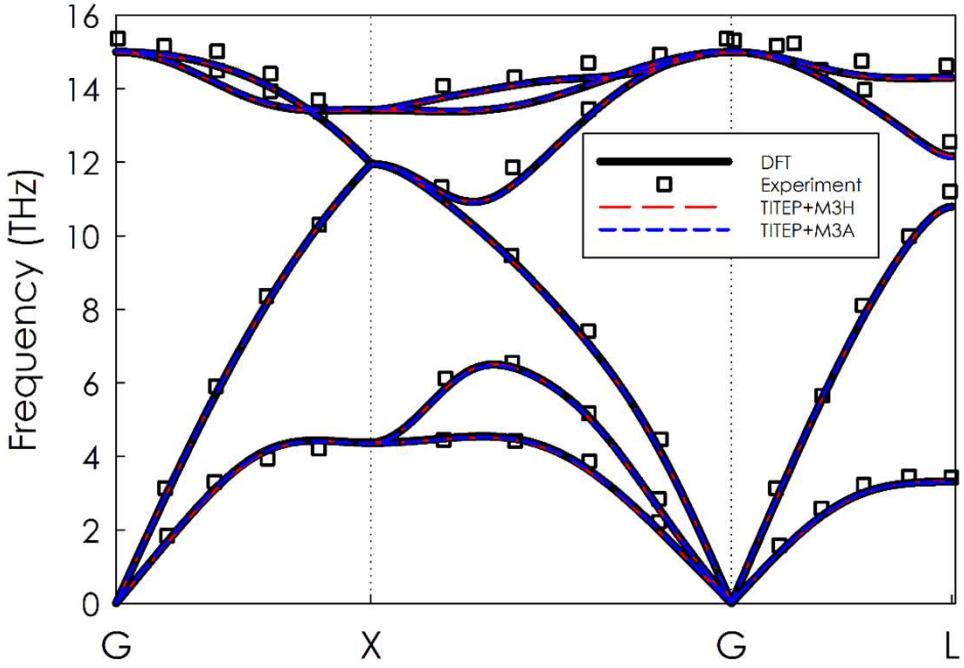
Red: Potential force

Silicon

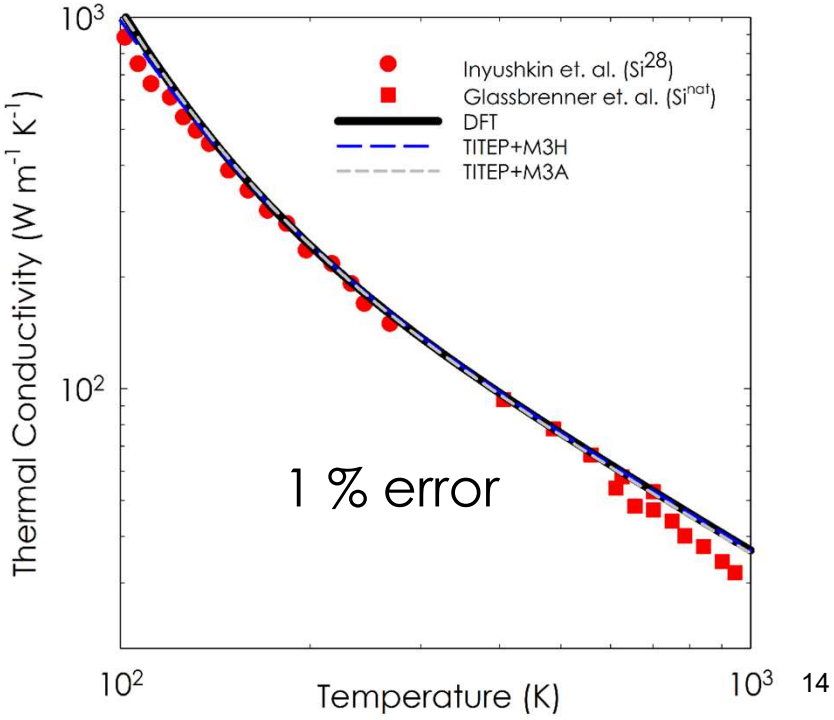


$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + \lambda_1 \left[1 - \exp\left(-\lambda_2 \left(r - \lambda_3\right)\right)\right]^2 + \lambda_4 \left(\theta - \theta_0\right)^2$$

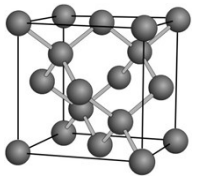
Dispersion



Thermal Conductivity

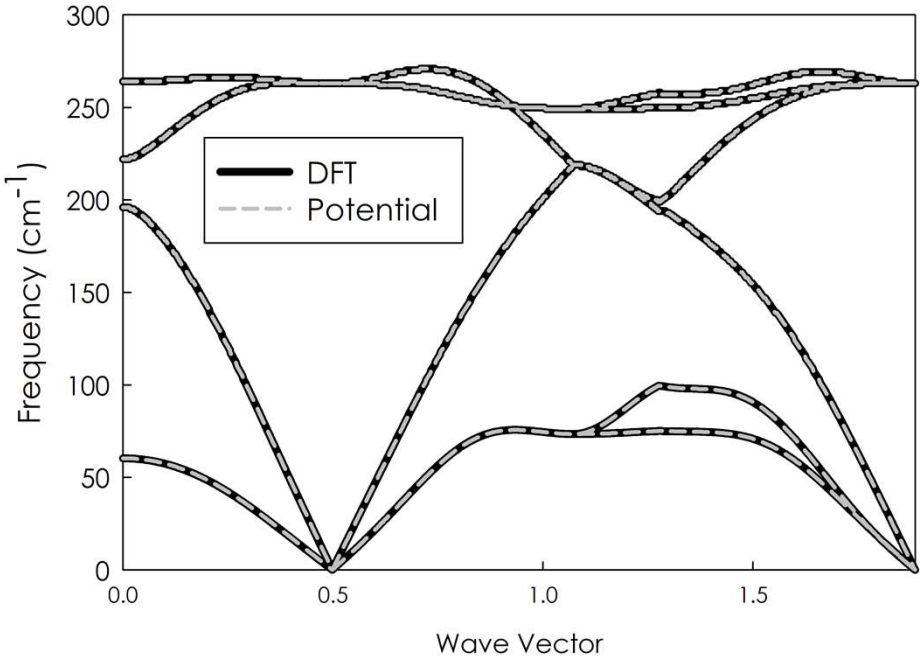


Germanium

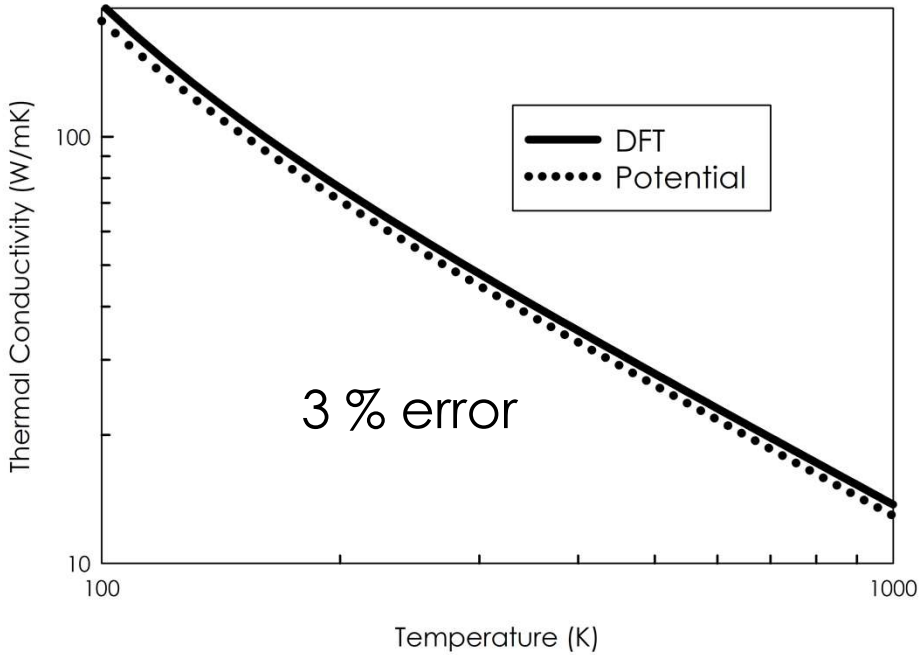


$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + \lambda_1 \left[1 - \exp\left(-\lambda_2 \left(r - \lambda_3\right)\right)\right]^2 + \lambda_4 \left(\theta - \theta_0\right)^2$$

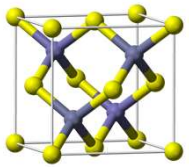
Dispersion



Thermal Conductivity

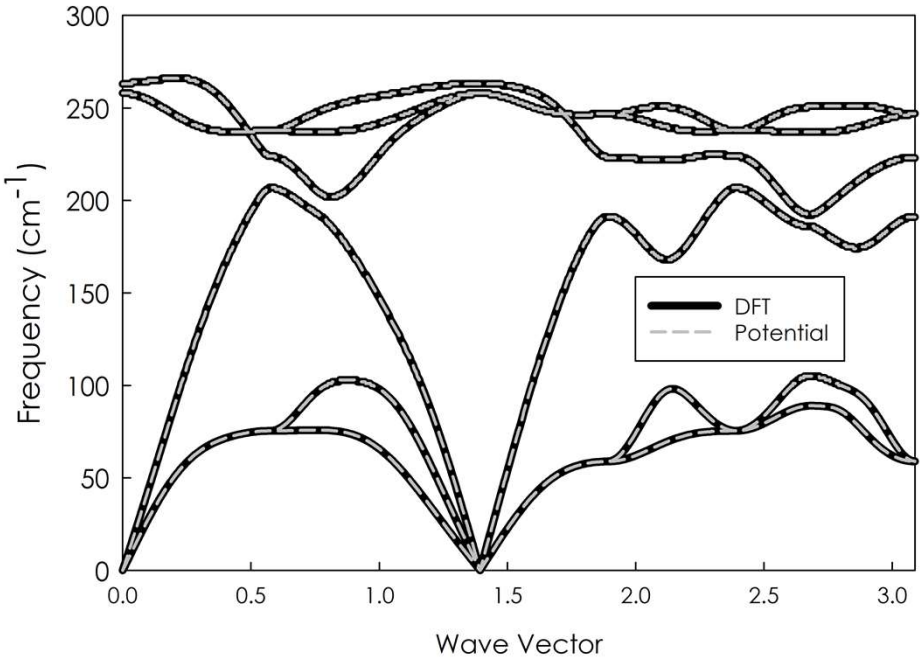


Gallium Arsenide

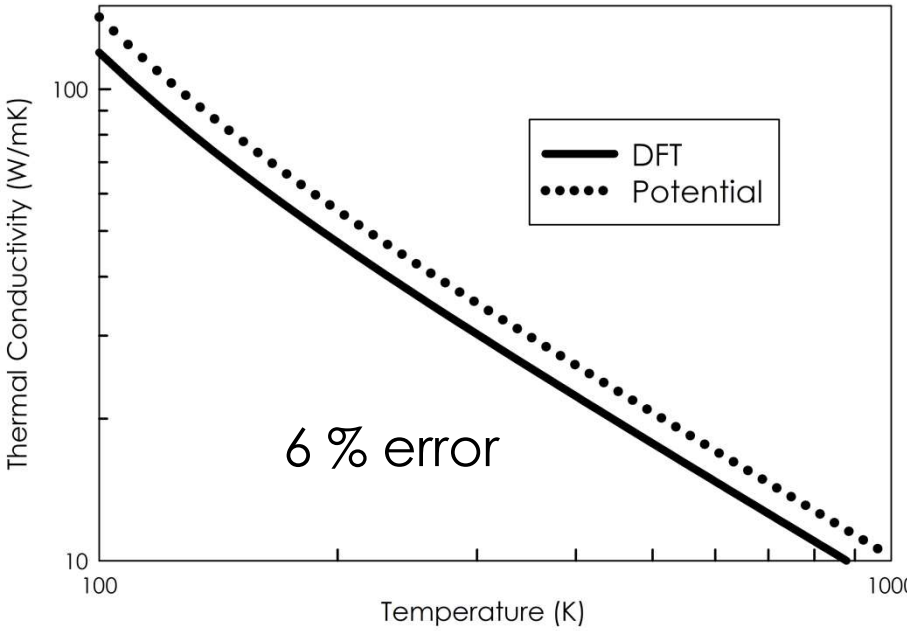


$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + \lambda_1 \left[1 - \exp\left(-\lambda_2 \left(r - \lambda_3\right)\right)\right]^2 + \lambda_4 \left(\theta - \theta_0\right)^2$$

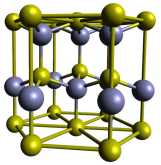
Dispersion



Thermal Conductivity

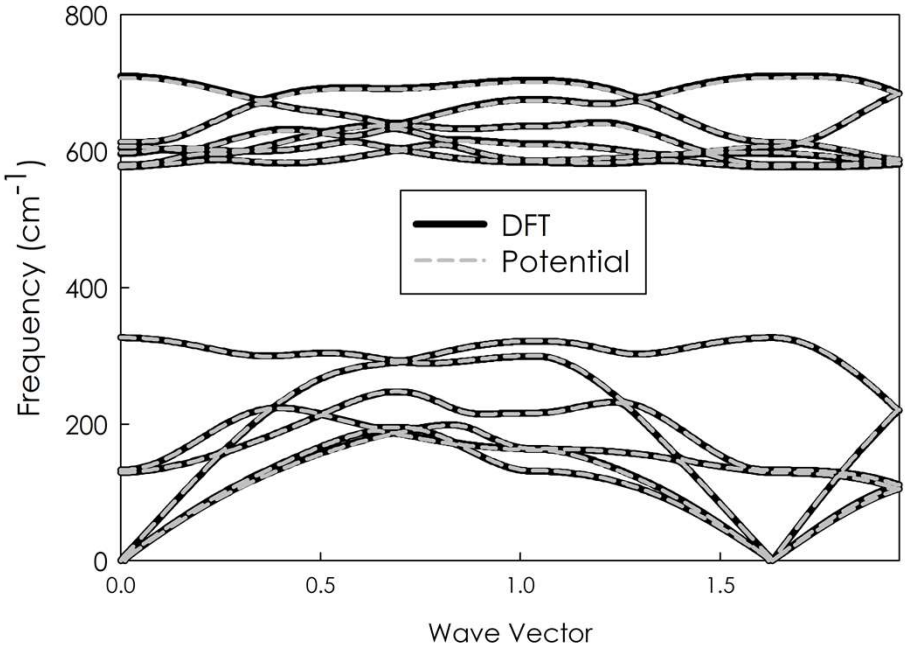


Gallium Nitride

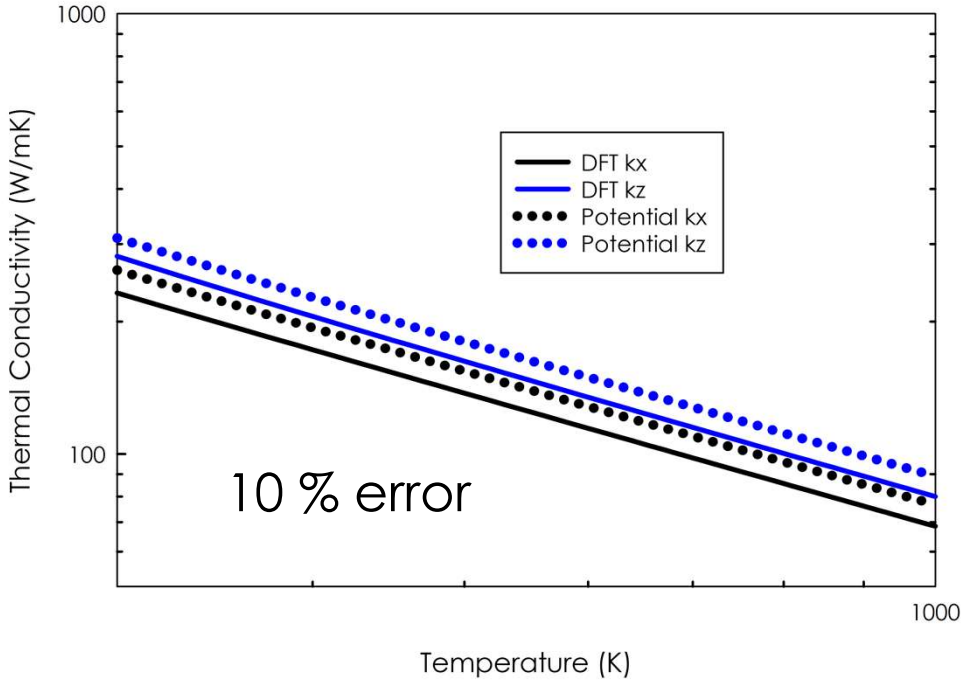


$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + \beta_0 + \sum_k \beta_k B_k \quad \text{(SNAP)}$$

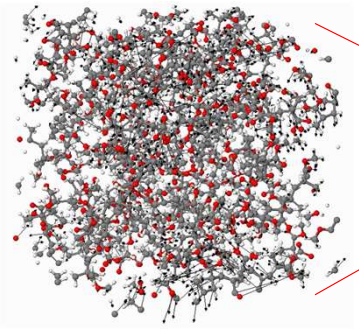
Dispersion



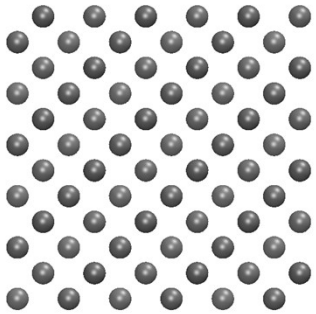
Thermal Conductivity

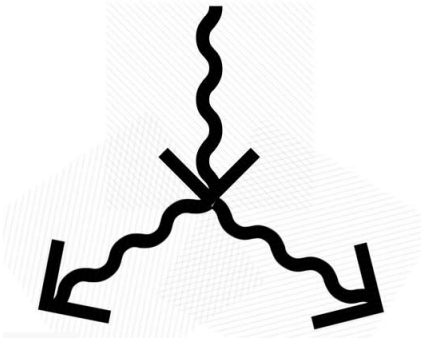


Conclusion



$$E = \frac{1}{2}\sum_{ij} K_{ij} u_i u_j + E_{anharmonic}$$





A Rohskopf, H Seyf, K Gordiz, T Tadano, A Henry. "*Empirical interatomic potentials optimized for phonon properties.*" *NPJ Computational Materials* 3 (2017)

M Muraleedharan, A Rohskopf, V Yang, A Henry. "*Phonon optimized interatomic potential for aluminum.*" AIP Advances 7 (2018)

A Rohskopf, S Wyant, A Henry. "*Fast and accurate empirical interatomic potentials for describing thermal vibrations*". In progress

OPEN-SOURCE
https://github.com/rohskopf