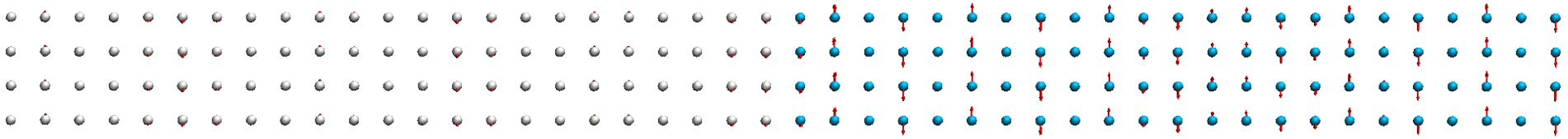
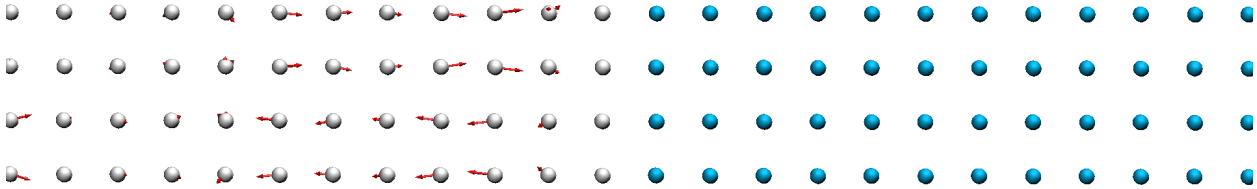
Not All Modes Propagate!

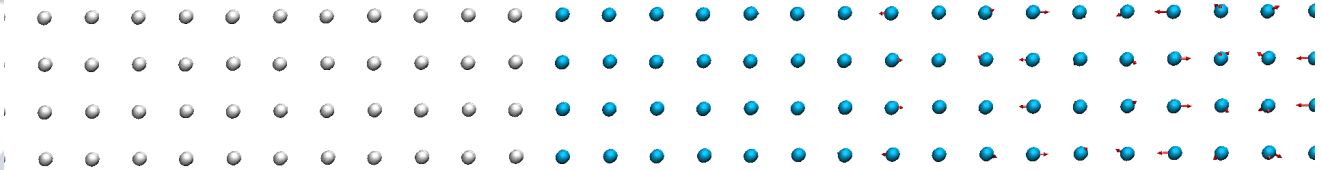
Extended Modes



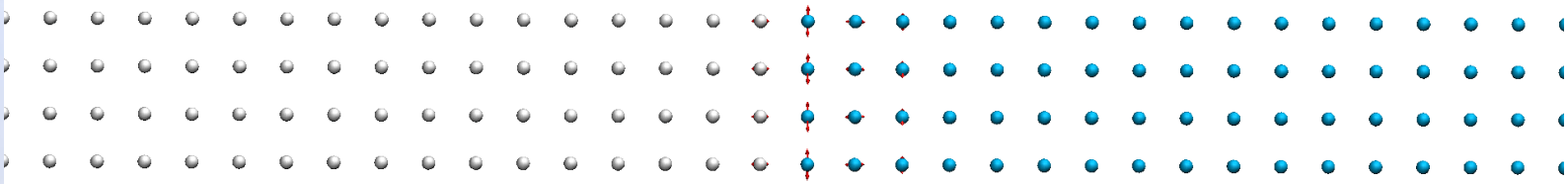
Partially Extended Modes



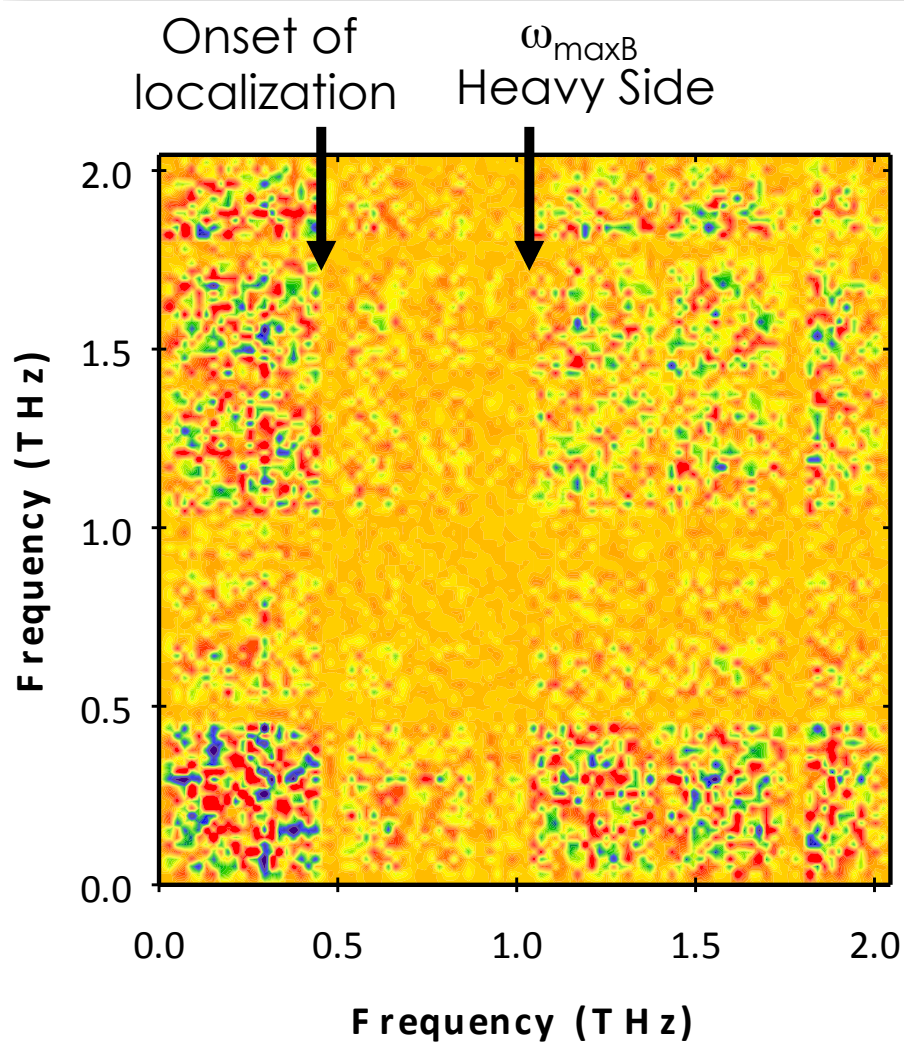
Isolated Modes

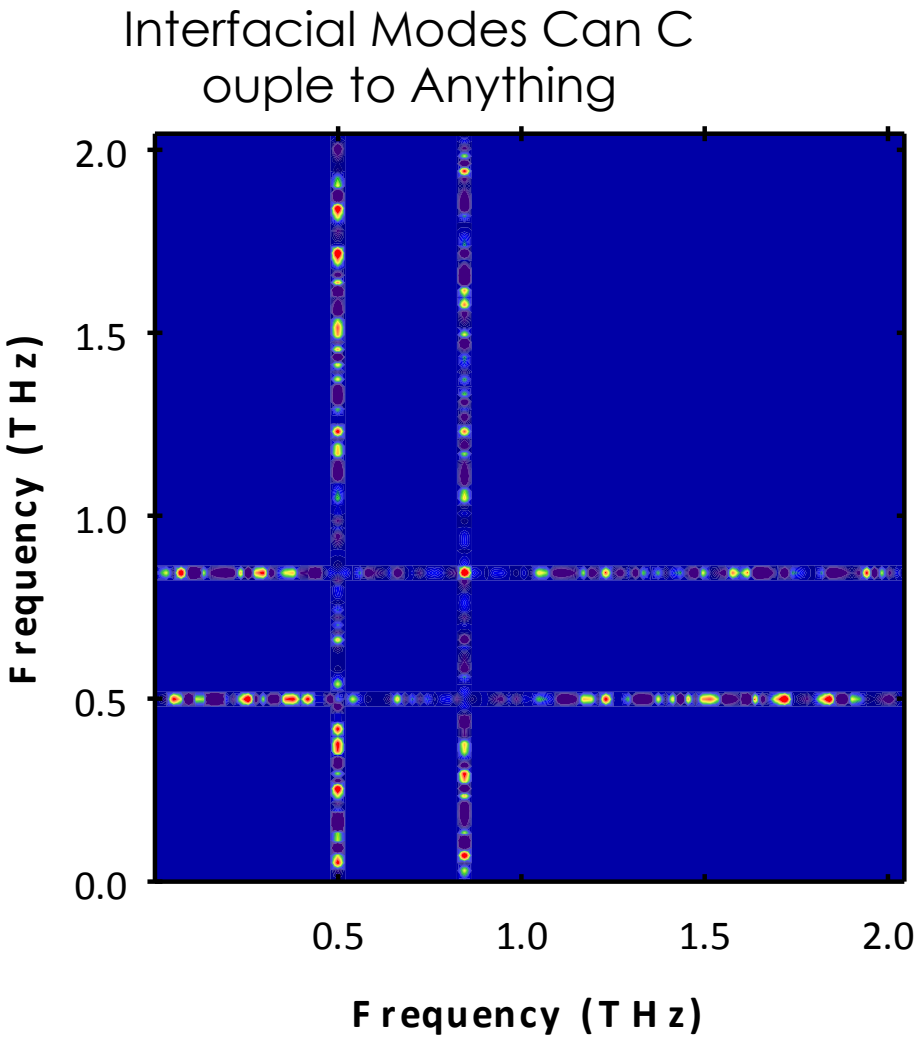


Interfacial Modes

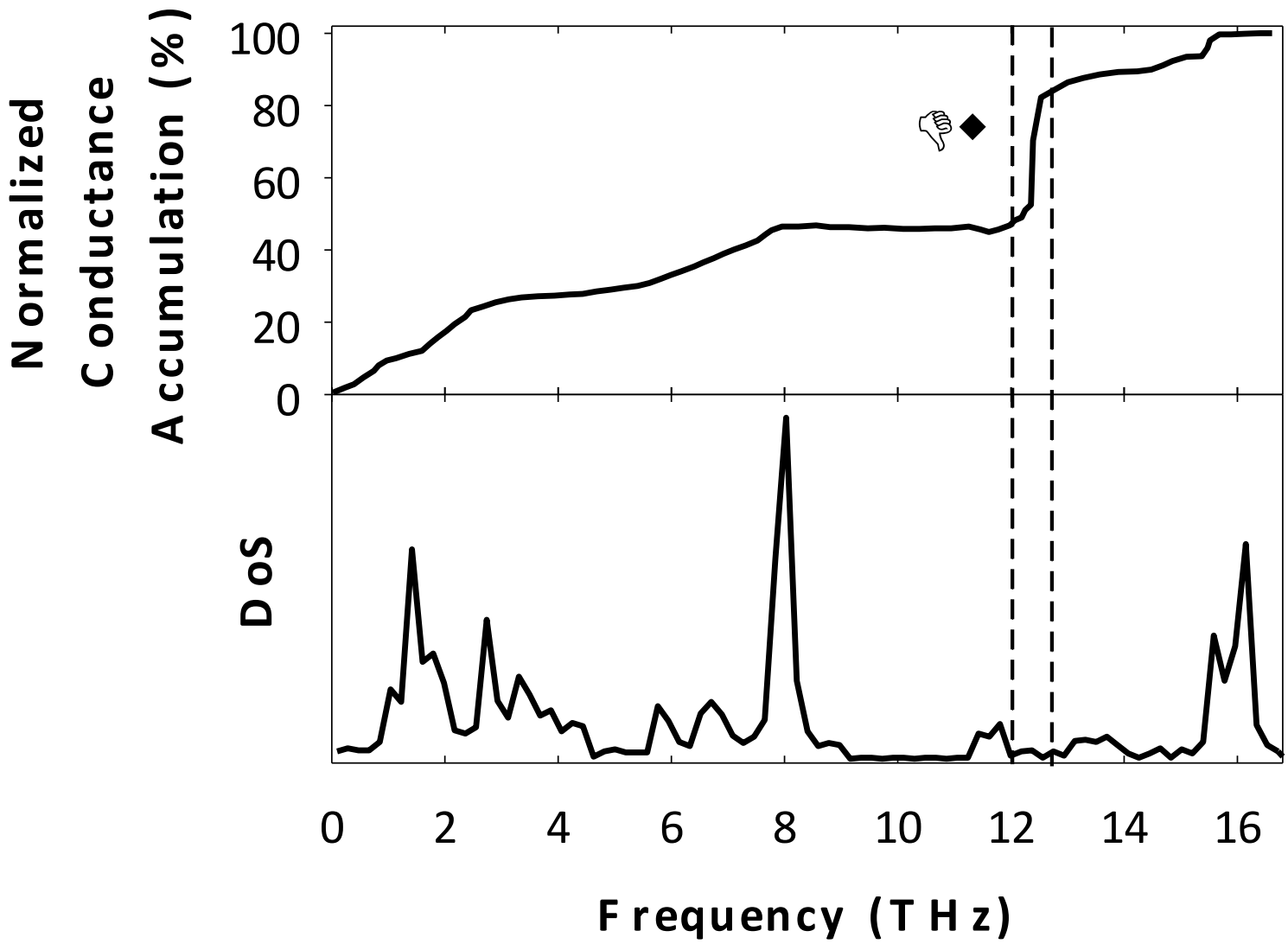


Mode-Mode Correlation

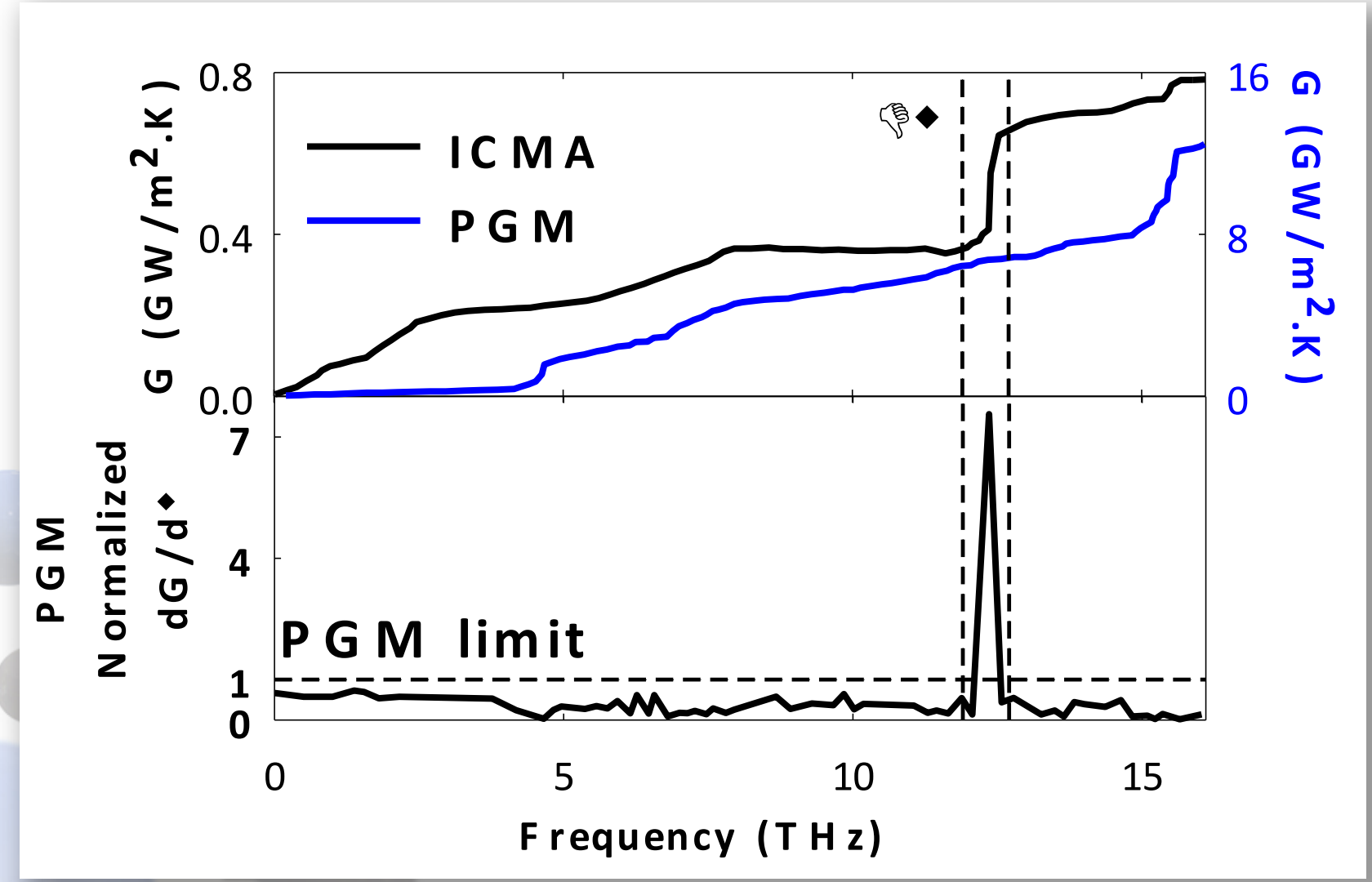




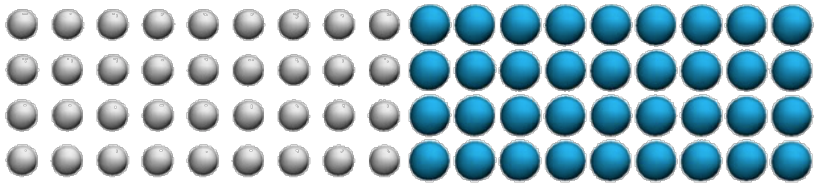
Silicon (m) : Silicon (4m)

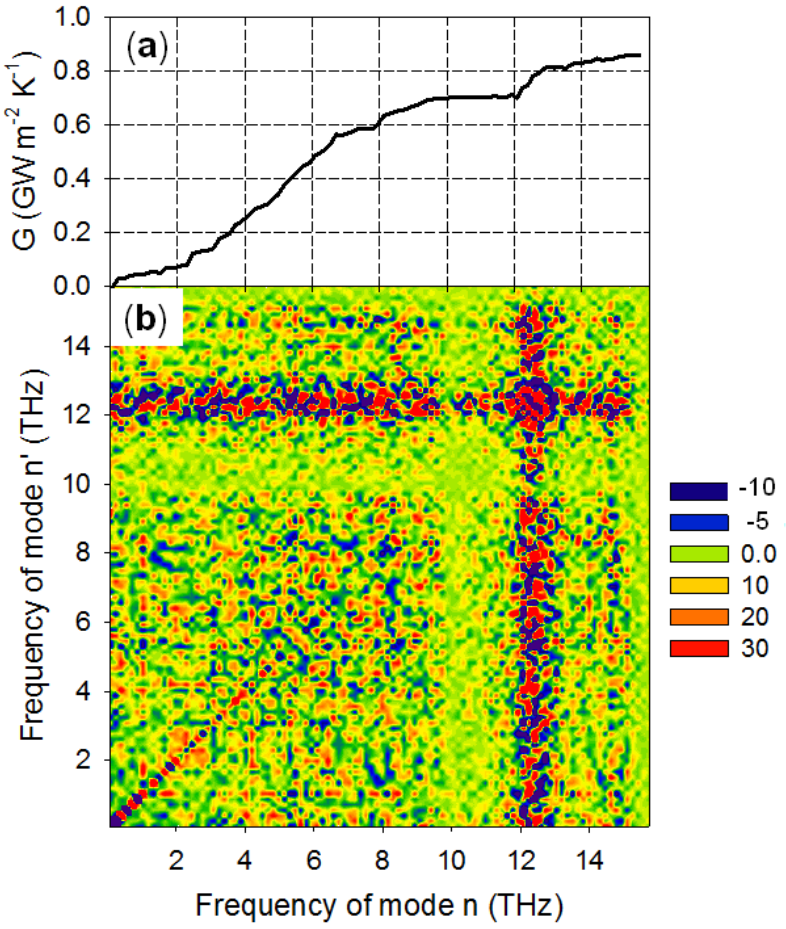


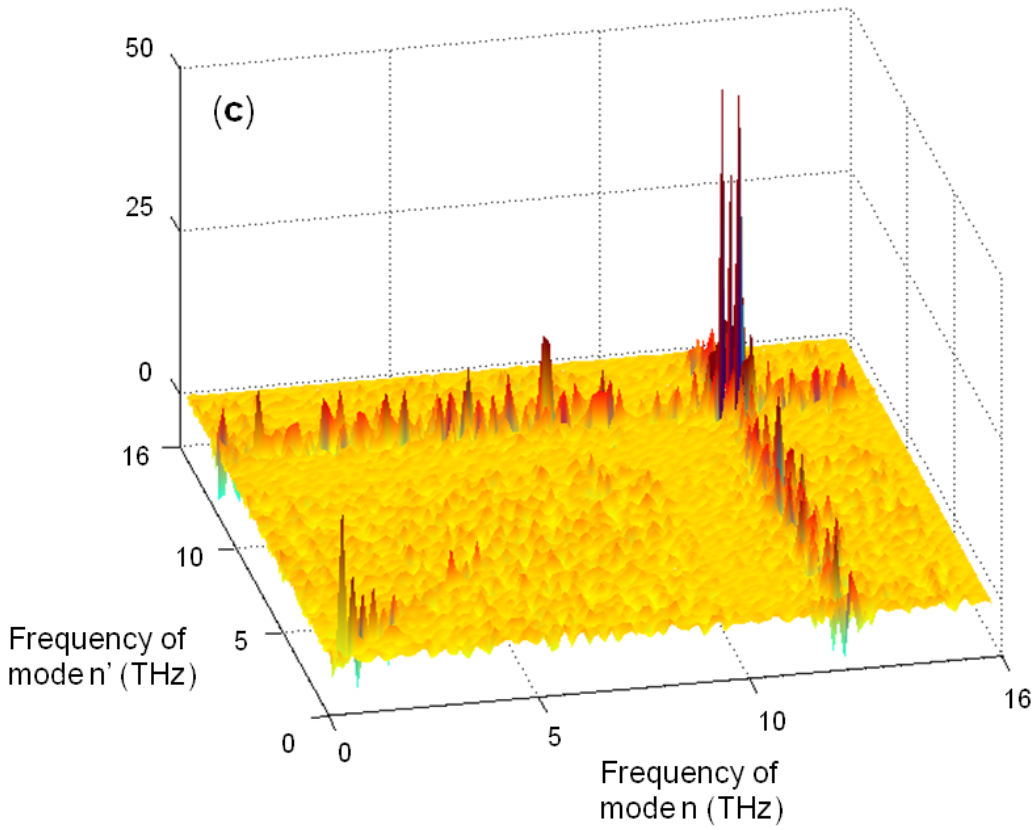
Silicon (m) : Silicon (4m)



Crystalline Si / crystalline Ge

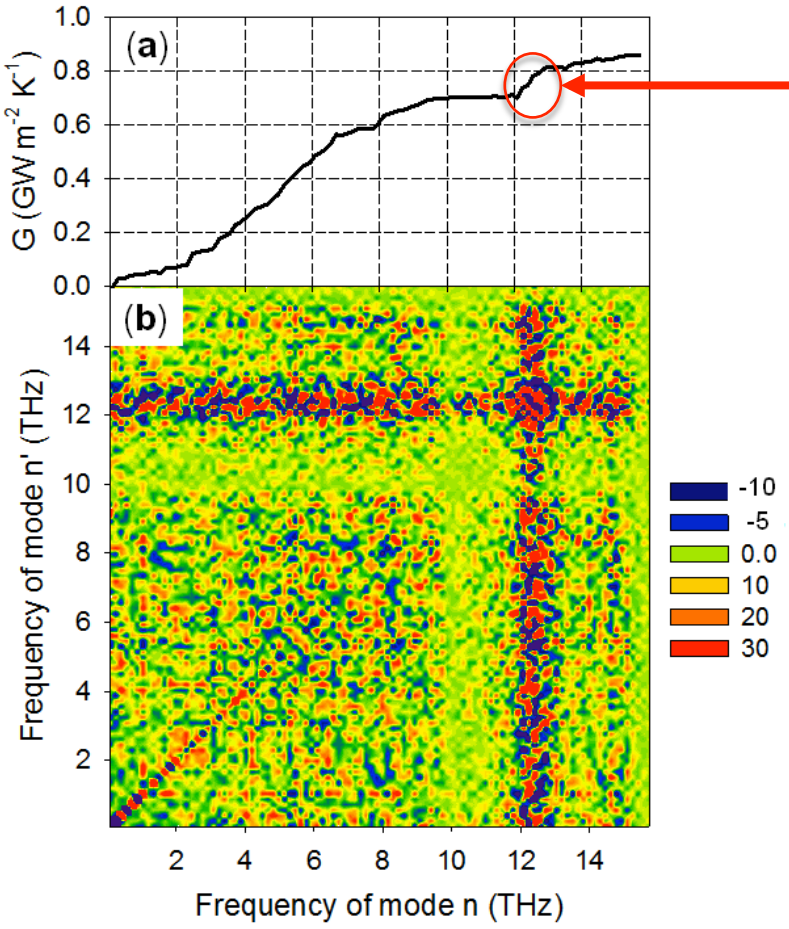


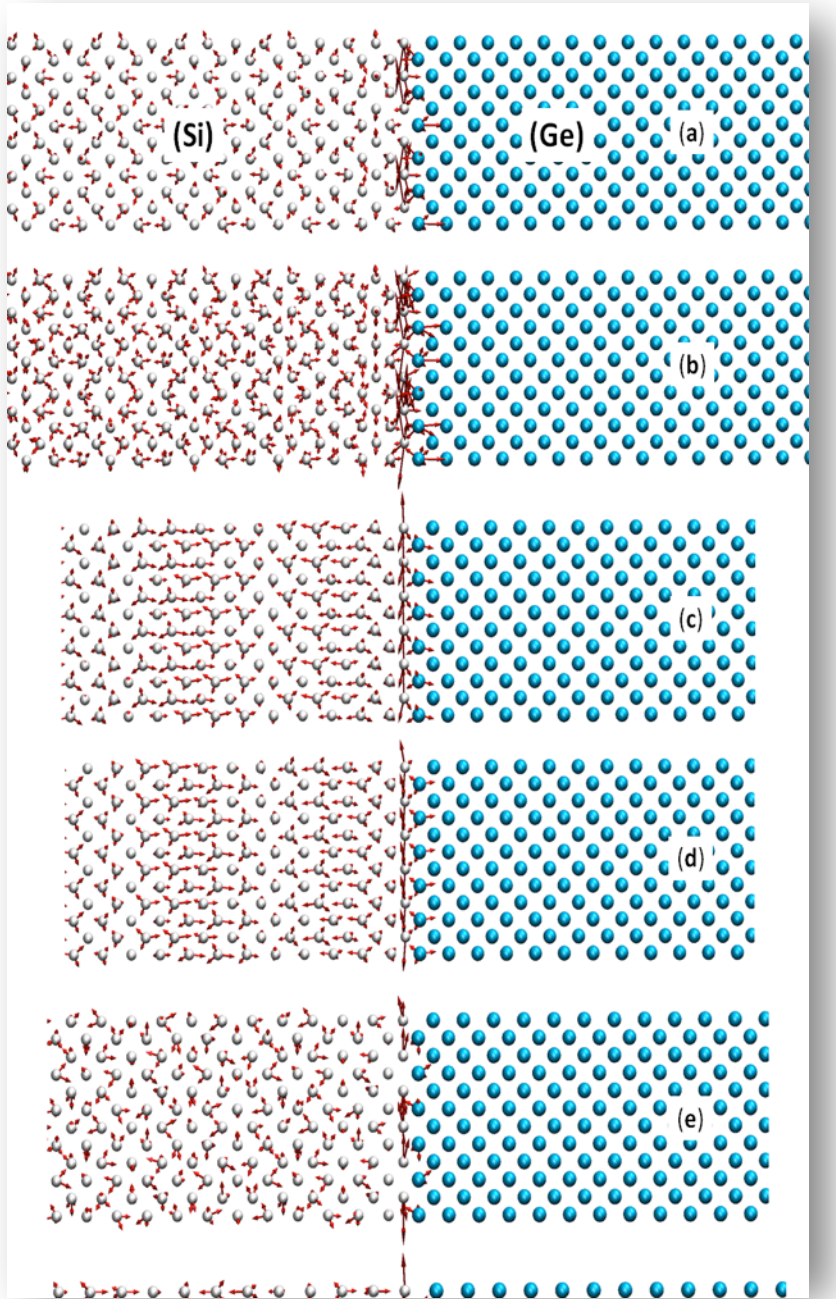




Gordiz & Henry, Sci. Rep. 6, 23139 (2016).

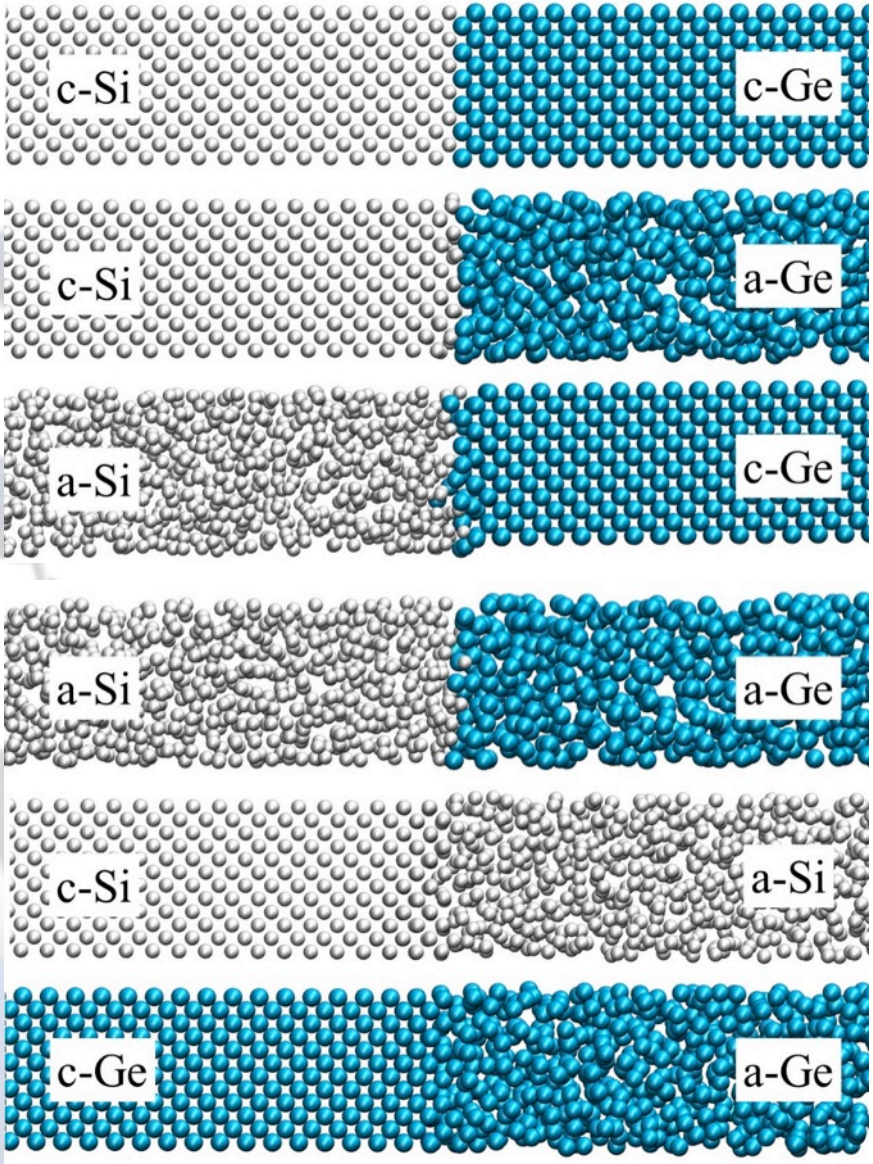
crystalline Si / crystalline Ge

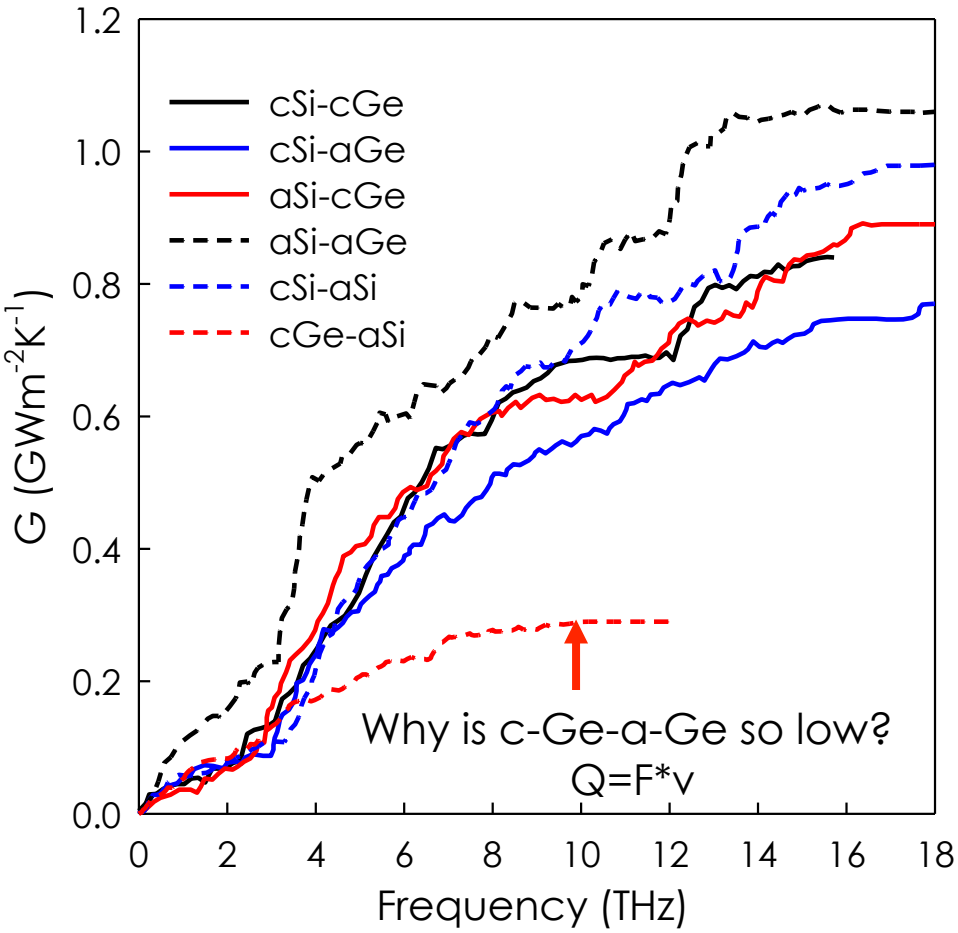




Gordiz & Henry, Sci. Rep. 6, 23139 (2016).

What About Different Phases?



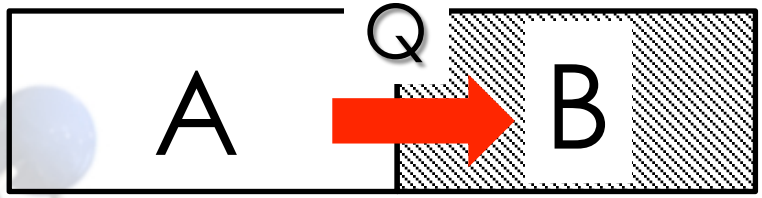


Gordiz & Henry, J. Appl. Phys. 121, 025102 (2017).

Equilibrium vs. Non-Equilibrium

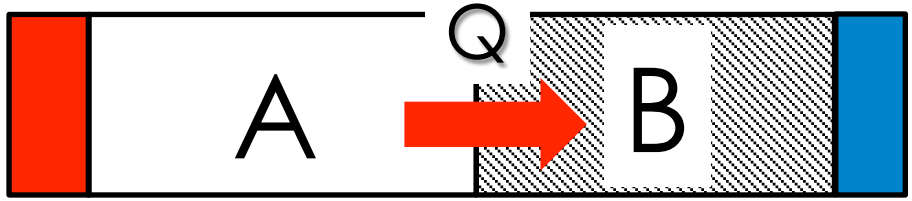
Molecular Dynamics (MD)

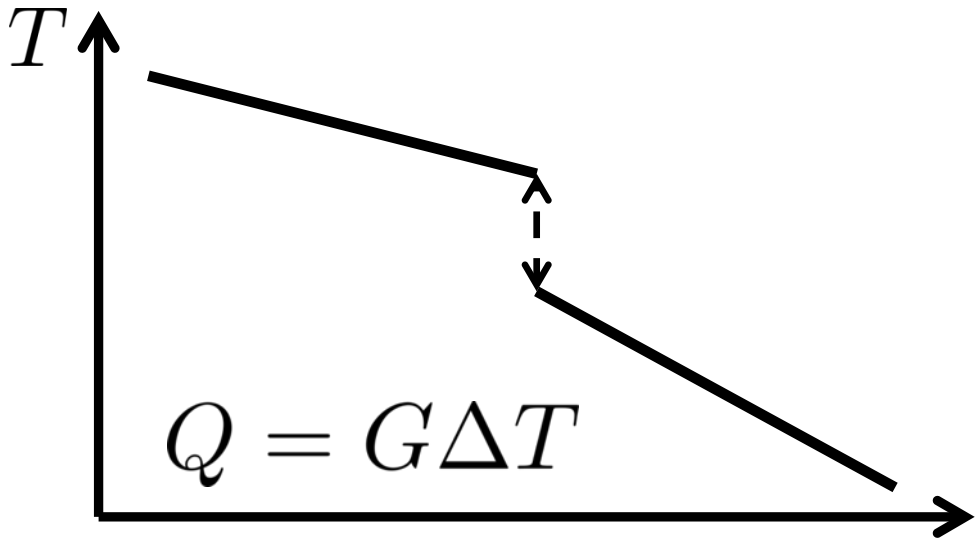
Equilibrium MD



$$G = \frac{1}{k_B T^2 A} \int \langle Q(0) \cdot Q(\tau) \rangle \, d\tau$$

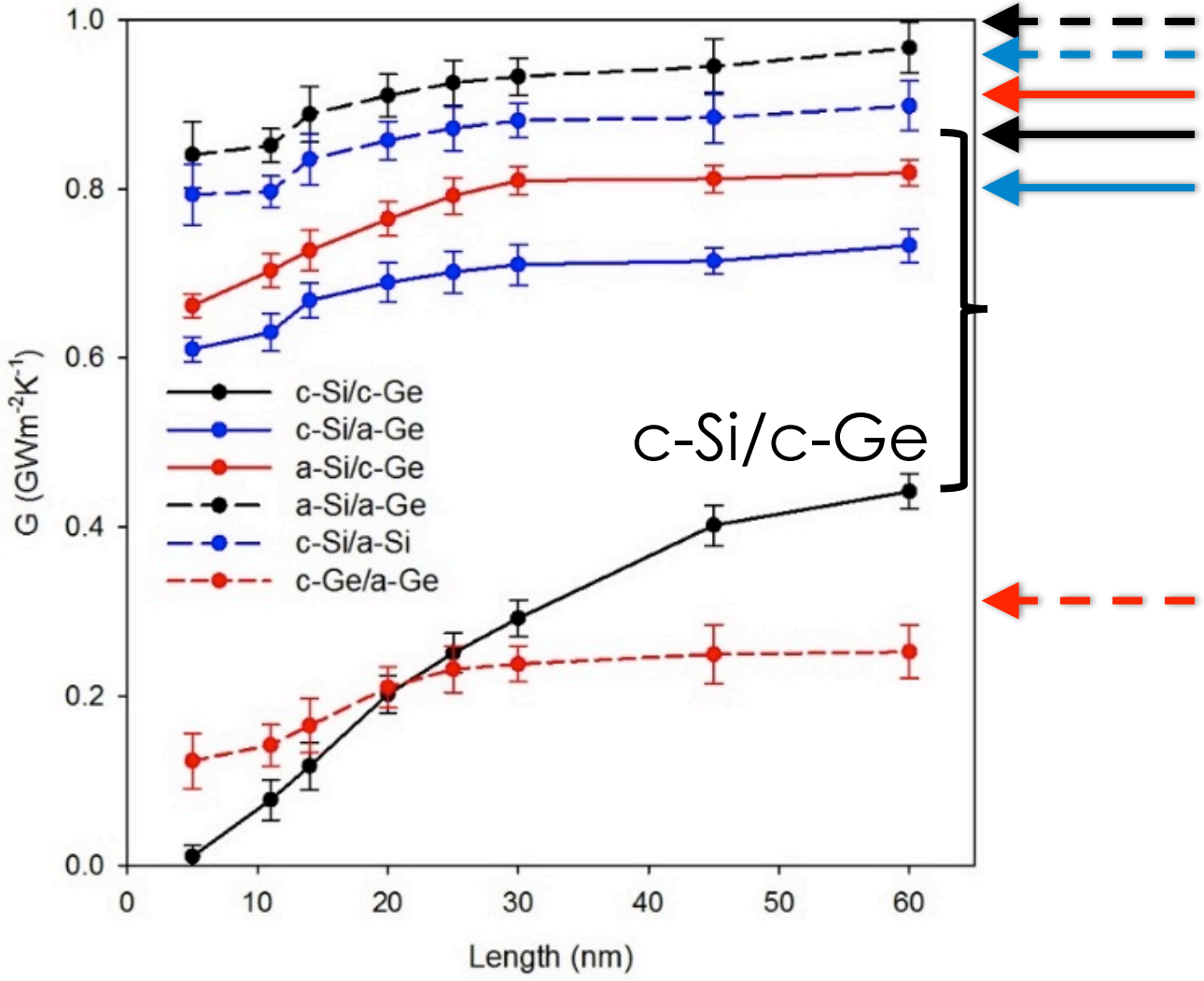
Non-equilibrium MD



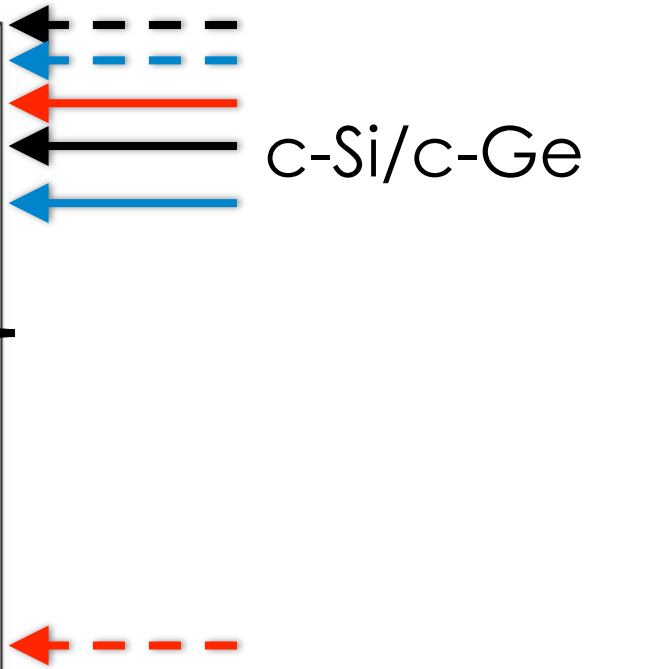


Equilibrium vs. Non-Equilibrium

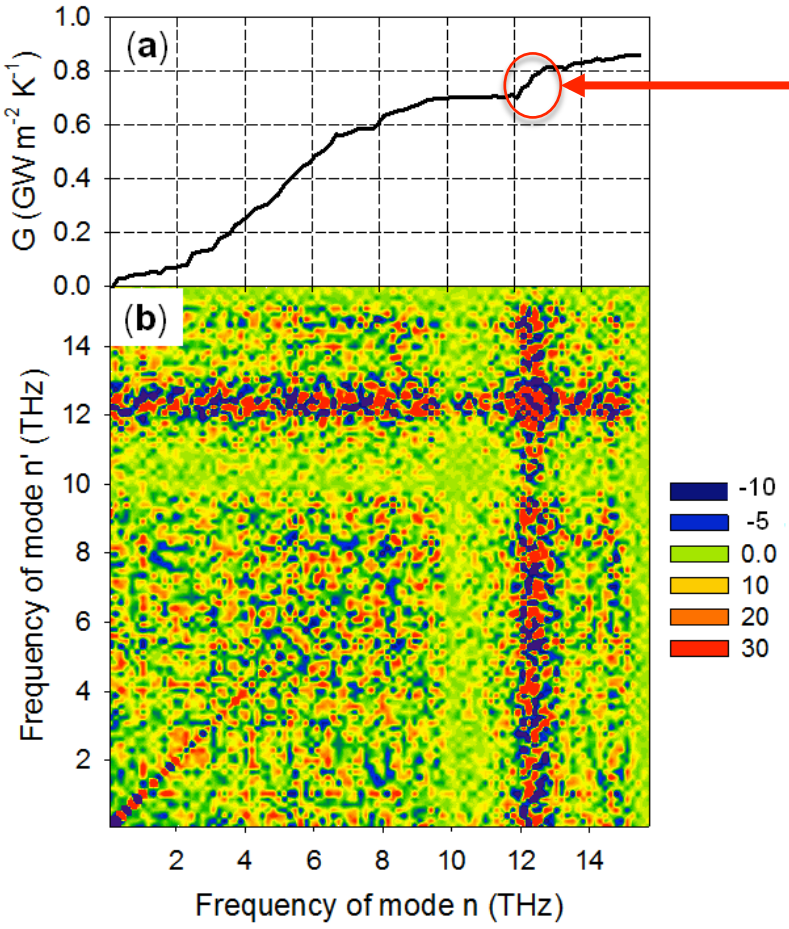
Non-equilibrium results

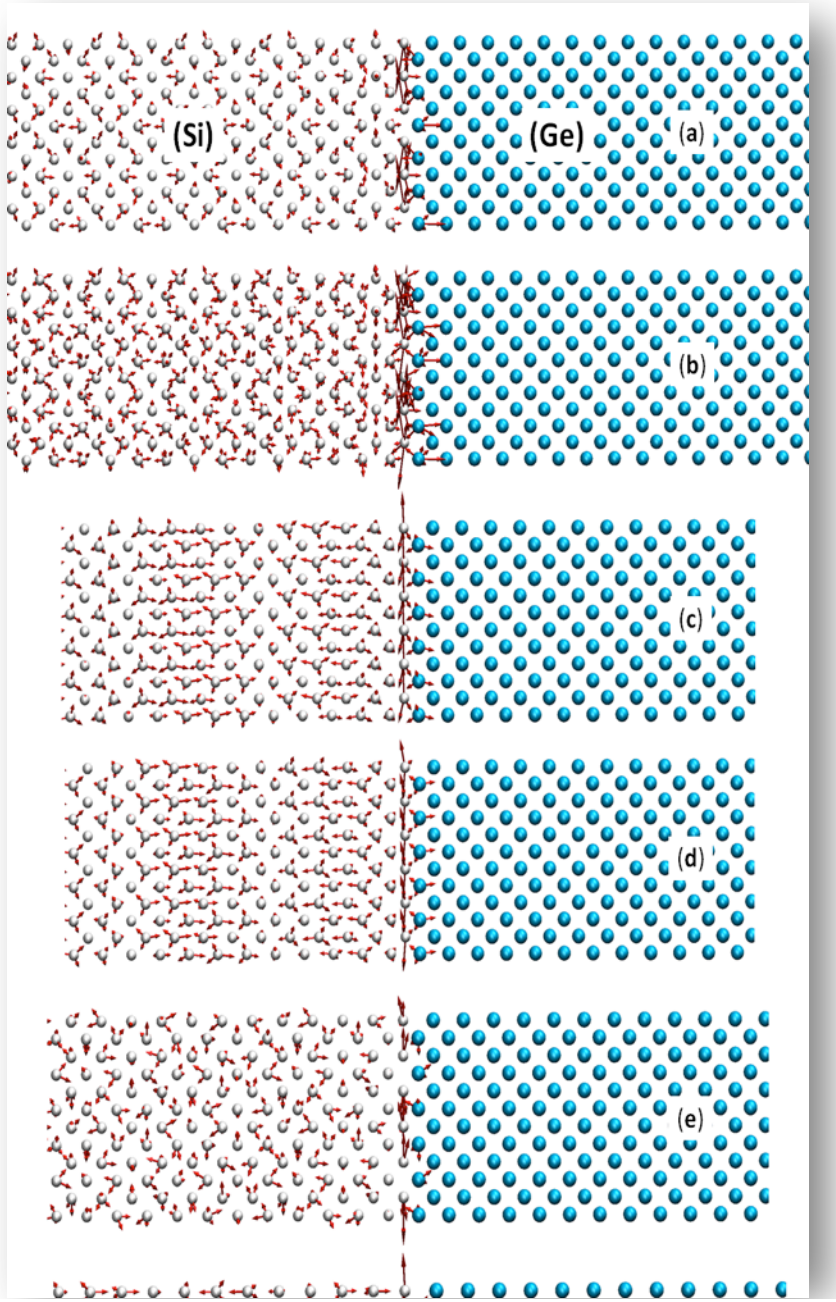


Equilibrium results

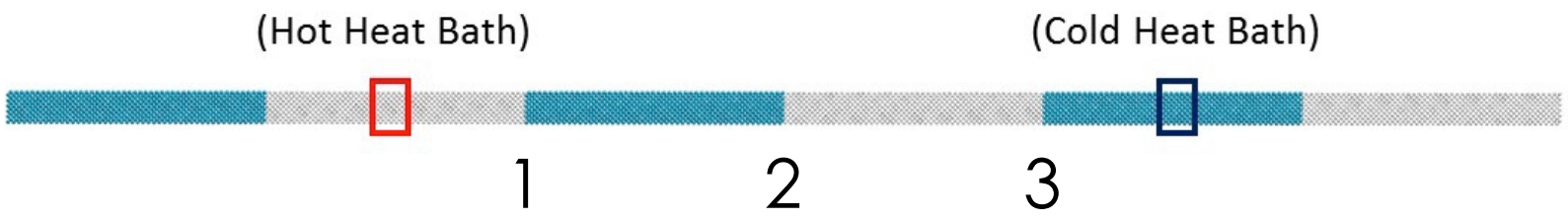


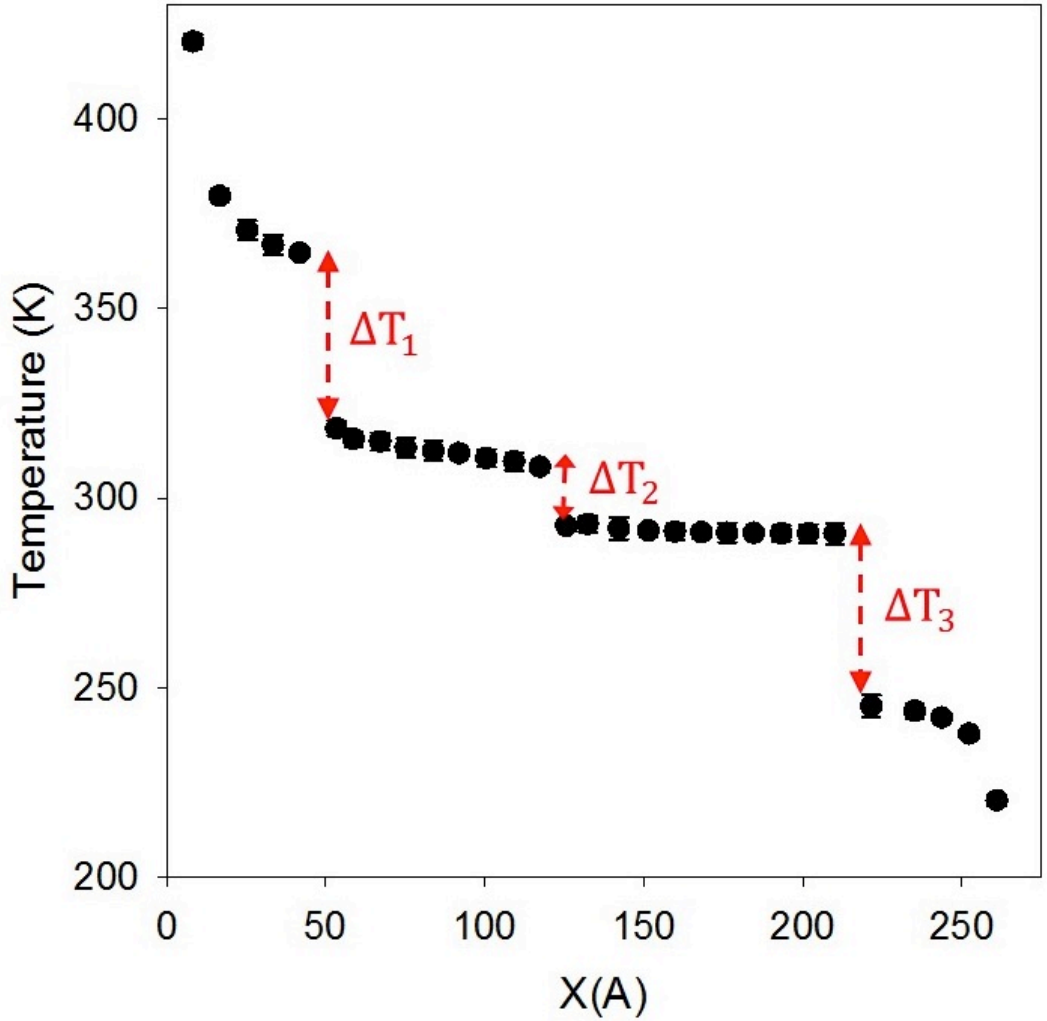
Remember the Interfacial Modes?



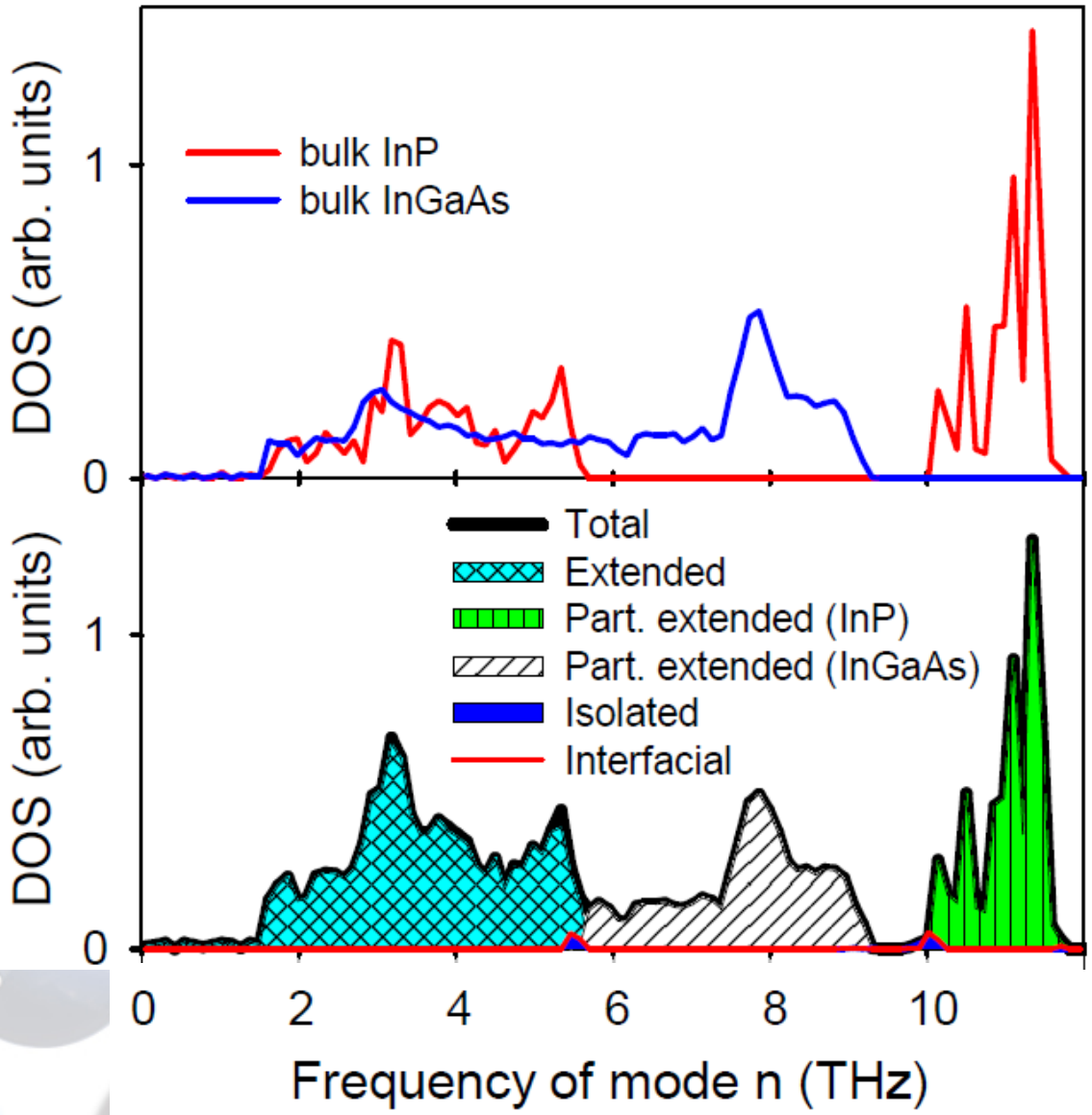


Gordiz & Henry, Sci. Rep. 6, 23139 (2016).


(Hot Heat Bath)
(Cold Heat Bath)
1
2
3

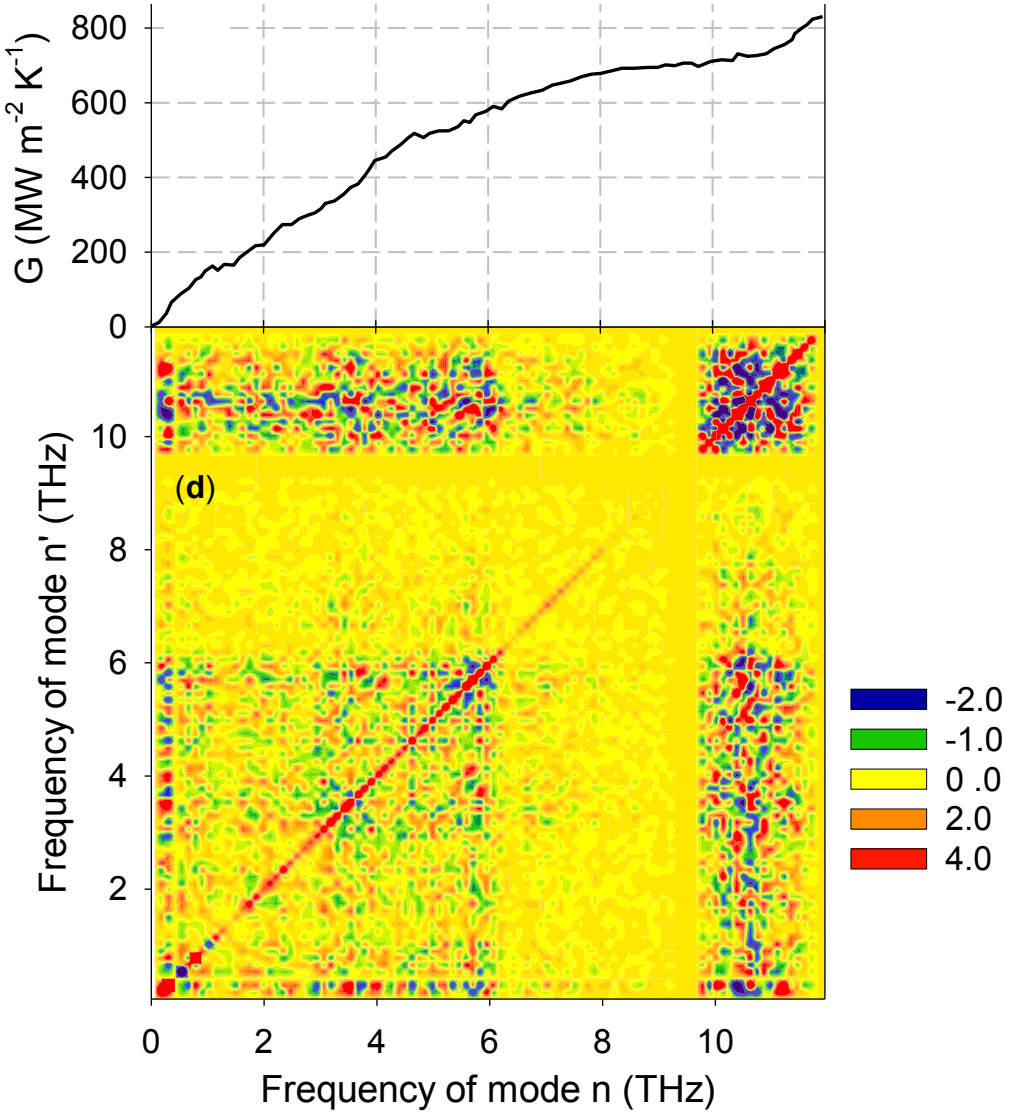

400
350
300
250
200
Temperature (K)
ΔT_1
ΔT_2
ΔT_3
0
50
100
150
200
250
X(A)

Lots of Extended Modes?



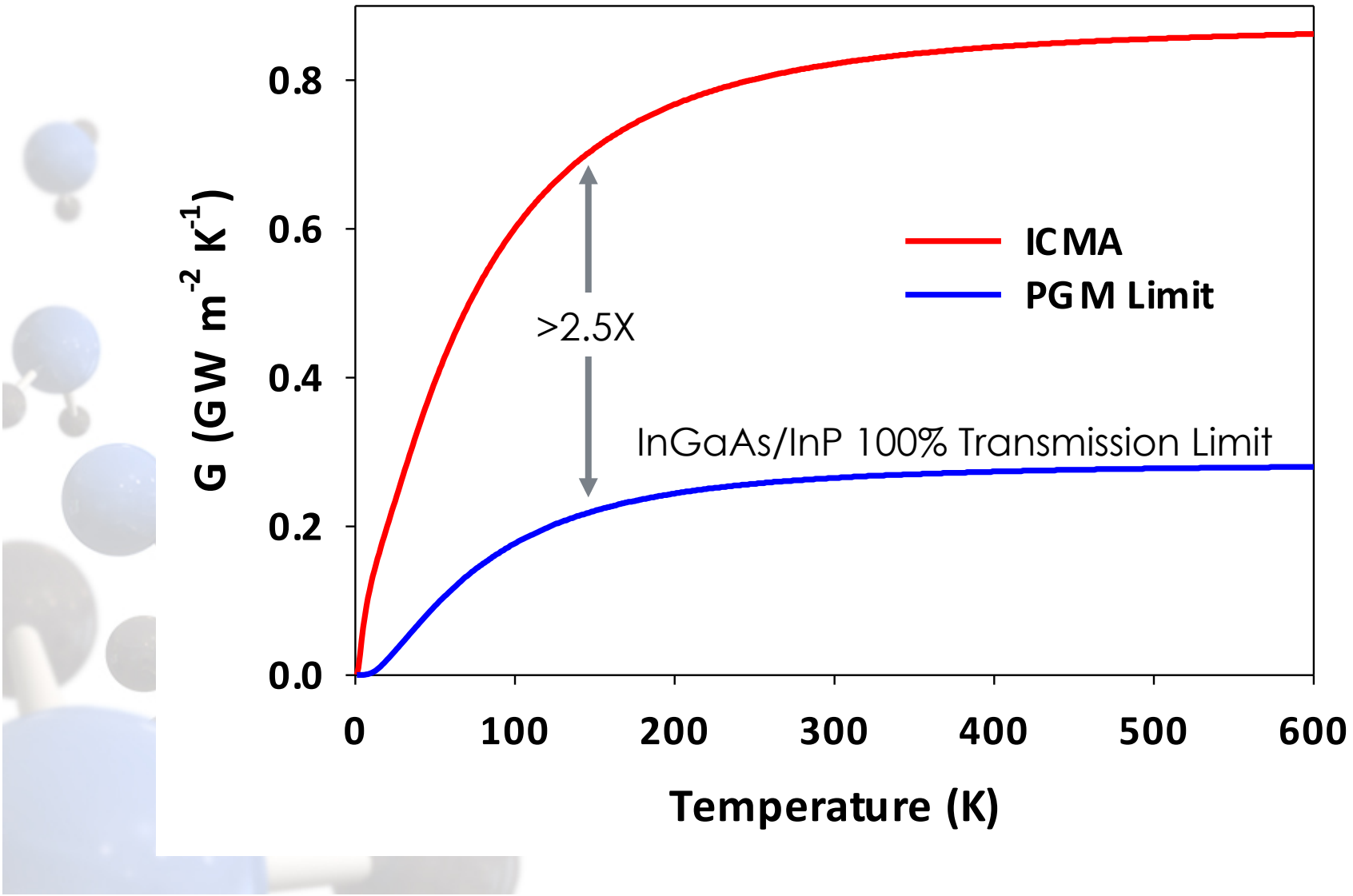
Gordiz & Henry, Appl. Phys. Lett., 108, 181606 (2016)

InP/InGaAs Conductance Accumulation

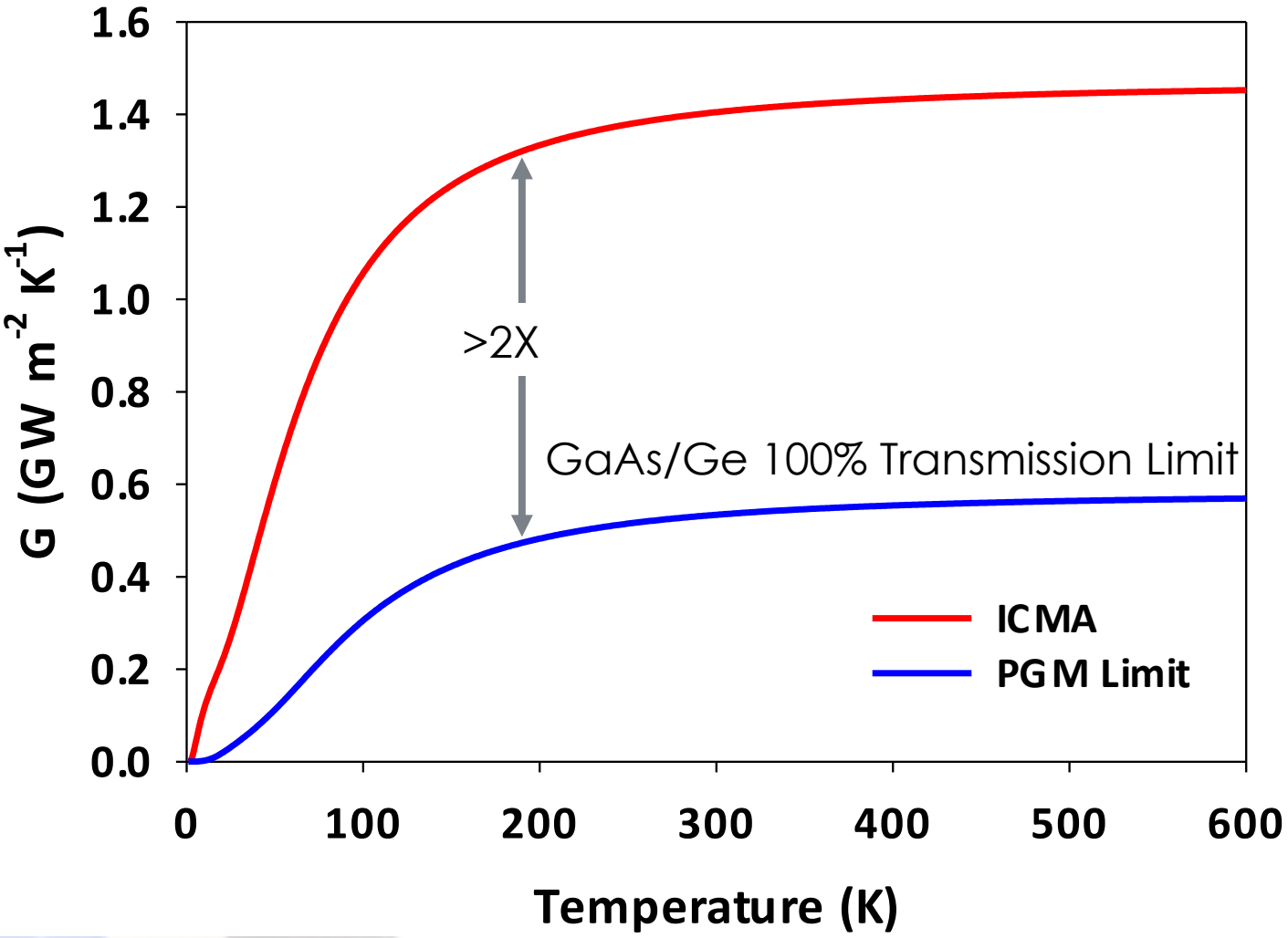


Gordiz & Henry, A. Appl. Phys. Lett., 108, 181606 (2016).

Total Conductance Can Exceed The PGM Limit



Total Conductance Can Exceed The PGM Limit



Conclusions

- LD and MD can be used together
- Phonons exist in all rigid bodies
- Phonons = steps in normal mode amplitude
- Phonons do not require periodicity
- Phonons in disordered systems (non-propagon)
- Modal analysis is the connection
- An alternative perspective is correlation
- Correlation can explain all contributions
- GKMA yields excellent agreement
- ICMA yields a new perspective

Acknowledgements

- Wei Lv
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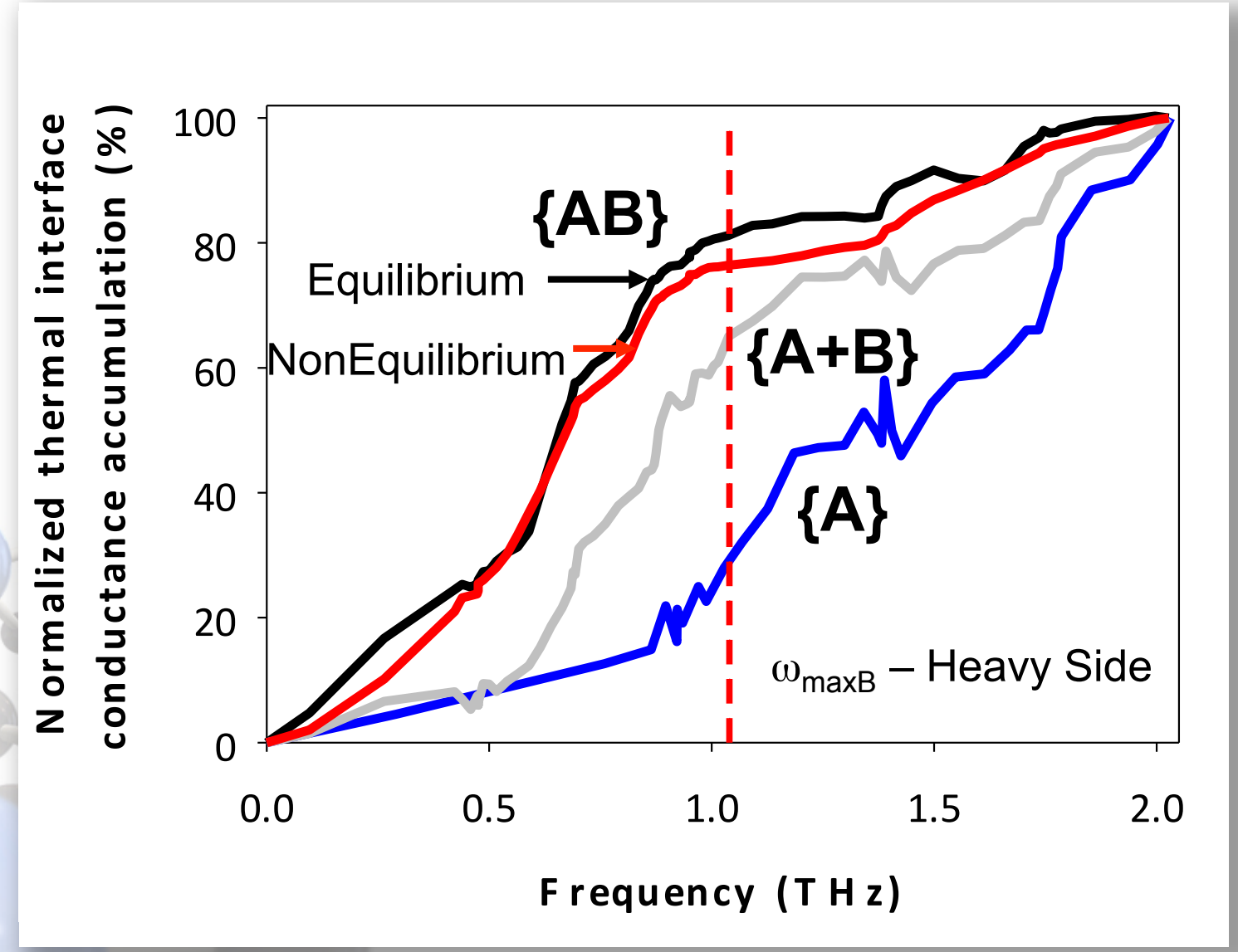
- Andrew Rohskopf
- Freddy DeAngelis

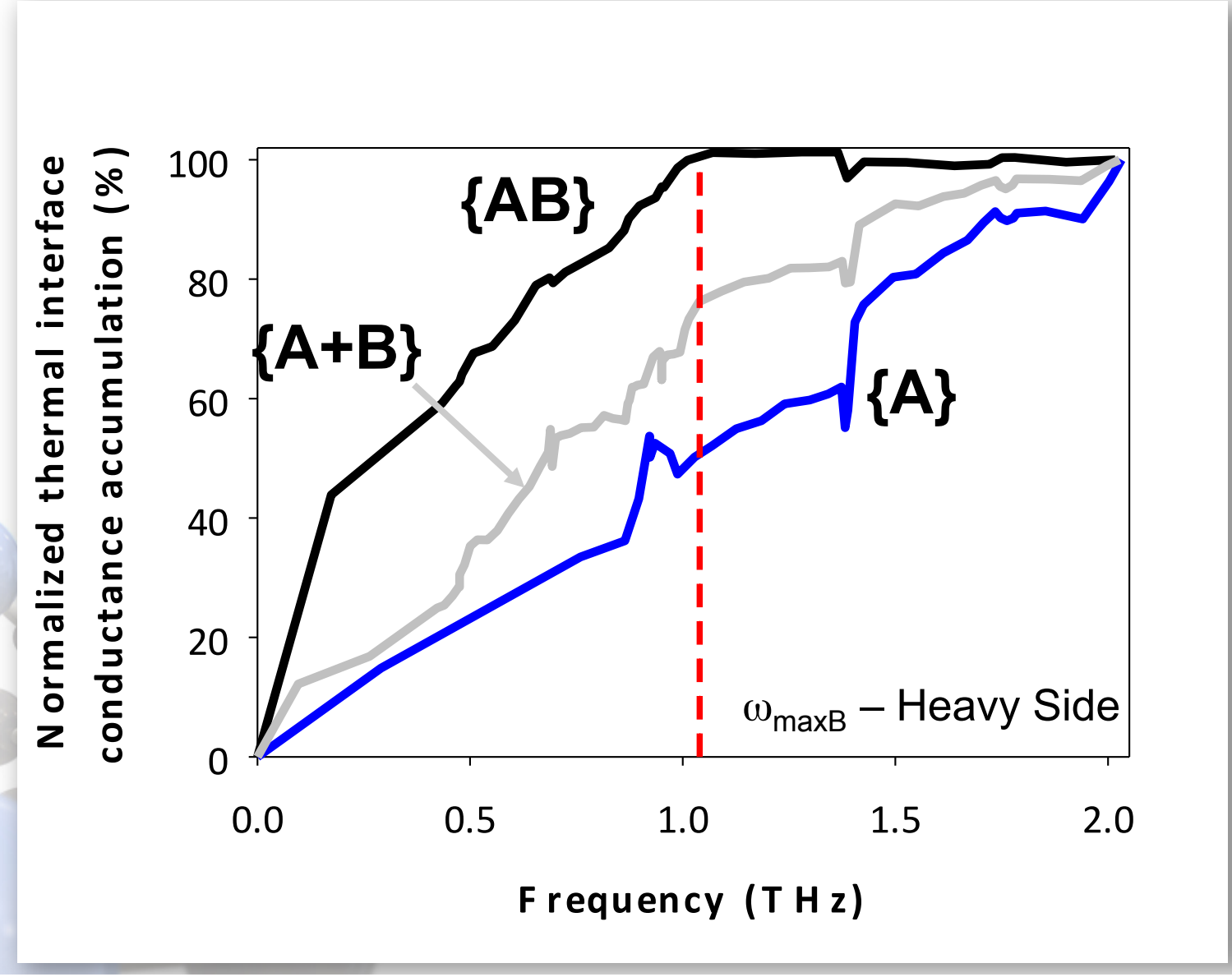
- NSF Career Award
- Intel Project
- ARPA-E
- DOE SunShot

Backup Slides

Conductance Accumulation – 60°K



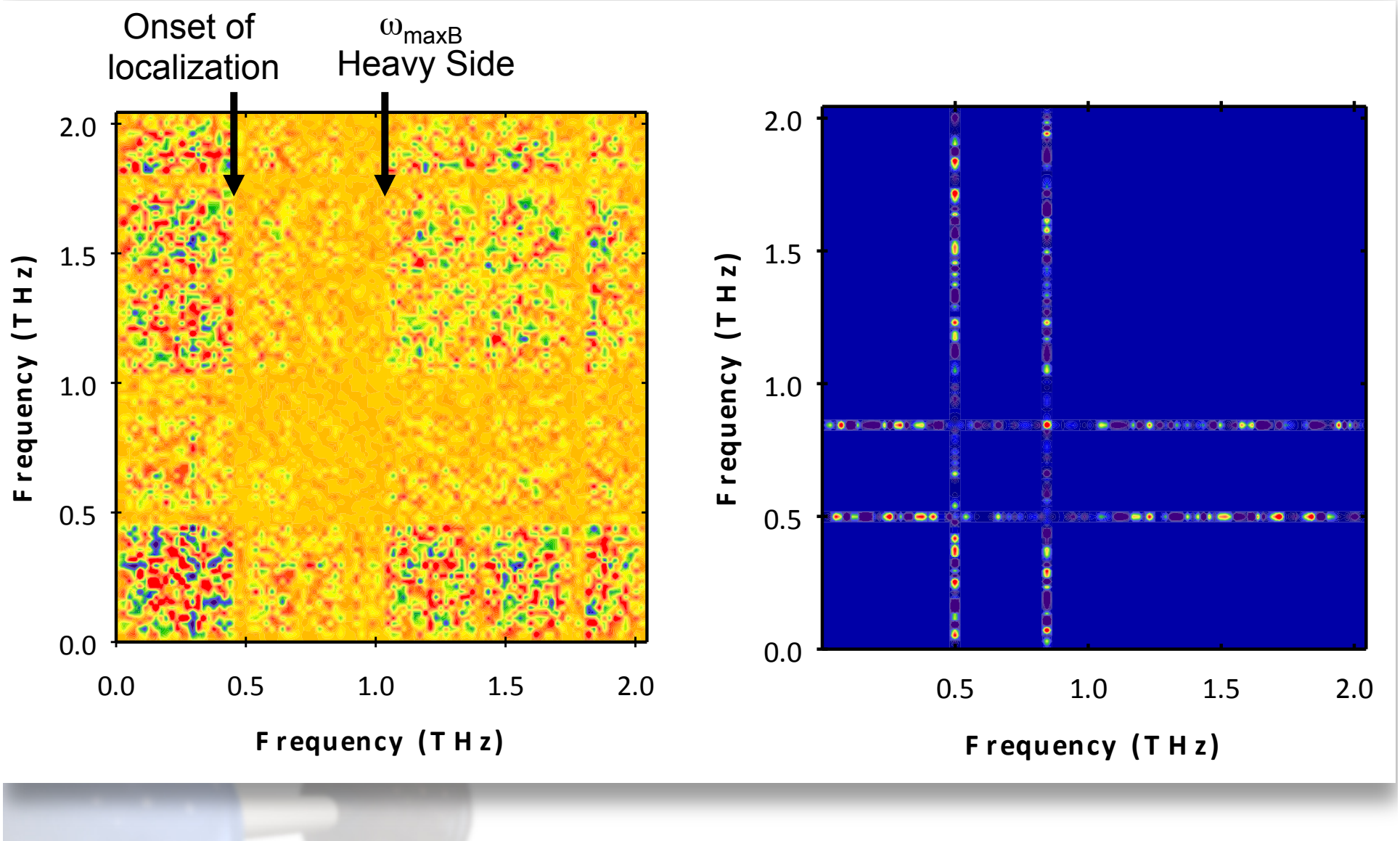
Conductance Accumulation – 1°K



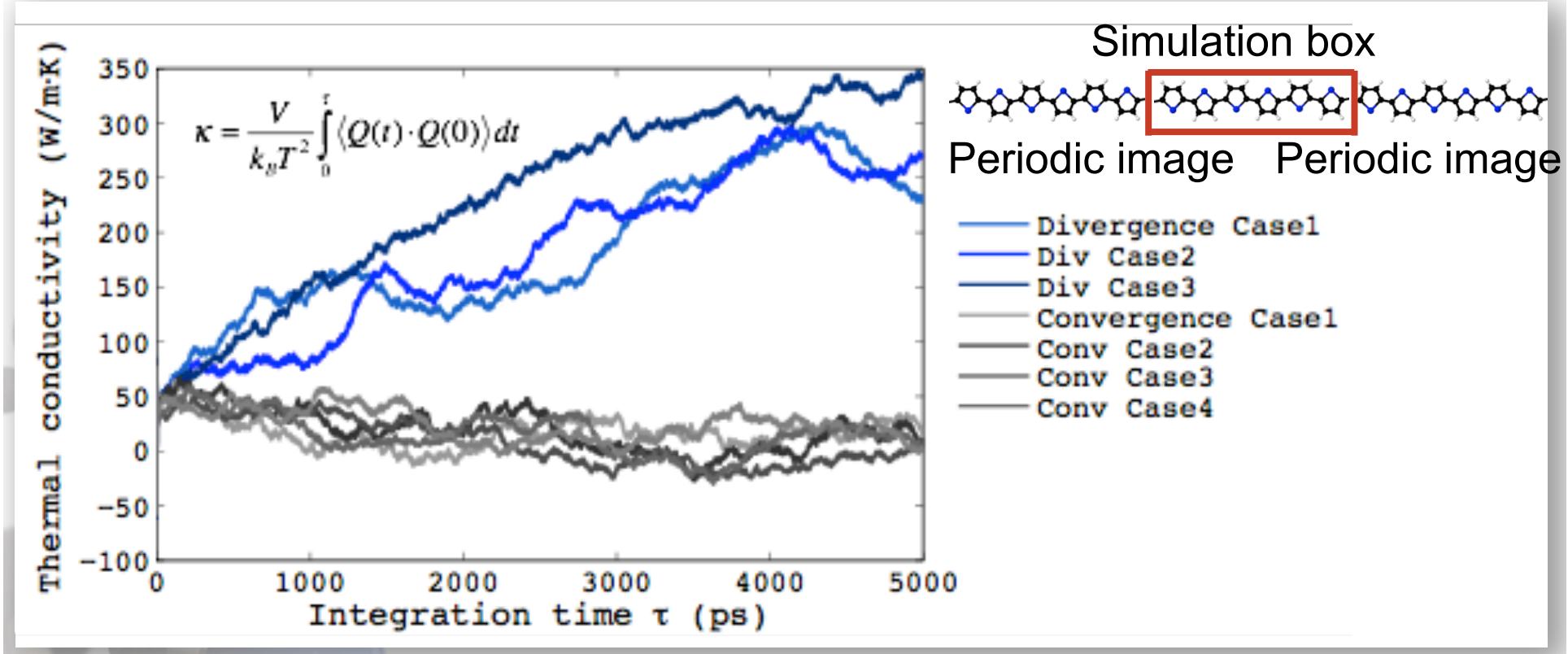
Modal Contributions

Mode Type	Percent of total # of modes (%)	Contribution to G (%)	Contribution to G per % of total modes
Extended	10.73	42.89	3.99
Partially extended	83.19	53.40	0.64
Isolated	5.76	0.55	0.095
Interfacial	0.31	3.16	10.19

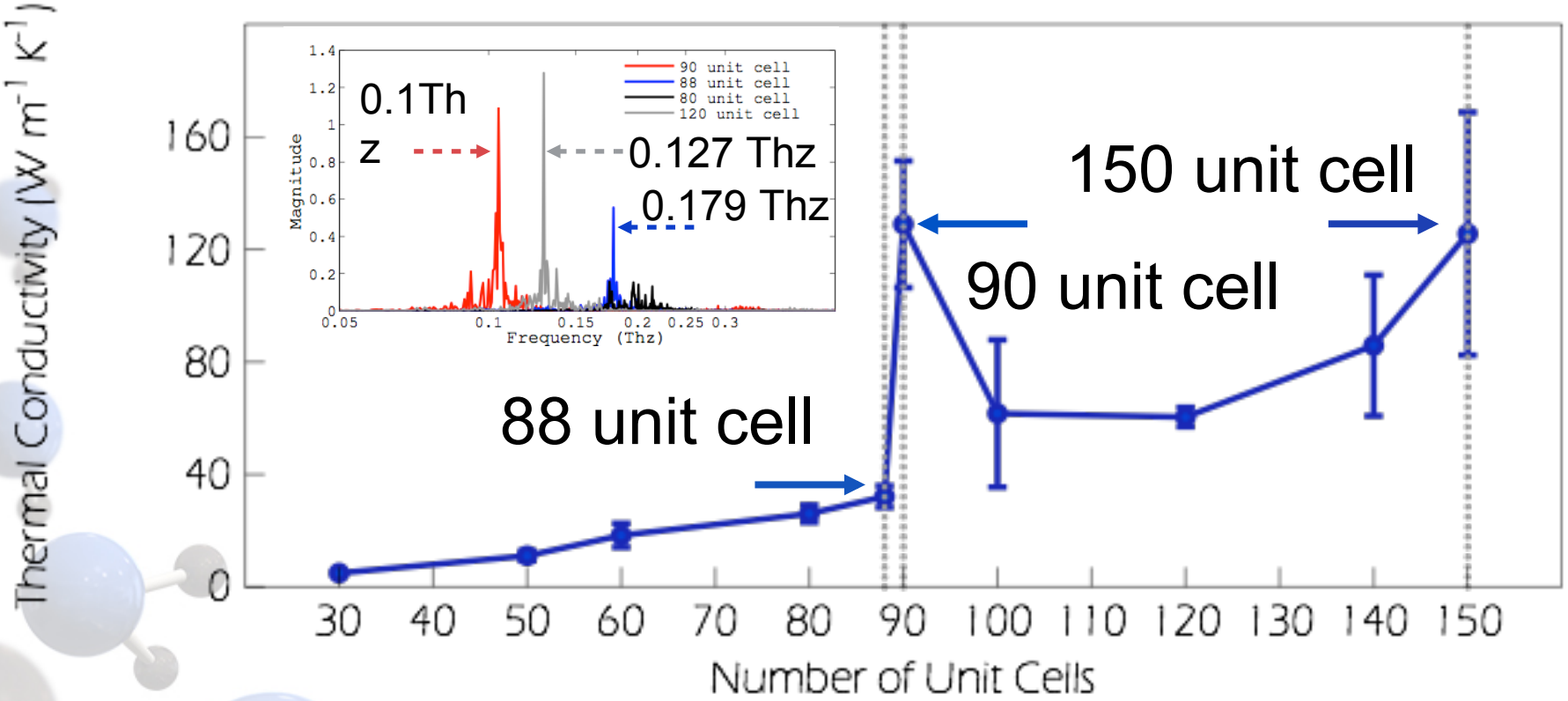
Mode-Mode Correlation

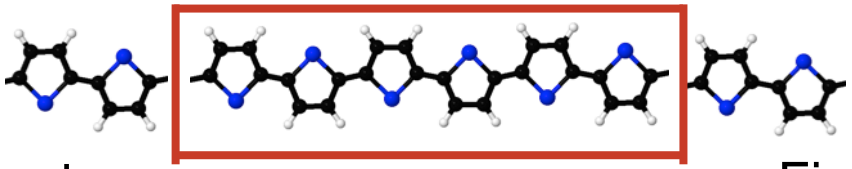


Divergent κ in Polymers



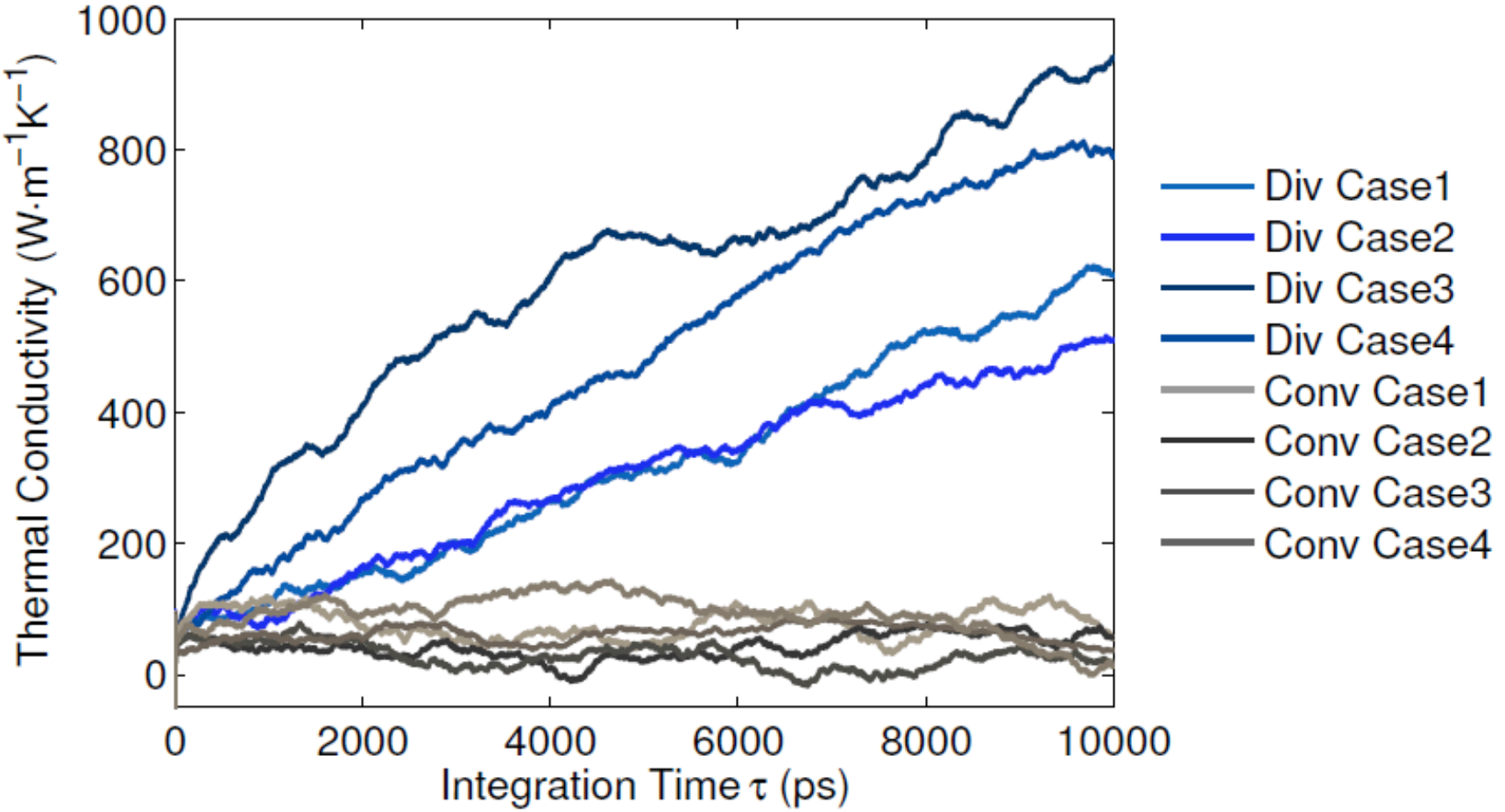
Anomalous Behavior Without PBC





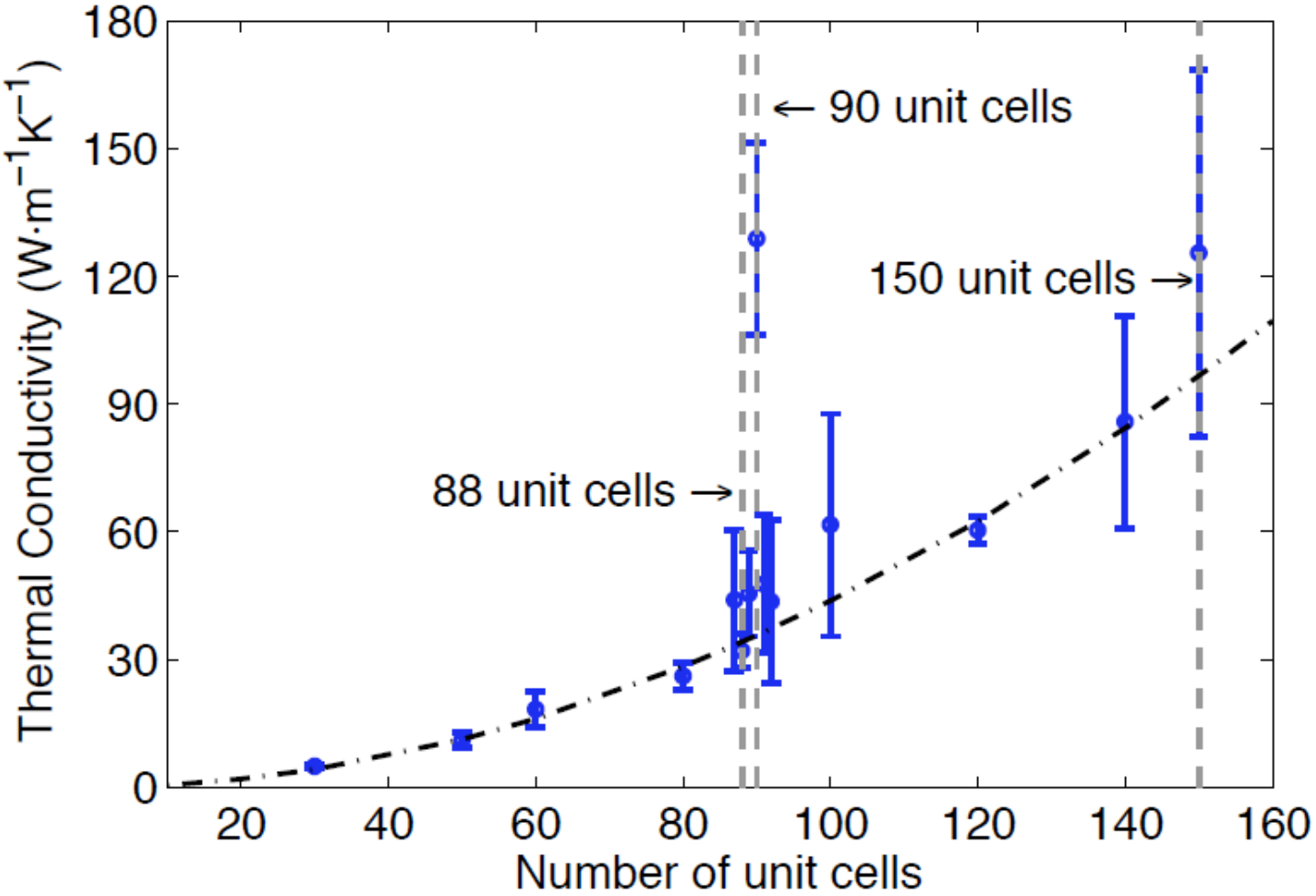
New Understanding

Single Polythiophene Chains



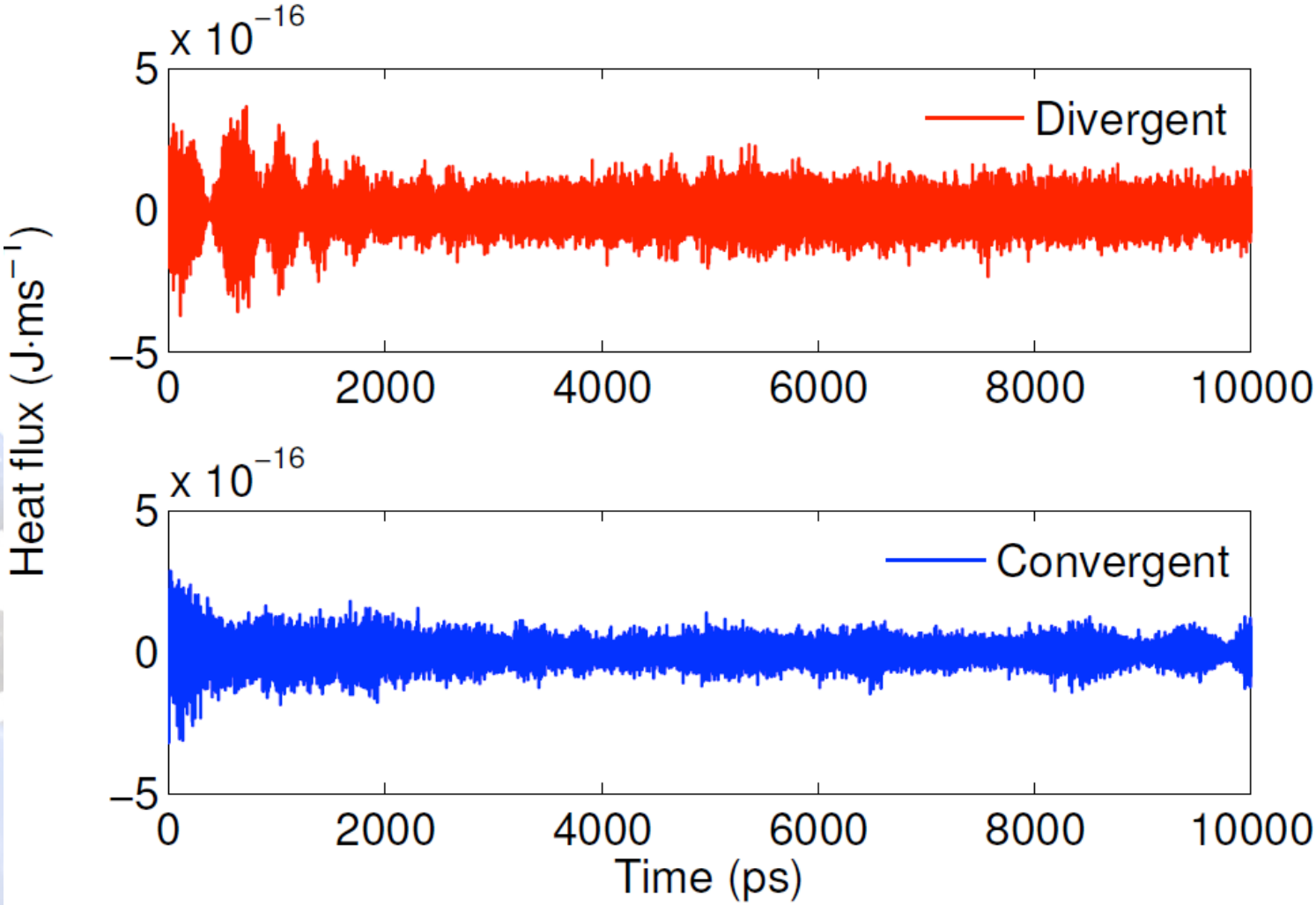
New Understanding

Single Finite Length Polythiophene Chains

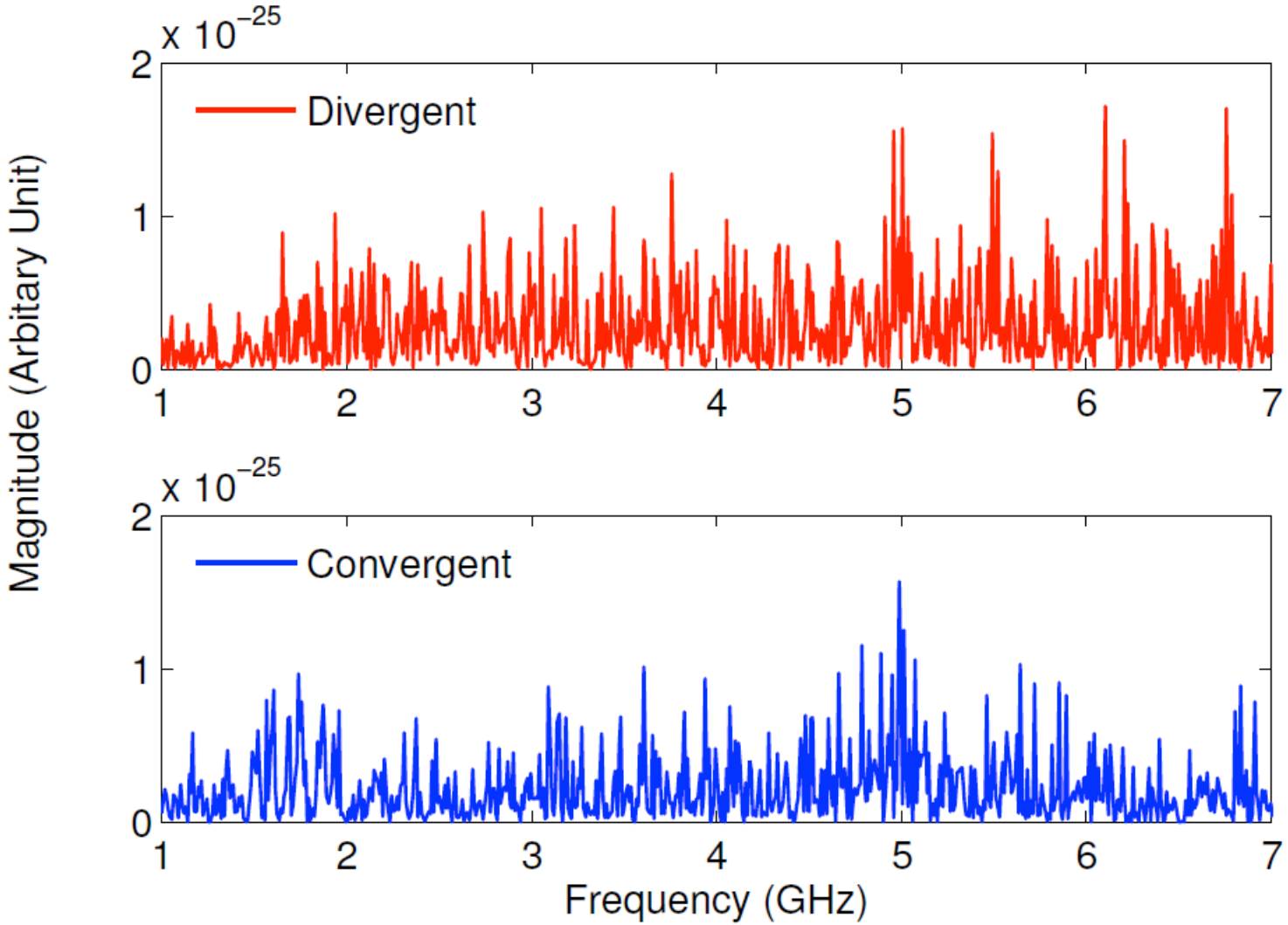


New Understanding

Convergent vs. Divergent

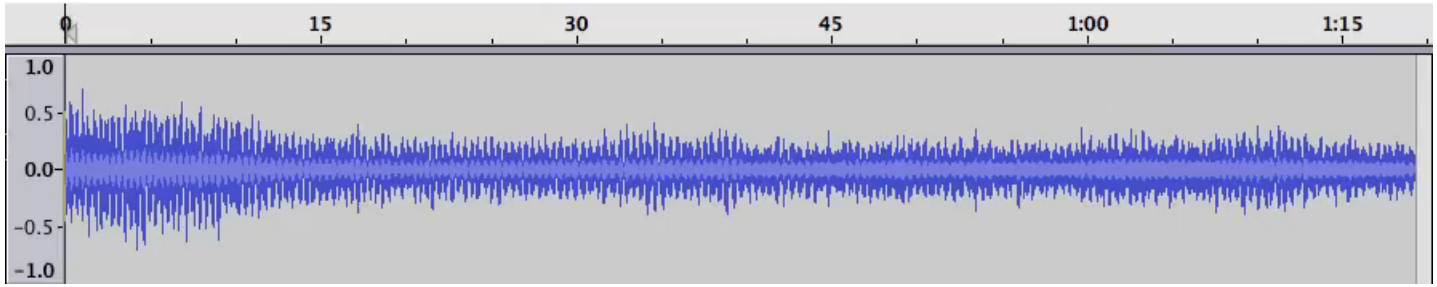


New Understanding



New Understanding

Convergent



Divvergent