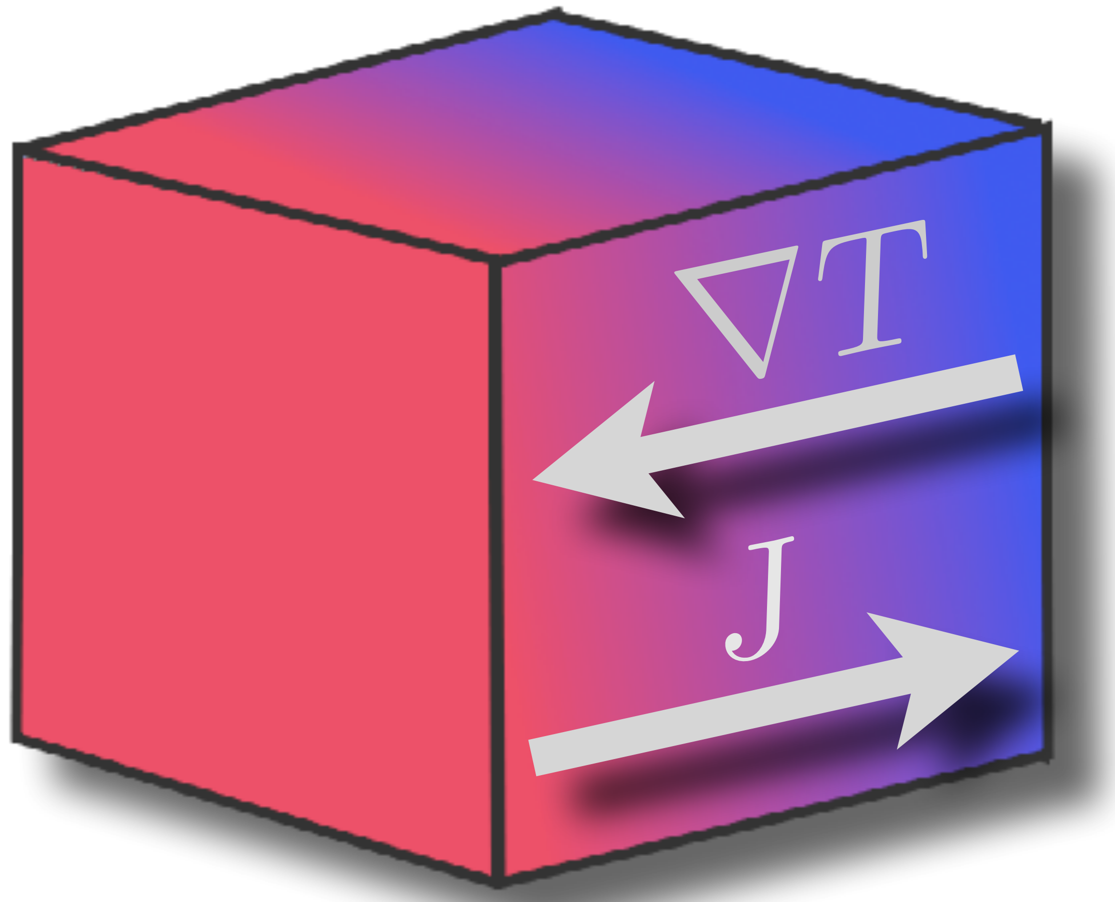
# High-Throughput *Ab initio* Green-Kubo Simulations for Thermal Insulator Discovery

*Christian Carbogno*

*Nomad Laboratory, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin*

# HEAT TRANSPORT

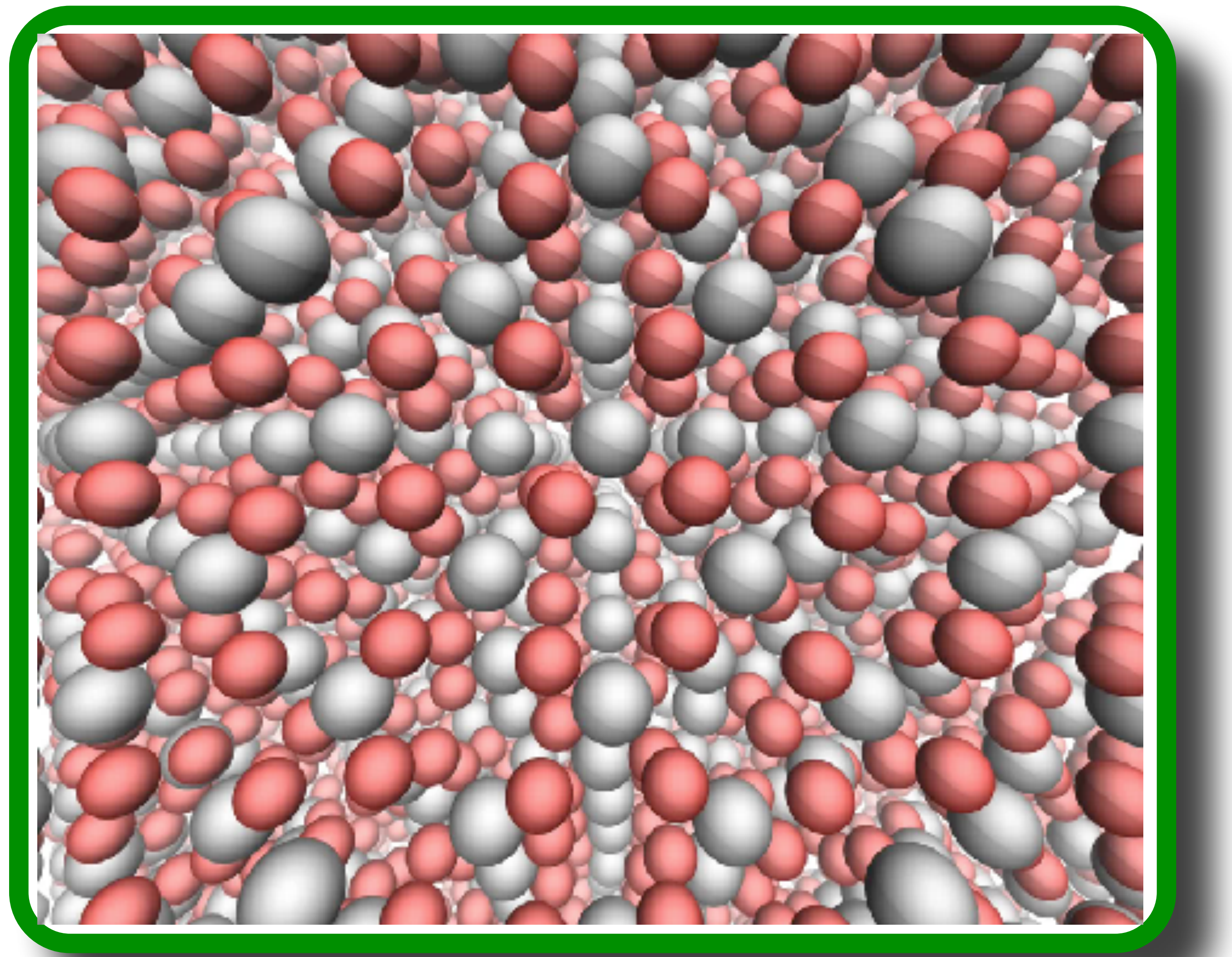
**Macroscopic Effect:**




Fourier's Law:

$$\mathbf{J} = -\kappa\, \nabla T = -\alpha\, \rho\, c_V\, \nabla T$$

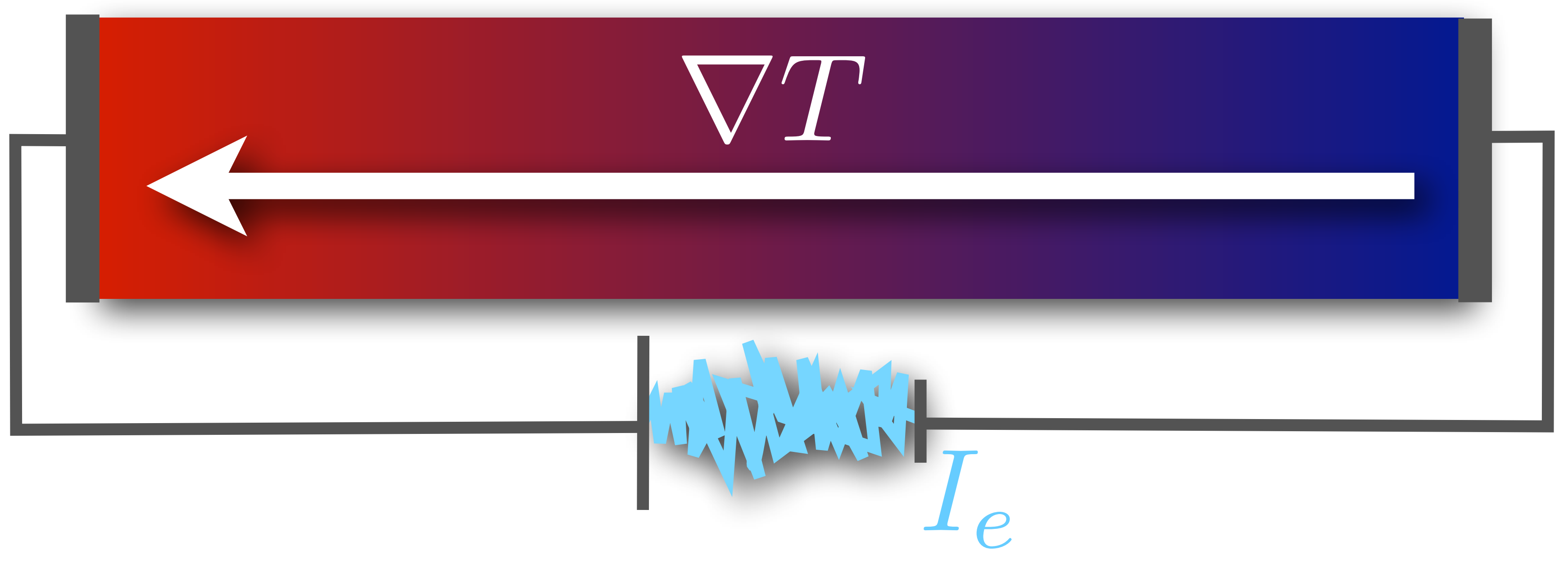
$$\kappa = \cancel{\kappa_{\text{photon}}} + \cancel{\kappa_{\text{elec.}}} + \boxed{\kappa_{\text{nucl.}}}$$



**Microscopic Mechanisms**

# Thermoelectric Elements

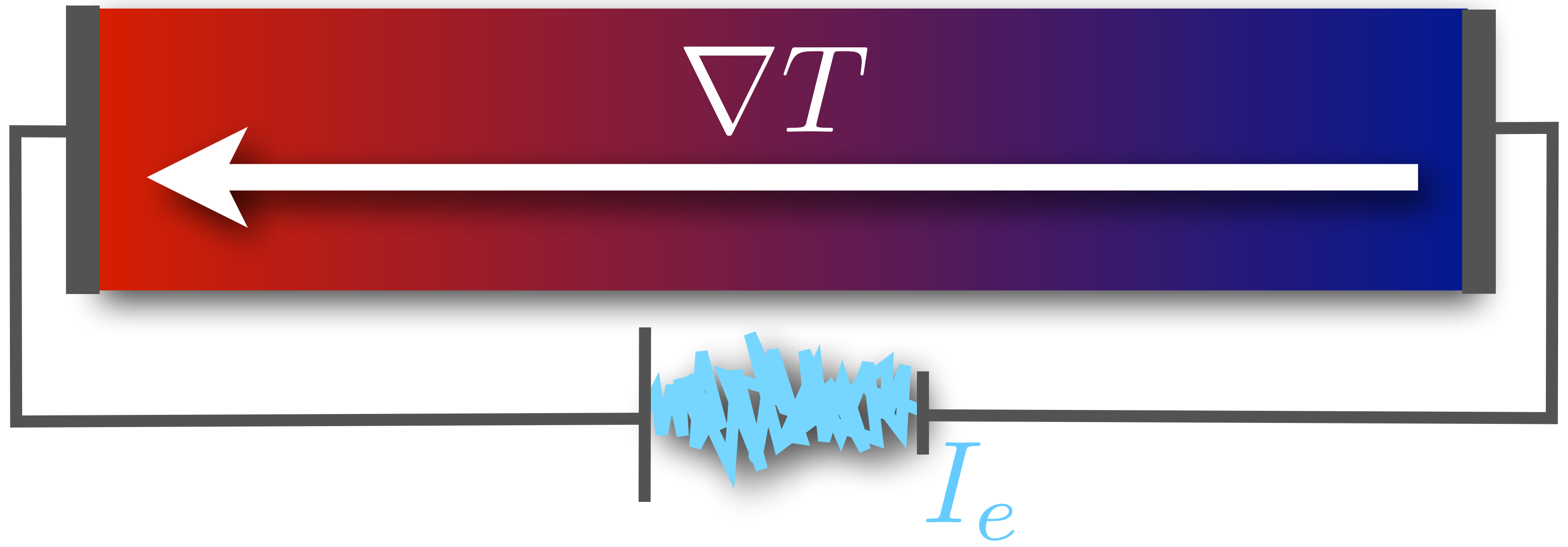
Conversion of **temperature gradient** into **electric current**.




**Efficiency** $\propto \dfrac{S_{el}^2\, \sigma_{el}\, T}{\kappa_{ph} + \kappa_{el}}$

# Thermoelectric Elements

Conversion of **temperature gradient** into **electric current**.

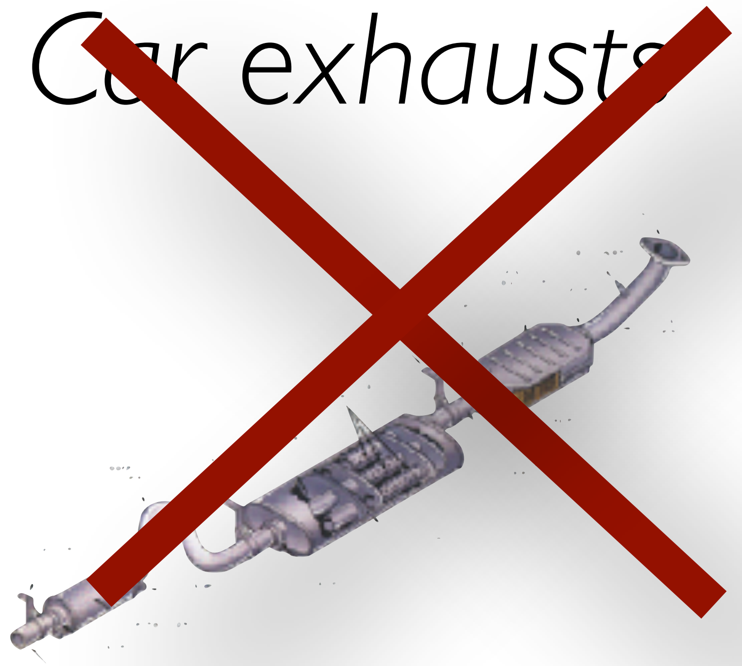



$$\textbf{Efficiency} \propto \frac{S_{el}^2\, \sigma_{el}\, T}{\kappa_{ph} + \kappa_{el}}$$

**Potential “*waste heat recovery*” device!**

*Industrial plants*

*Car exhausts*

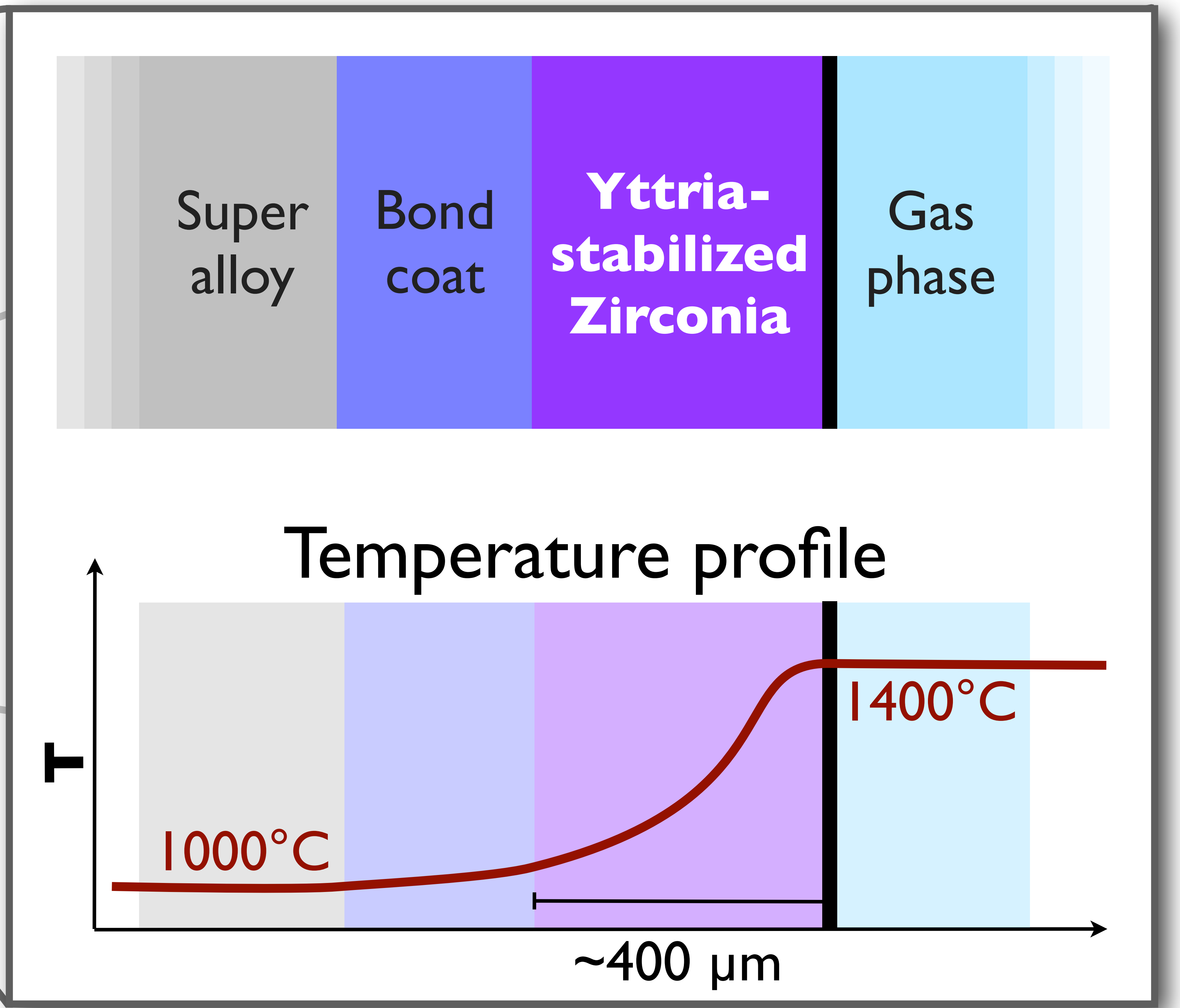


*Personal Computing*

**Too low efficiency inhibits** a large scale, economically attractive deployment of **thermoelectric devices.**

# Thermal-Barrier Coatings

CFM 56-7 airplane engine




**Suppressing** heat transport in **thermal barrier coatings** has driven the fuel-efficiency increase over the last 30 years.

D. R. Clarke & C. G. Levi, *Ann. Rev. Mat. Res.*, **33**, 383 (2003).

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e.g. GaAs, benzene, Cd-Te, band gap

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thermal conductivity

**Data collections**

| | |
|---|---|
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| Landolt-Börnstein | 503 |
| MSI Eureka | 3 |
| Thermophysical Properties | 159 |
| Metal foam | 7 |

**1,222** results for

Filtered by: Inorganic Solid Phases   thermal conductivity

Inorganic Solid Phases

## TiC thermal conductivity

Element system: C-Ti; Phase prototype: NaCl; Pearson symbol: *cF*8; Space group: 225; Data points: 3; Samples: 3; Journal references: 3

Inorganic Solid Phases

## $CdSnAs_2$ rt thermal conductivity

Element system: As-Cd-Sn; Phase prototype: $CuFeS_2$; Pearson symbol: *tI*16; Space group: 122; Data points: 1; Samples: 1; Journal references: 1

Inorganic Solid Phases

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e.g. GaAs, benzene, Cd-Te, band gap

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Inorganic Solid Phases

TiC thermal conducti

Element system: C-Ti; Phase prot
3; Samples: 3; Journal references

Inorganic Solid Phases

$CdSnAs_2$ rt thermal c

Element system: As-Cd-Sn; Phas
points: 1; Samples: 1; Journal refe

Inorganic Solid Phases

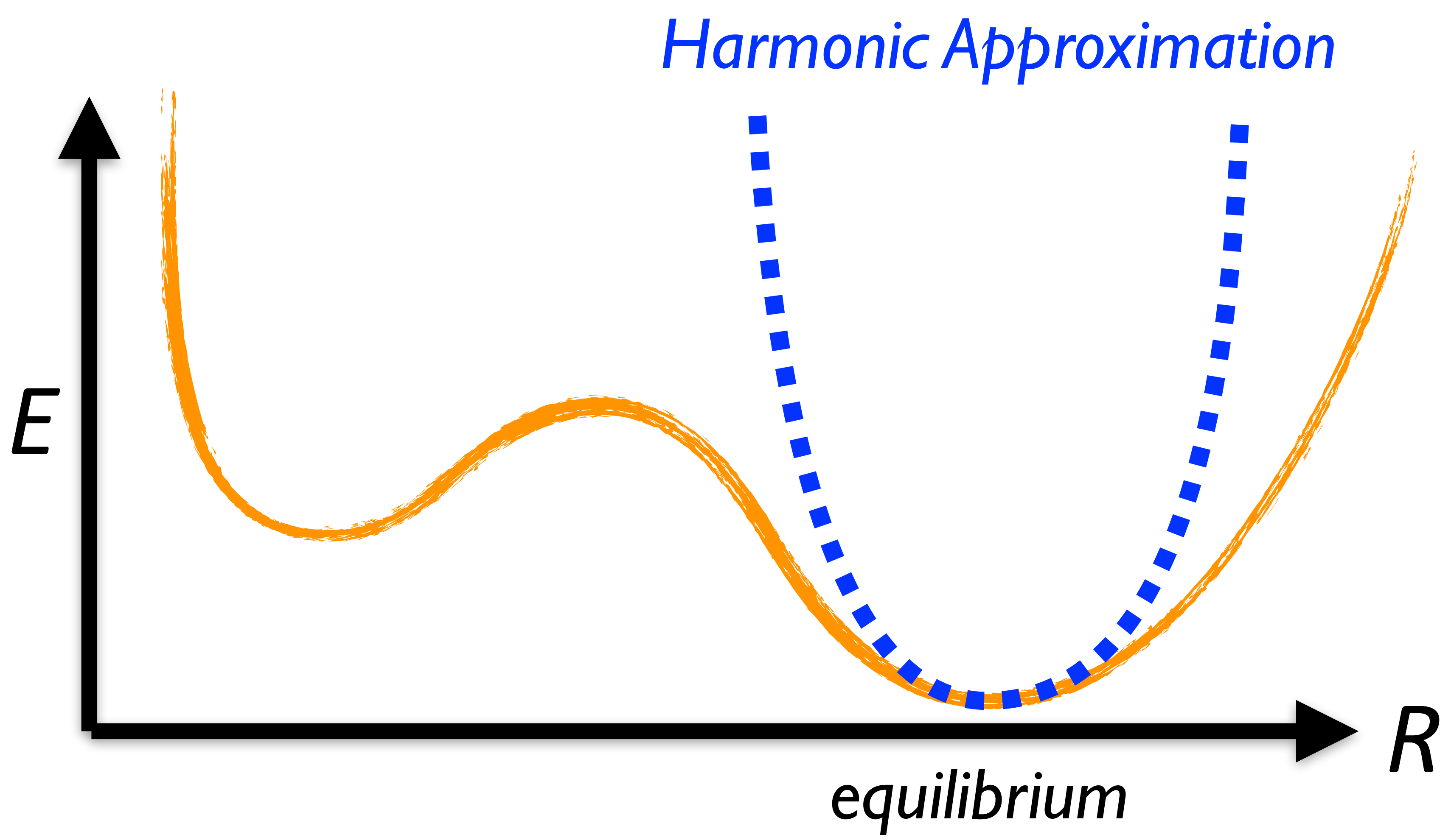
- Consolidate data for different temperatures
- Remove duplicates
- Remove liquids
- Remove metals
- Remove doped/non-pristine materials

$\Longrightarrow$ Much less than 150 materials left!

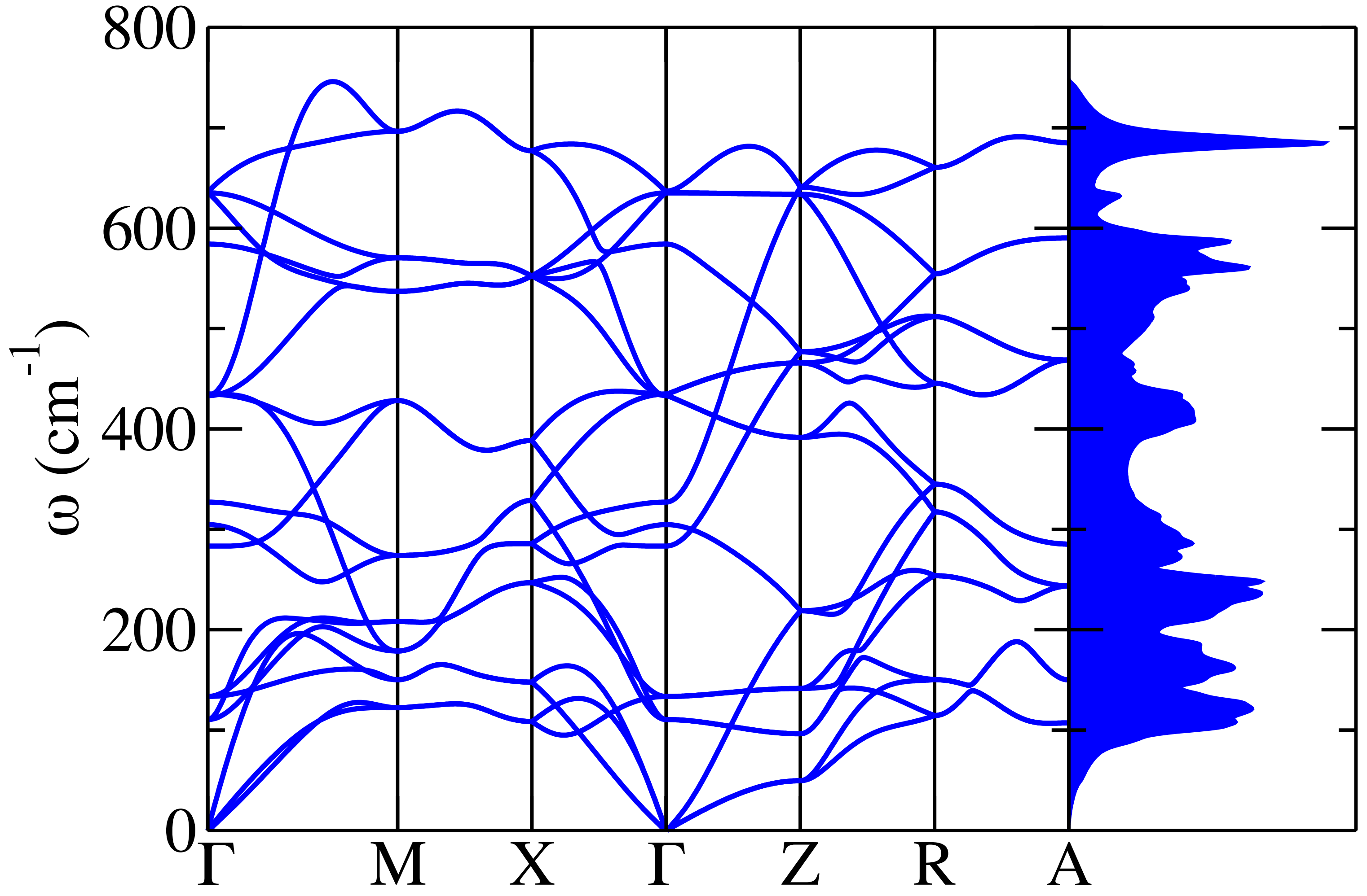
# MORE DATA URGENTLY NEEDED!

# Heat Transport Theory 101

*Real-Space Representation*




*Reciprocal-Space Representation*



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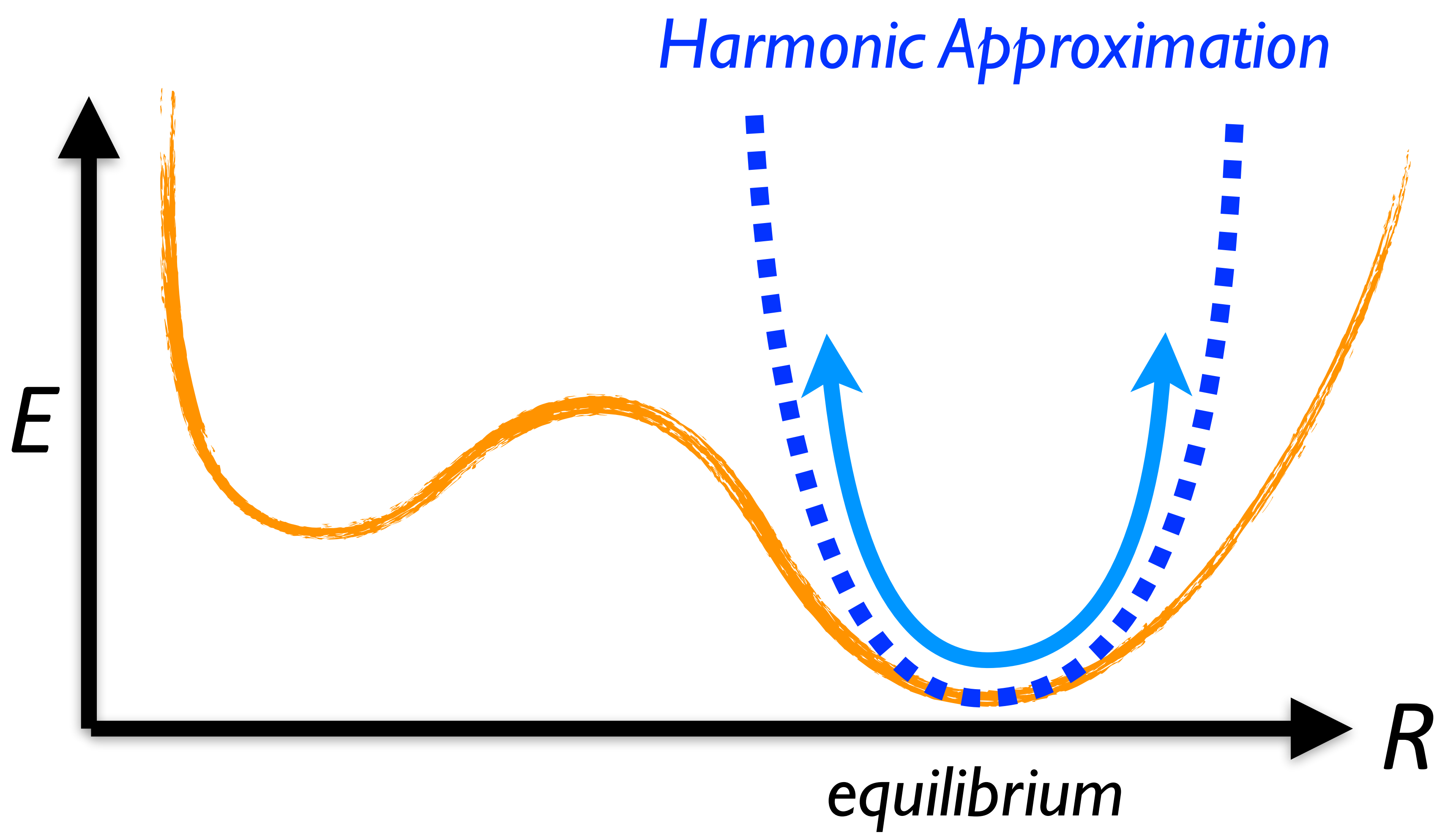
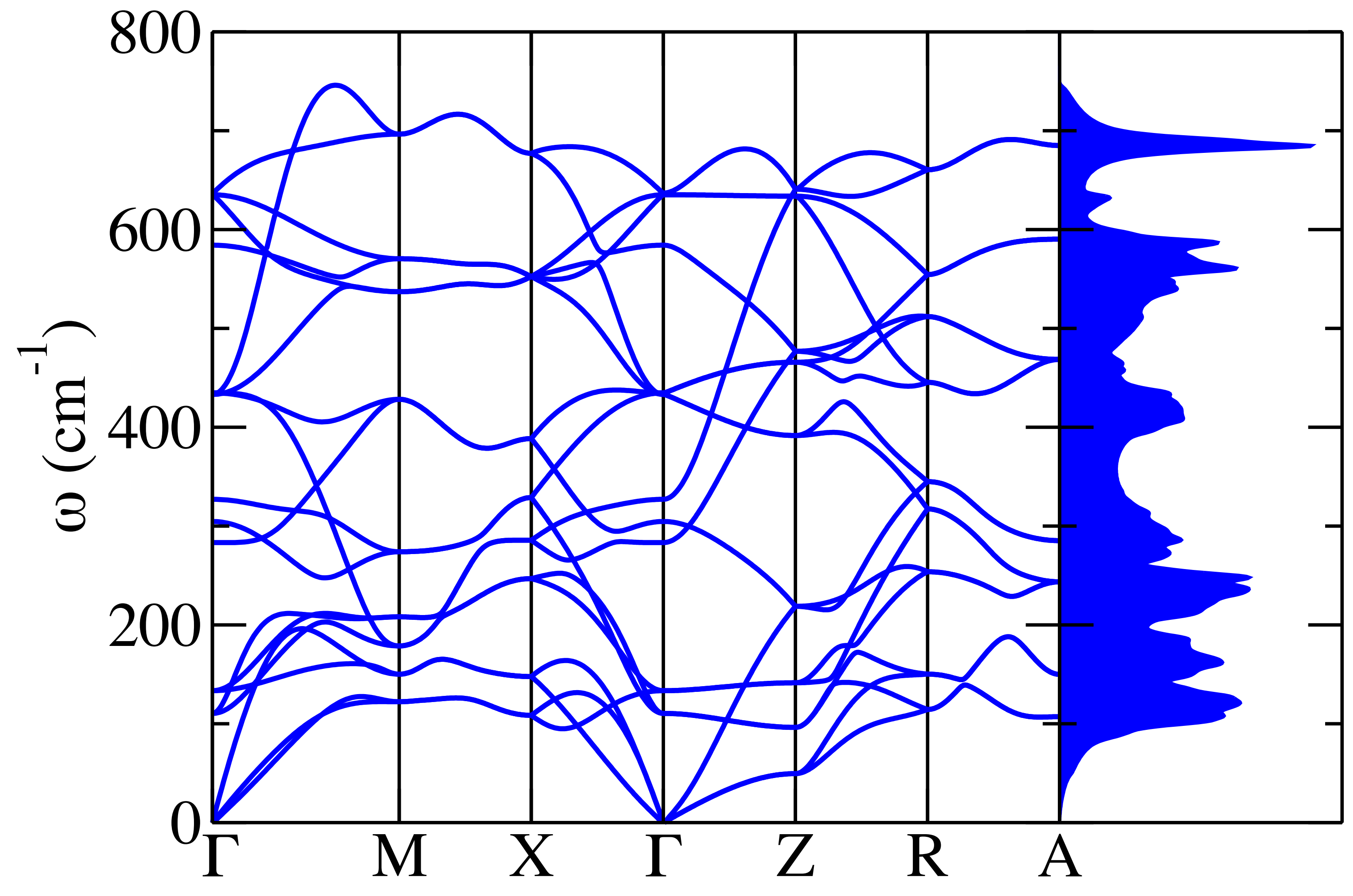
*Real-Space Representation*




**Decoupled Modes**

*Reciprocal-Space Representation*

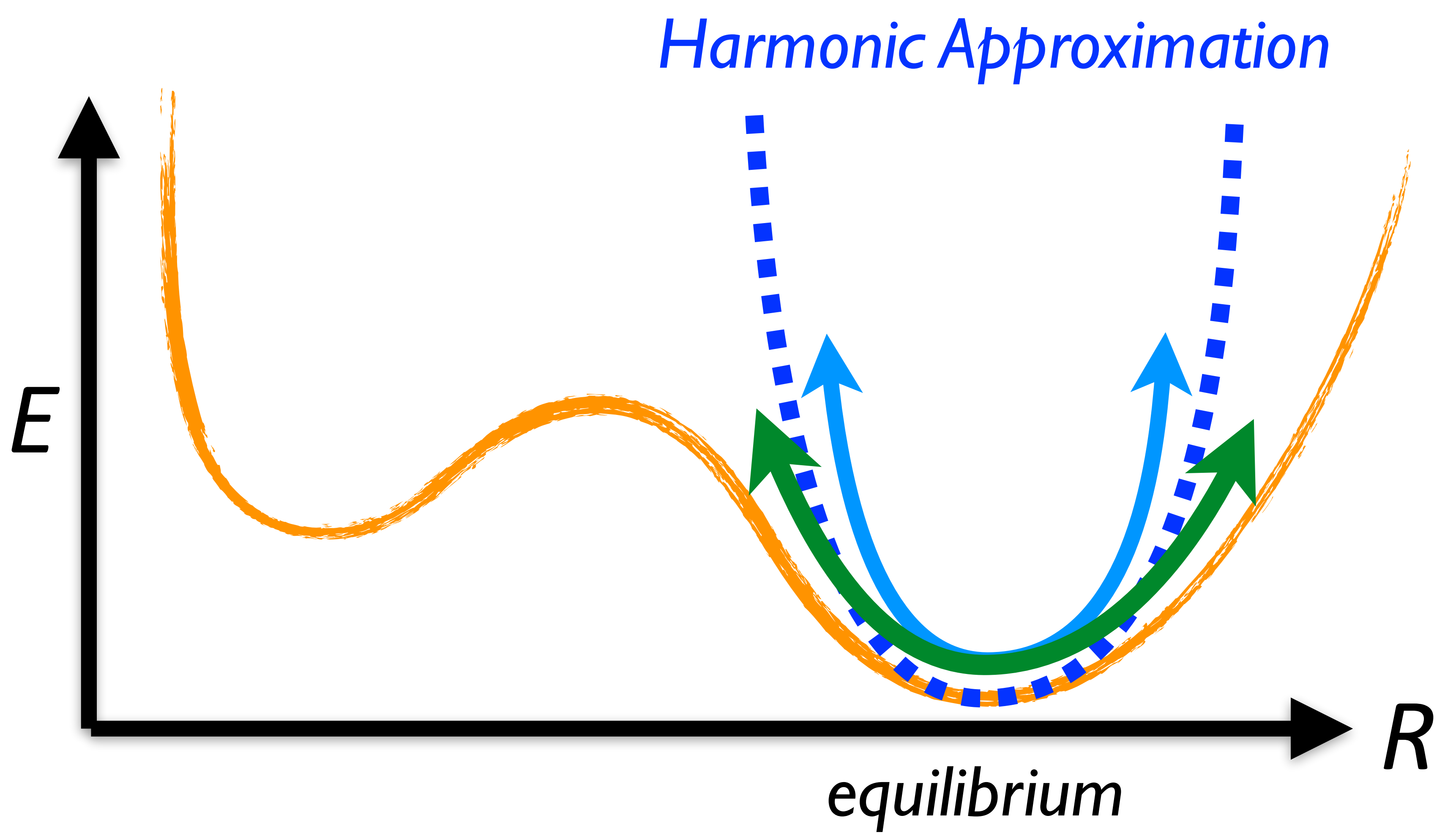



**Infinite Lifetime**

**Infinite Thermal Conductivity**

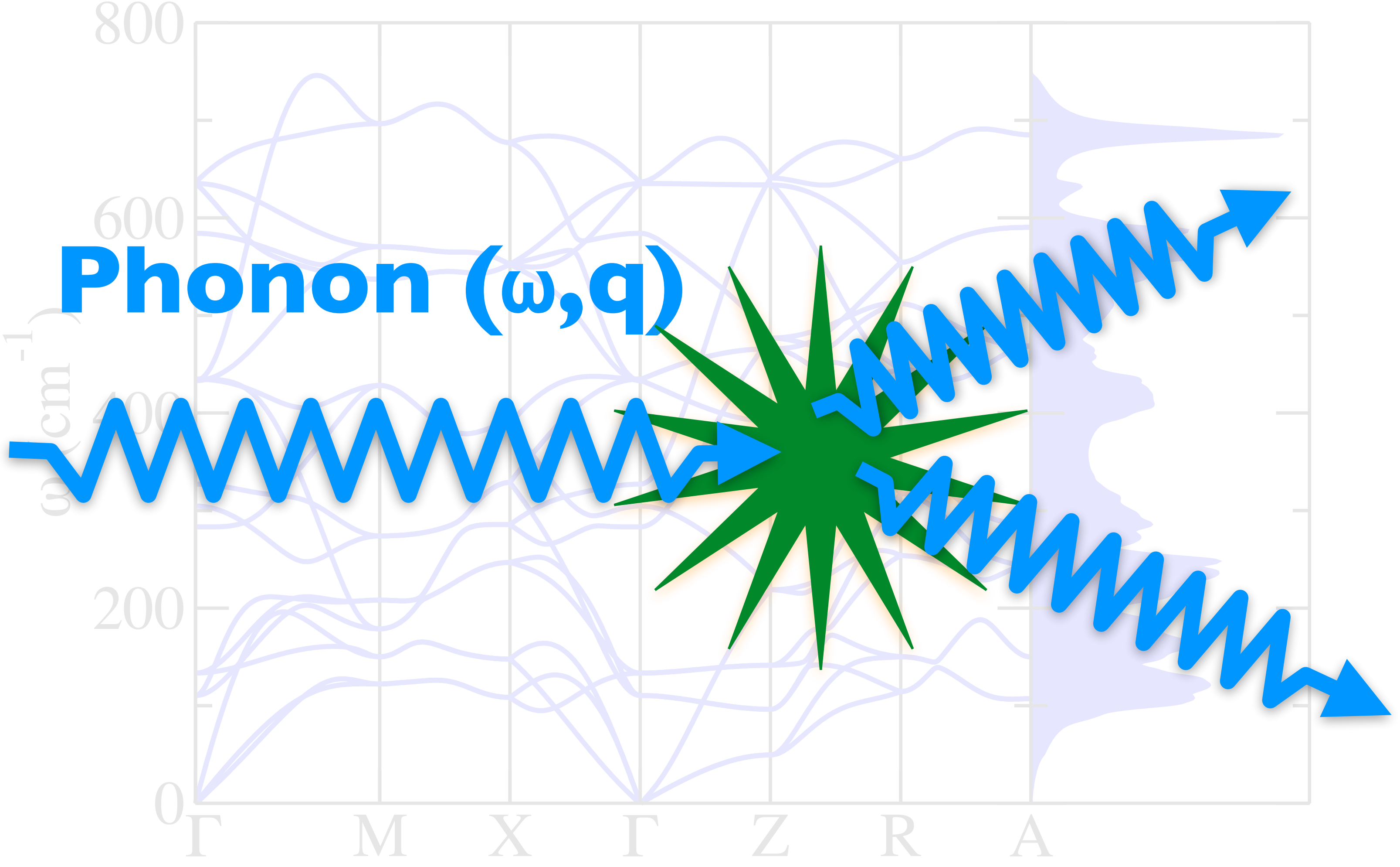
# Heat Transport Theory 101

*Real-Space Representation*




**Anharmonic** Dynamics

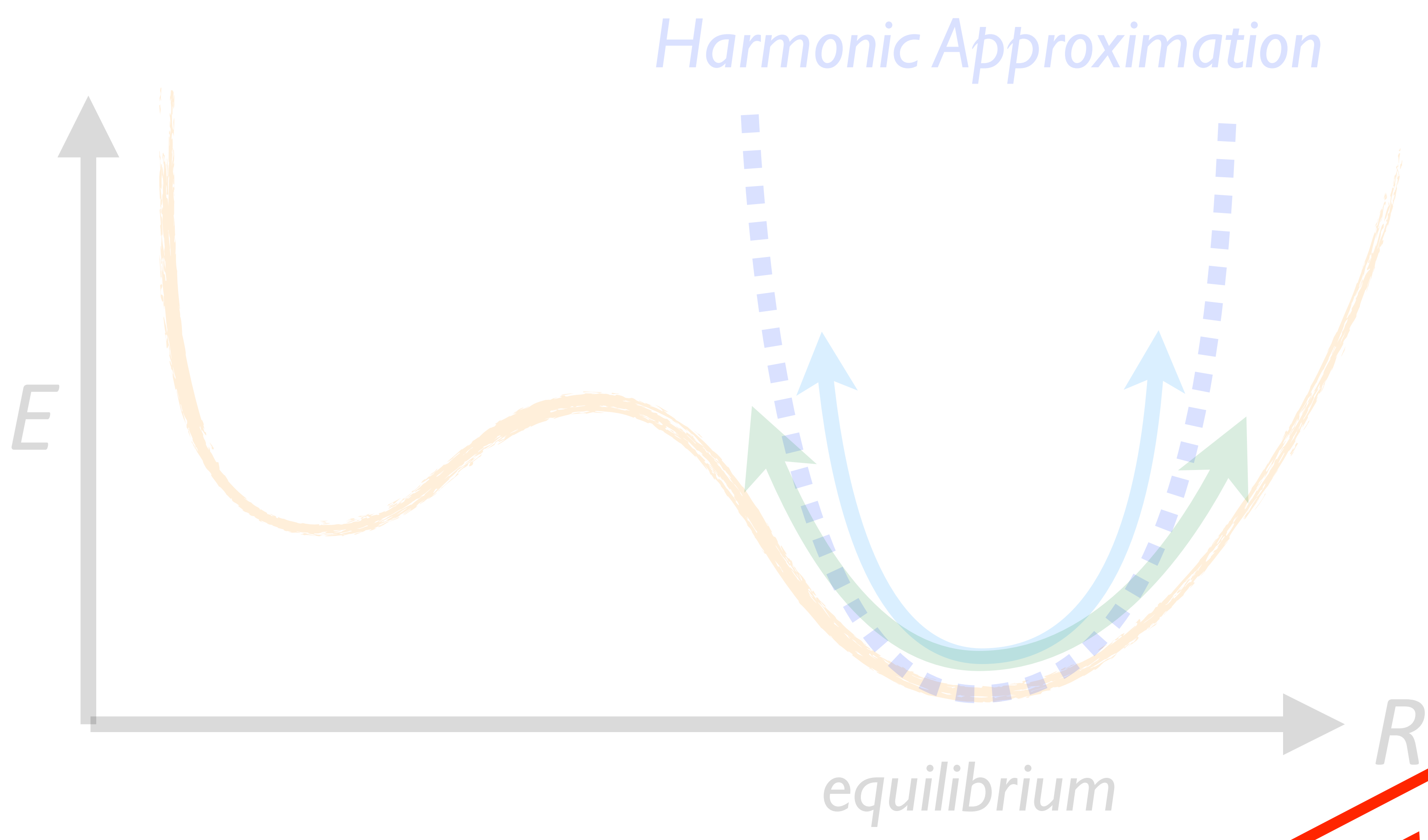
*Reciprocal-Space Representation*



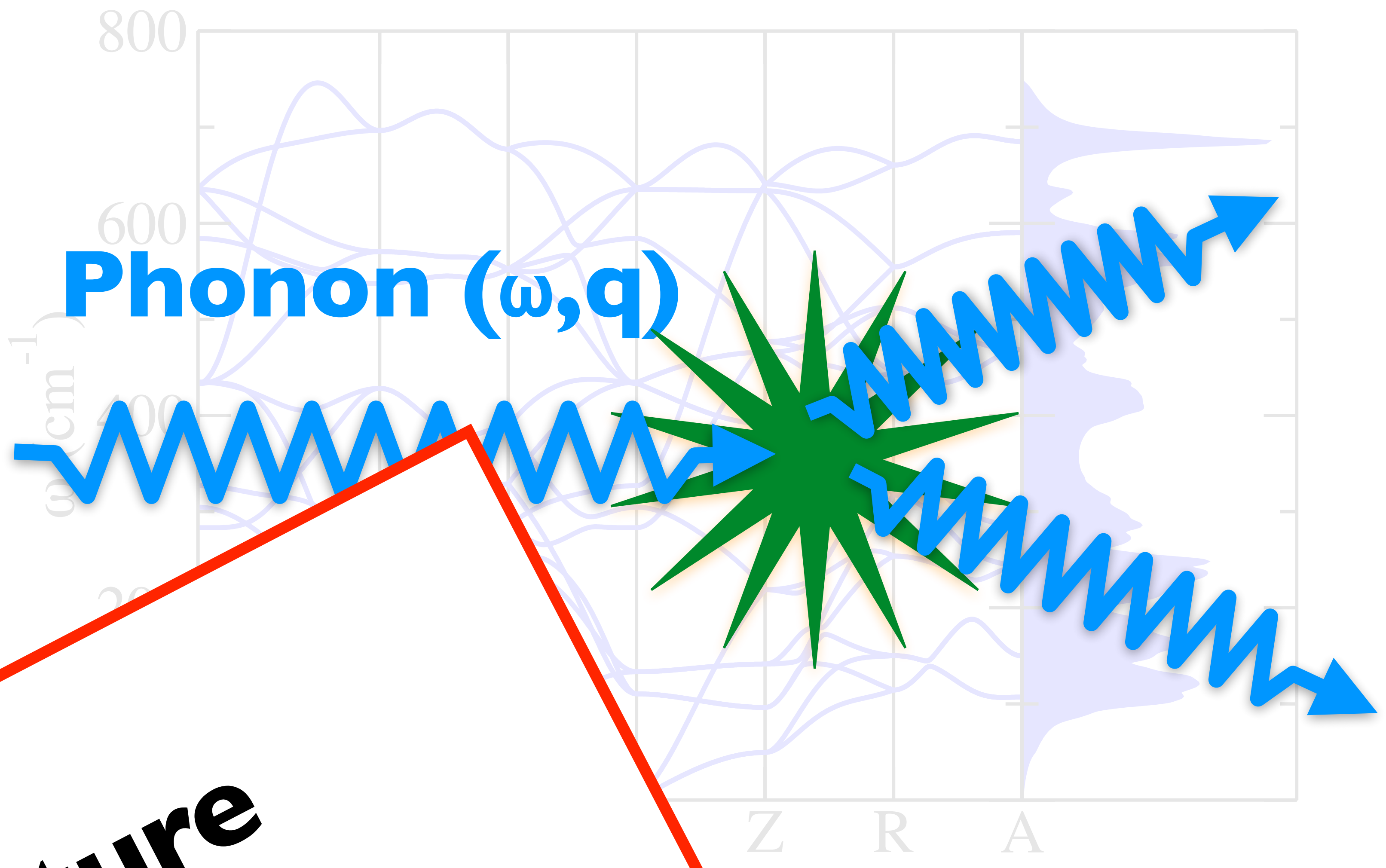

Phonon **Scattering**

# Heat Transport Theory 101

*Real-Space Representation*




*Reciprocal-Space Representation*




**Anharmonic D**

**n Scattering**

**CAVEAT:**

**Low Temperature Approximation!**

$E_{harm} \gg E_{anha}$ !

**Perturbative Treatment:**

D. A. Broido, *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).

*Density Functional Perturbation Theory*

\+ *Boltzmann Transport Equation*

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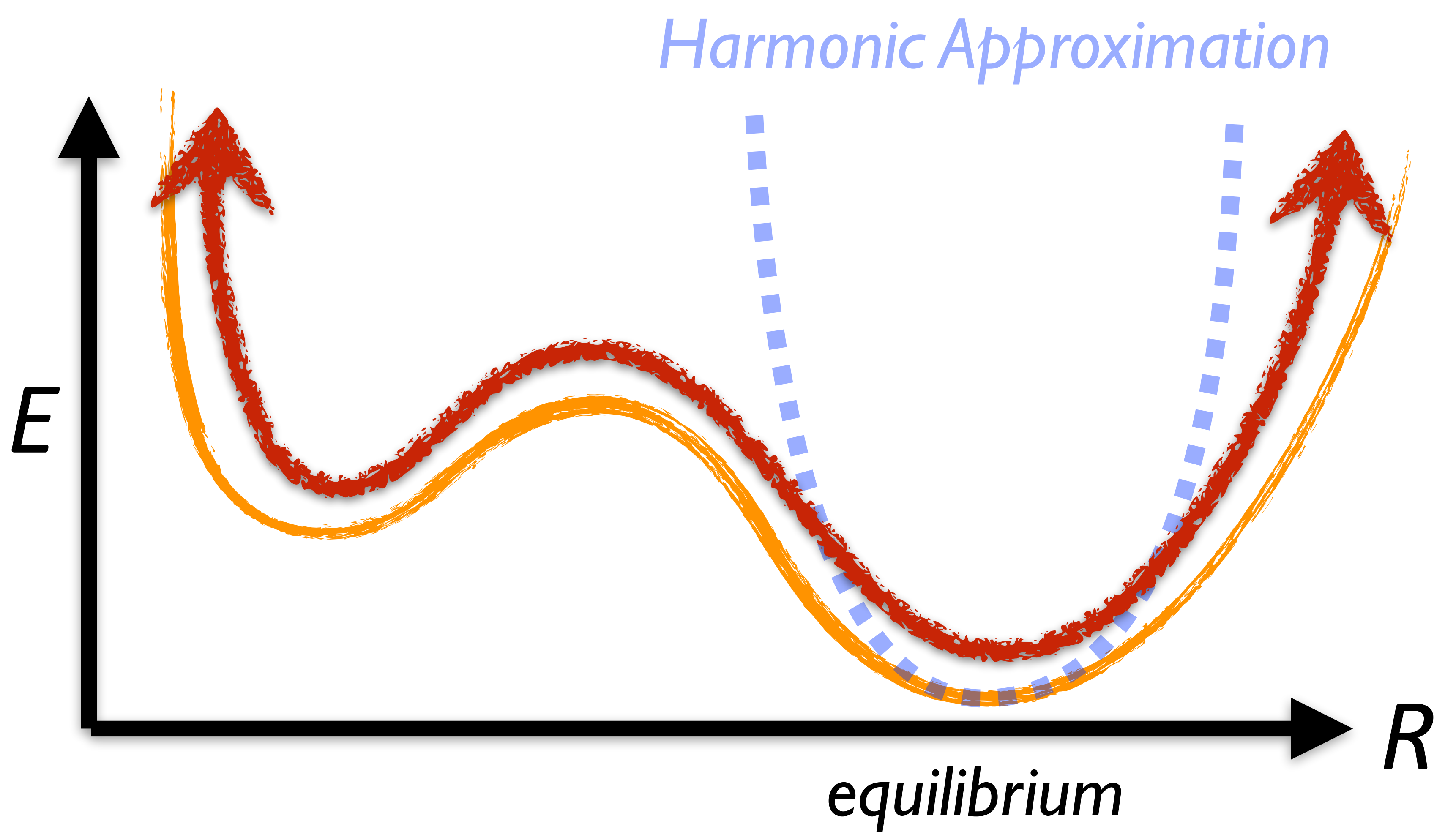
*Real-Space Representation*

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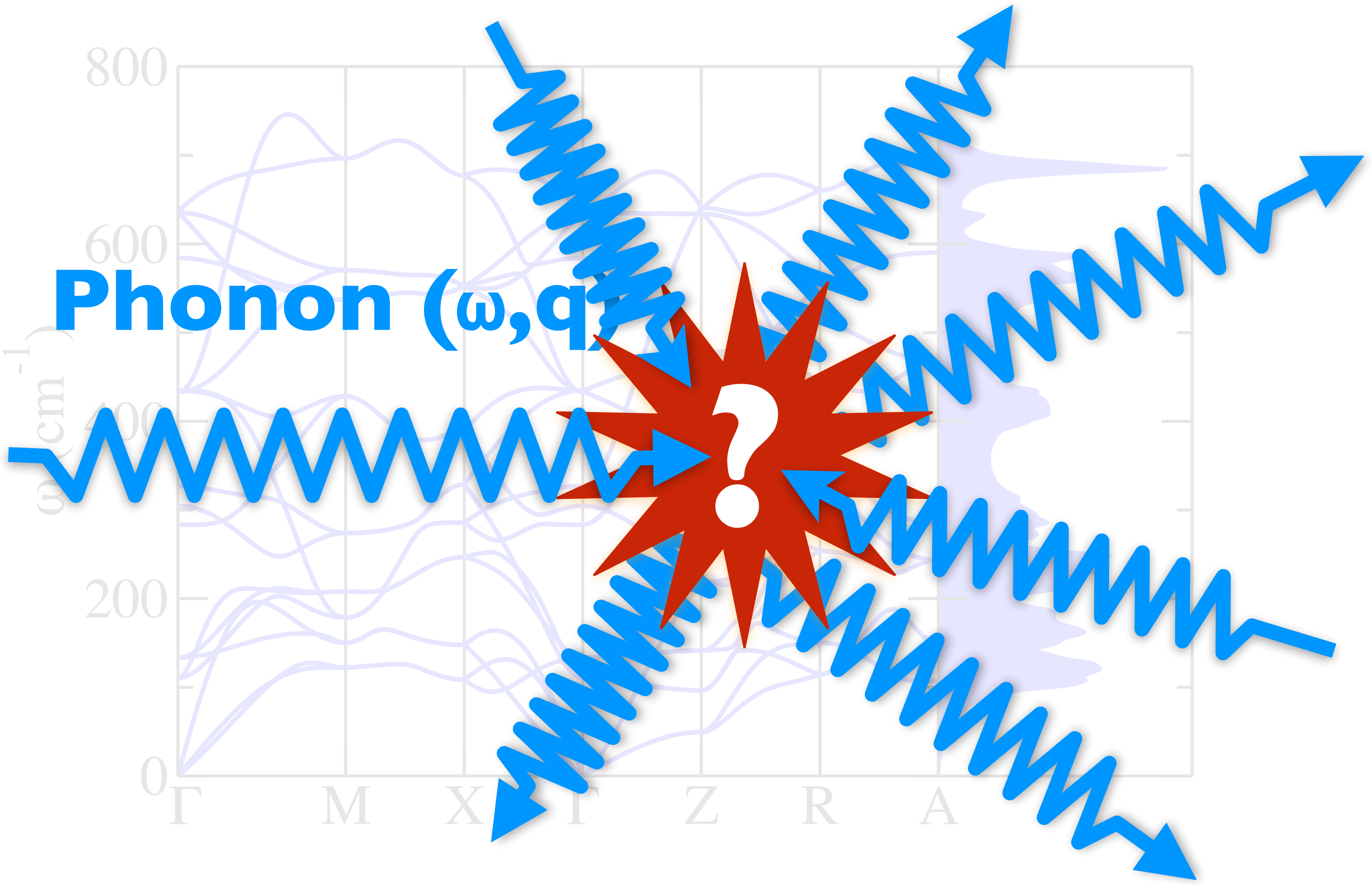


**Anharmonic** Dynamics

Phonon **Scattering**

**Strong Anharmonic Effects beyond the Realm of Perturbation Theory:**

$E_{harm} \ll E_{anha}$ **!**

***⇒ A Fully Anharmonic Theory of Heat Transport is Needed!***

# GREEN-KUBO METHOD

R. Kubo, M. Yokota, and S. Nakajima, *J. Phys. Soc. Japan* **12**, 1203 (1957).

**Fluctuation-Dissipation Theorem**

**Simulations** of the **thermodynamic equilibrium**

$\Downarrow \qquad \Downarrow \qquad \Downarrow$

**Information** about **non-equilibrium processes**

$$\kappa \sim \int_0^\infty d\tau \, \langle \, \mathbf{J}(0) \, \mathbf{J}(\tau) \rangle_{eq}$$

The **thermal conductivity** is related to the **autocorrelation function** of the **heat flux**.

# GREEN-KUBO METHOD

R. Kubo, M. Yokota, and S. Nakajima, *J. Phys. Soc. Japan* **12**, 1203 (1957).

**Green-Kubo method**...

...works in **thermal equilibrium** (linear response)

...accounts for **anharmonic** effects **to all orders**

A **first-principles** implementation of the **Green-Kubo method** faces severe...

...**conceptual challenges:** definition of the heat flux

...**numerical challenges:** size and time convergence

# THE ATOMISTIC HEAT FLUX

E. Helfand, *Phys. Rev.* **119**, 1 (1960).

*Continuity Equation:*

$$\frac{\partial E(\mathbf{r})}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{r}) = 0 \qquad \mathbf{J}(t) = \int \mathbf{j}(\mathbf{r})\, d\mathbf{r}$$

*Energy decomposition* — *Heat flux*

$$E(\mathbf{r}) = \sum_I E_I\, \delta(\mathbf{r} - \mathbf{R}_I) \quad \Rrightarrow \quad \mathbf{J}(t) = \frac{d}{dt}\left(\sum_I \mathbf{R}_I E_I\right)$$

**Correct** heat flux definition requires a **decomposition** of the **energy**, which **is not unique** by definition.

# THE VIRIAL HEAT FLUX

R. J. Hardy, *Phys. Rev.* **132**,168 (1963).

**Helfands' Heat Flux** | **Hardys' Heat Flux**

$$\mathbf{J}(t) = \boxed{\frac{d}{dt}\left(\sum_I \mathbf{R}_I \; E_I\right)} = \boxed{\cancel{\sum_I \mathbf{V}_I E_I} + \sum_I \mathbf{R}_I \dot{E}_I}$$

~~**Convective Heat Flux**~~

**Liquids & Gases:**

⇛ use **energy density**

A. Marcolongo, P. Umari, and S. Baroni, *Nat. Phys.* **12**, 80 (2016).

***Virial Heat Flux:***

- **Unique:**
  Does **not** depend on **partitioning**
- Describes **phonon** transports
- **Well-defined** for **classical** potentials
- **Well-defined**
  in ***first-principles*** **frameworks**

# ALL-ELECTRON FORMALISM FOR TOTAL ENERGY STRAIN DERIVATIVES

F. Knuth, C. Carbogno, V. Atalla, V. Blum, and M. Scheffler, *Comp. Phys. Comm.* **190**, 33 (2015).

## Formulas for analytical stress

$$\sigma_{ij} = \sigma_{ij}^{\mathrm{HF}} + \sigma_{ij}^{\mathrm{MP}} + \sigma_{ij}^{\mathrm{Pulay}} + \sigma_{ij}^{\mathrm{kin}} + \sigma_{ij}^{\mathrm{Jac}}.$$

$$\sigma_{ij}^{\mathrm{HF}} = \frac{1}{2V} \sum_{\alpha,\beta\neq\alpha} \frac{\partial v_{\beta}^{\mathrm{es,tot}}(|\mathbf{R}_\alpha - \mathbf{R}_\beta|)}{\partial R_i^\alpha} (\mathbf{R}_\alpha - \mathbf{R}_\beta)_j$$

$$\sigma_{ij}^{\mathrm{MP}} = \frac{1}{V} \sum_{\alpha} \int_{\mathrm{UC}} \mathrm{d}\mathbf{r} \left[ n(\mathbf{r}) - \frac{1}{2} n_{\mathrm{MP}}(\mathbf{r}) \right] \frac{\partial v_{\alpha}^{\mathrm{es,tot}}(|\mathbf{r} - \mathbf{R}_\alpha|)}{\partial r_i} (\mathbf{r} - \mathbf{R}_\alpha)_j$$
$$- \frac{1}{2V} \sum_{\alpha} \int_{\mathrm{UC}} \mathrm{d}\mathbf{r} \frac{\partial n_{\alpha}^{\mathrm{MP}}(\mathbf{r} - \mathbf{R}_\alpha)}{\partial r_i} (\mathbf{r} - \mathbf{R}_\alpha)_j v_{\mathrm{es,tot}}(\mathbf{r})$$

$$\sigma_{ij}^{\mathrm{Pulay}} = \frac{2}{V} \sum_{k} \sum_{\alpha,l(\alpha)} \sum_{\beta,m(\beta)} f_k c_{kl} c_{km} \int_{\mathrm{UC}} \mathrm{d}\mathbf{r} \frac{\partial \varphi_l(\mathbf{r} - \mathbf{R}_\alpha)}{\partial r_i} (\mathbf{r} - \mathbf{R}_\alpha)_j \left[ \hat{h}_{\mathrm{KS}} - \varepsilon_k \right] \varphi_m(\mathbf{r} - \mathbf{R}_\beta)$$

$$\sigma_{ij}^{\mathrm{kin}} = \frac{1}{V} \sum_{k} \sum_{\alpha,l(\alpha)} \sum_{\beta,m(\beta)} f_k c_{kl} c_{km} \int_{\mathrm{UC}} \mathrm{d}\mathbf{r}\, \varphi_l(\mathbf{r} - \mathbf{R}_\alpha)(\mathbf{r} - \mathbf{R}_\alpha)_j \left[ \frac{\partial}{\partial r_i} \frac{\partial}{\partial r_j} \varphi_m(\mathbf{r} - \mathbf{R}_\beta) \right]$$

$$\sigma_{ij}^{\mathrm{Jac}} = \frac{1}{V} \delta_{ij} \left[ E_{\mathrm{xc}}[n] - \int \mathrm{d}\mathbf{r}\, n(\mathbf{r}) v_{\mathrm{xc}}(\mathbf{r}) - \frac{1}{2} \int \mathrm{d}\mathbf{r}\, n_{\mathrm{MP}}(\mathbf{r}) v_{\mathrm{es,tot}}(\mathbf{r}) \right]$$

# ALL-ELECTRON FORMALISM FOR TOTAL ENERGY STRAIN DERIVATIVES

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$$\sigma_{ij}^{\mathrm{HF}} = \frac{1}{2V} \sum \frac{\partial v_{\beta}^{\mathrm{es,tot}}(|\mathbf{R}_\alpha - \mathbf{R}_\beta|)}{\partial R^{\alpha}} (\mathbf{R}_\alpha - \mathbf{R}_\beta)_j$$

**⇛ Unique and well-defined!**

$$\sigma_{ij}^{\mathrm{Pulay}} = \frac{2}{V} \sum_k \sum_{\alpha,l(\alpha)} \sum_{\beta,m(\beta)} f_k c_{kl} c_{km} \int_{\mathrm{UC}} \mathrm{d}\mathbf{r}\, \frac{\partial \varphi_l(\mathbf{r} - \mathbf{R}_\alpha)}{\partial r_i} (\mathbf{r} - \mathbf{R}_\alpha)_j \left[\hat{h}_{\mathrm{KS}} - \varepsilon_k\right] \varphi_m(\mathbf{r} - \mathbf{R}_\beta)$$

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$$\sigma_{ij}^{\mathrm{Jac}} = \frac{1}{V}\delta_{ij}\left[E_{\mathrm{xc}}[n] - \int \mathrm{d}\mathbf{r}\, n(\mathbf{r}) v_{\mathrm{xc}}(\mathbf{r}) - \frac{1}{2}\int \mathrm{d}\mathbf{r}\, n_{\mathrm{MP}}(\mathbf{r}) v_{\mathrm{es,tot}}(\mathbf{r})\right]$$

# VALIDATION OF THE HEAT FLUX

C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

*Simple Recipe:*

1) Run aiMD to obtain trajectories $\boldsymbol{R}_I^{DFT}(t)$, $\boldsymbol{V}_I^{DFT}(t)$ as well as $\boldsymbol{J}^{DFT}(t)$
2) Compute $\boldsymbol{J}^{harm}(t)$ via the harmonic potential at $\boldsymbol{R}_I^{DFT}(t)$ and $\boldsymbol{V}_I^{DFT}(t)$
3) Compare $\boldsymbol{J}^{DFT}(t)$ *and* $\boldsymbol{J}^{harm}(t)$

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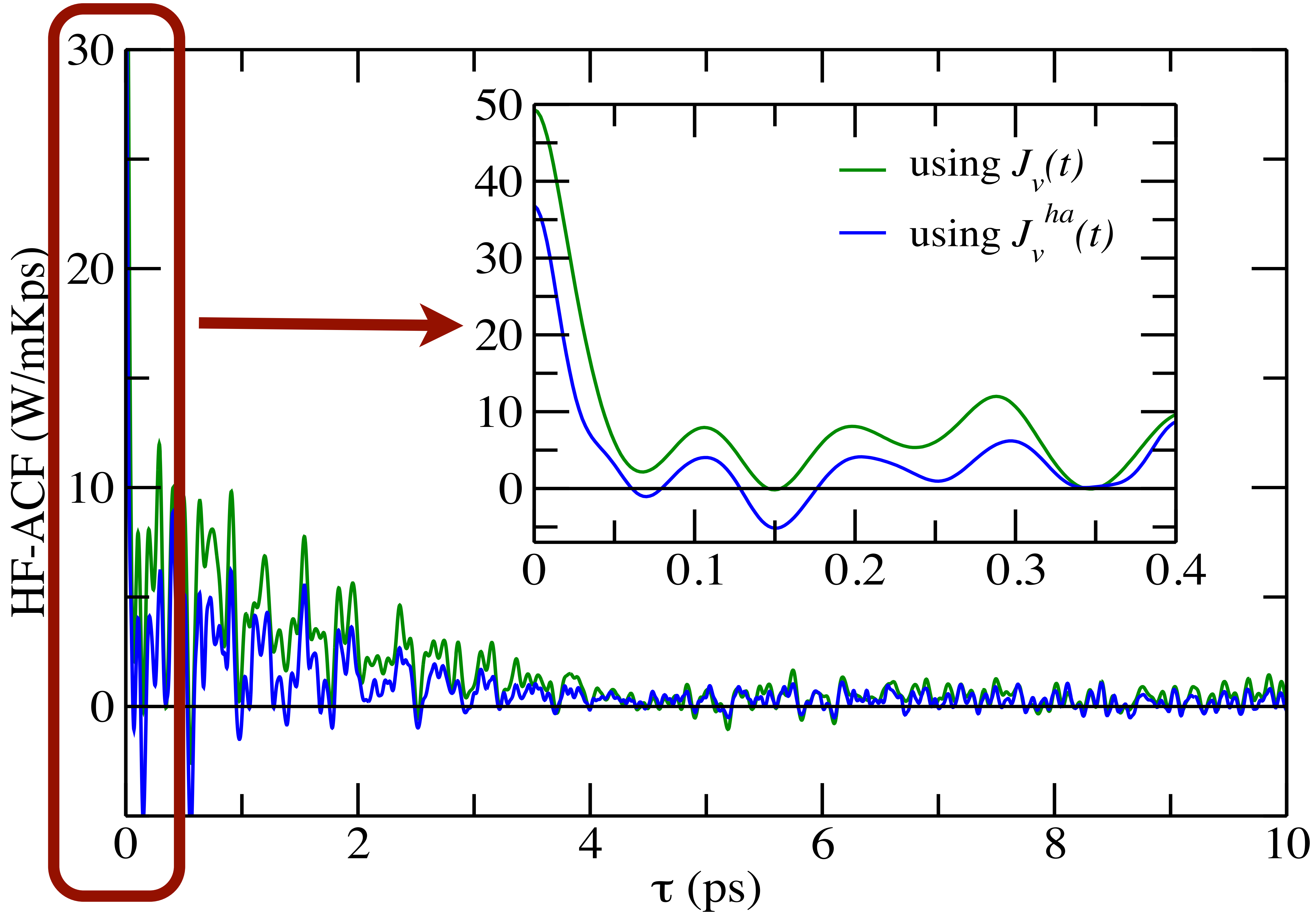


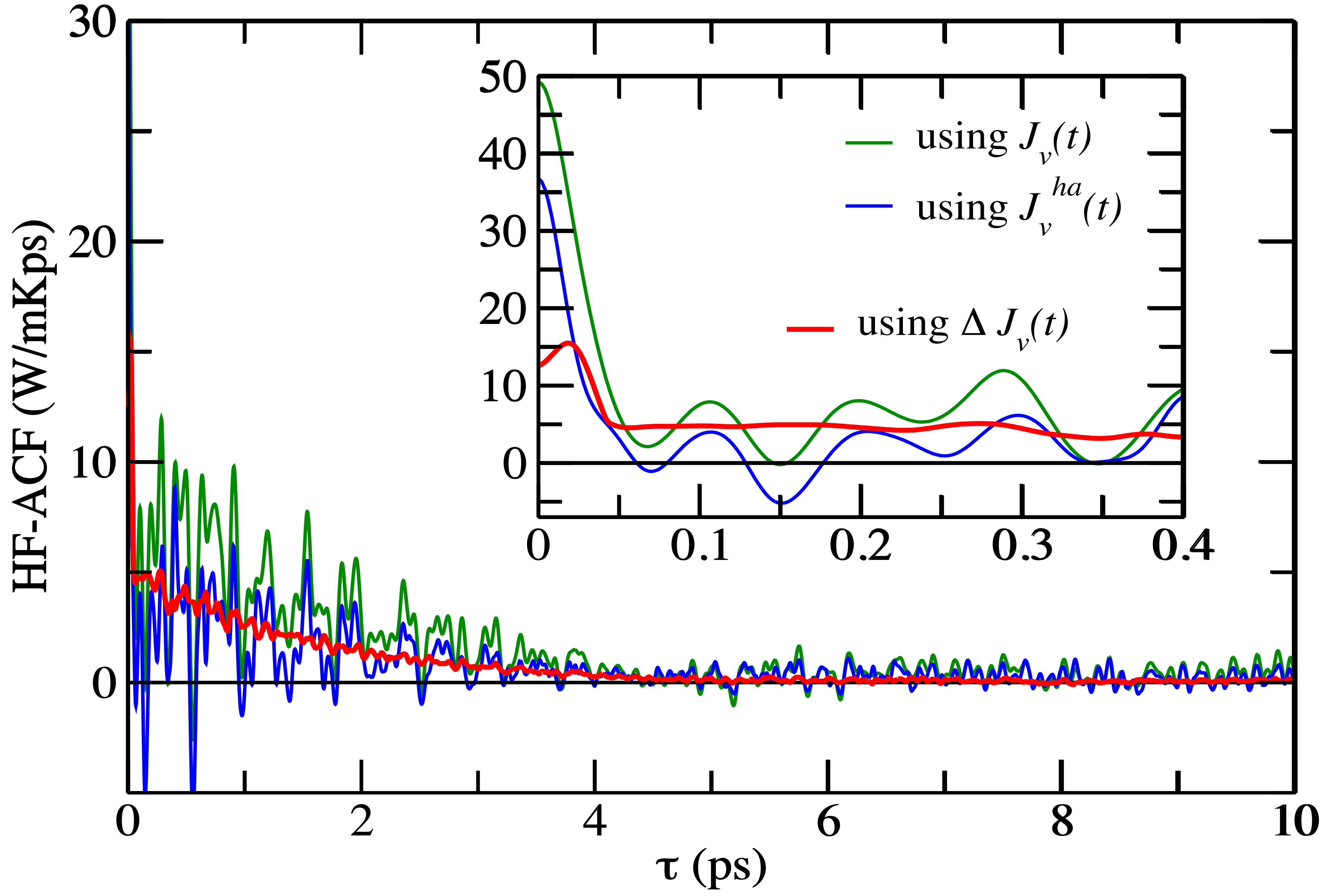

*Computational Details:*

- **pristine Si** (diamond)
- **64** atoms (2x2x2 cell)
- Temperature **1000K**
- **LDA** XC-Functional
- **>200ps** of *ab initio* MD

Full anharmonic DFT flux and harmonic flux (evaluated along the DFT trajectory) yield comparable auto-correlation functions.

**Numerical Challenge:**
Time and Size Convergence

# HOW TO BOOST CONVERGENCE?




Decompose heat flux into contributions from higher/lower orders of the Taylor expansion

$$J_v(t) = \Delta J_v(t) + J_v^{ha}(t)$$

$$\langle J_v, J_v \rangle = \langle \Delta J_v, \Delta J_v \rangle + \langle J_v^{ha}, \Delta J_v \rangle + \langle \Delta J_v, J_v^{ha} \rangle + \langle J_v^{ha}, J_v^{ha} \rangle$$

**Rapid Decay!**

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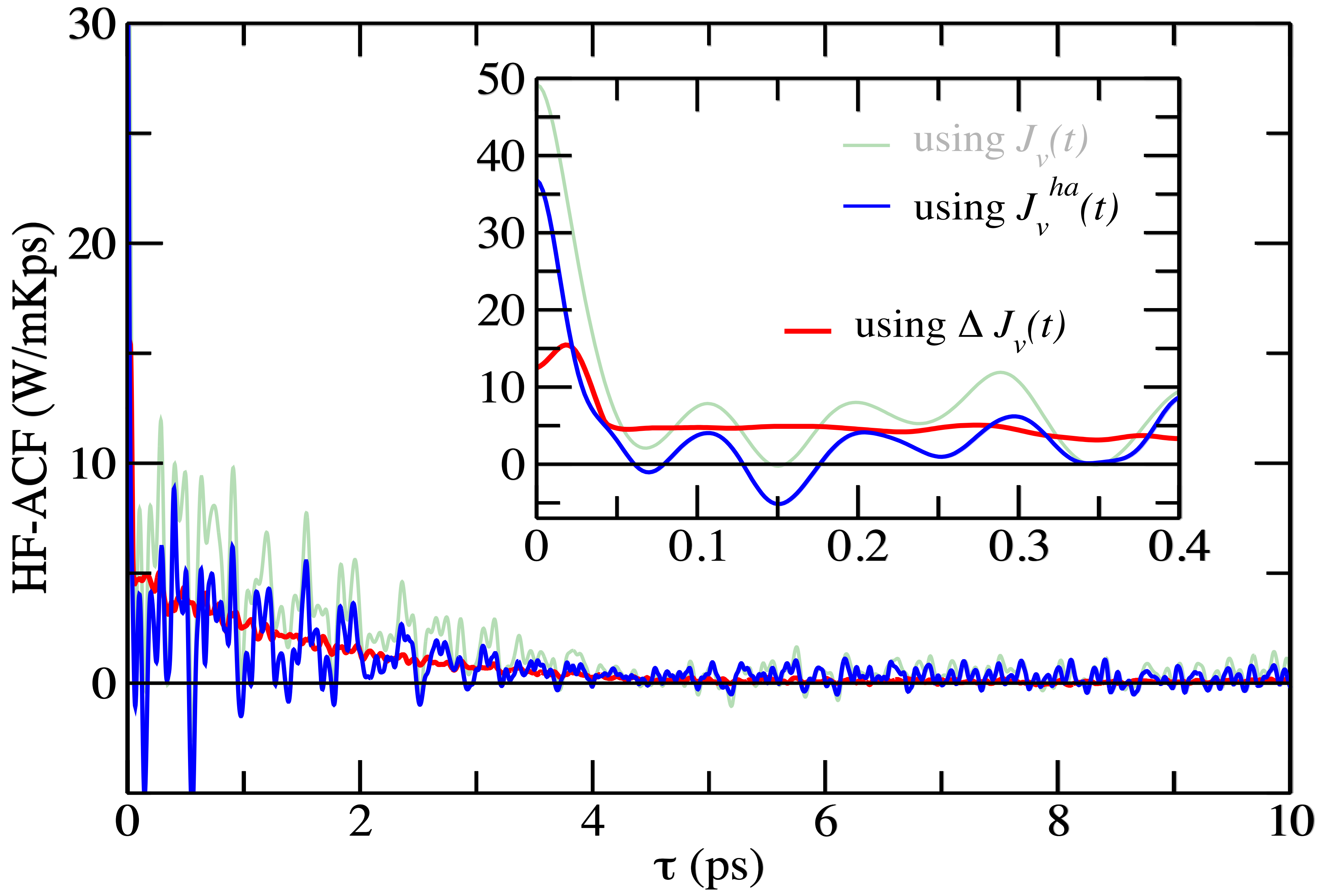


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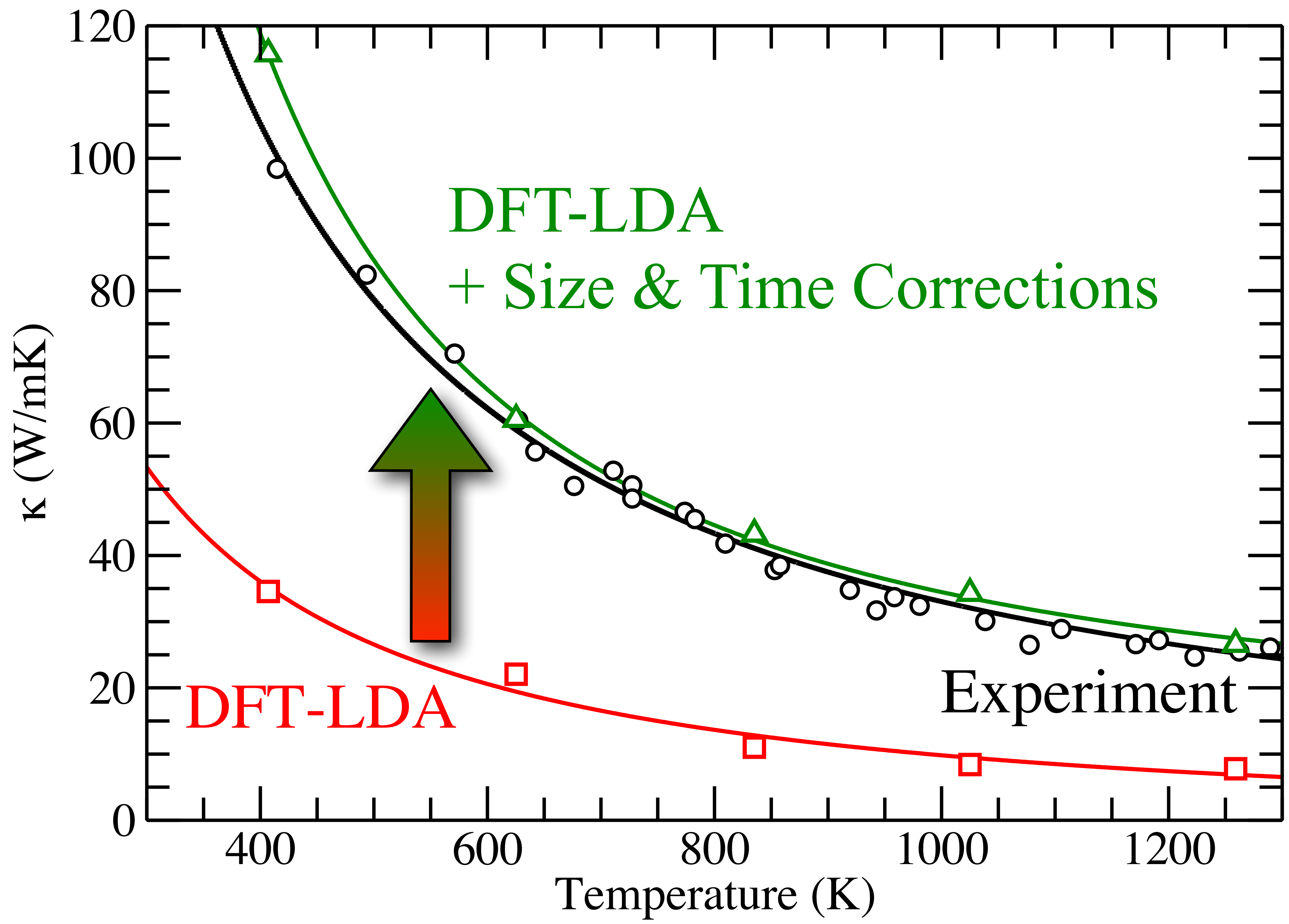
**Slow Decay!**

Can be (time and size) converged independently!

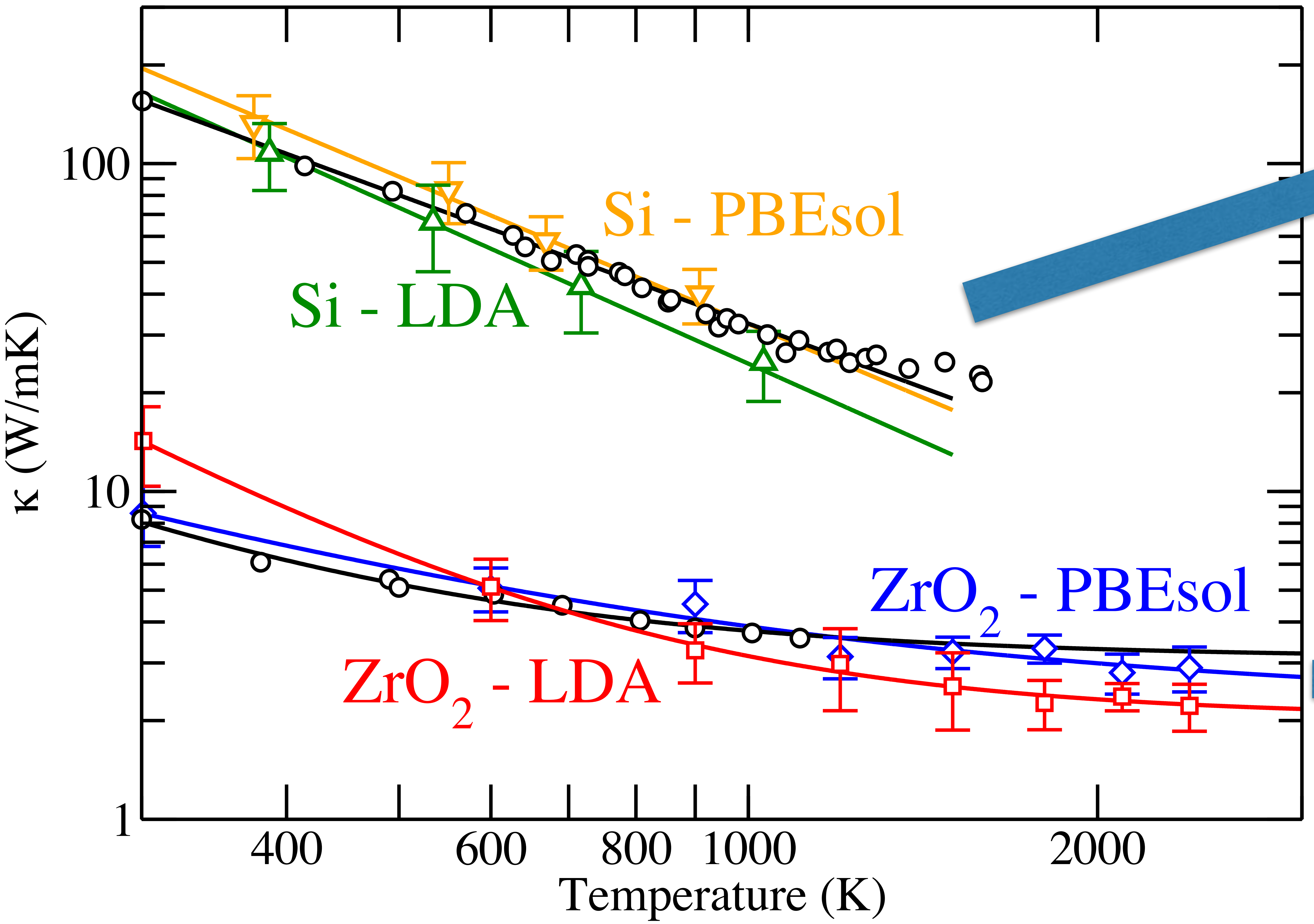
# EXTRAPOLATION FOR SILICON

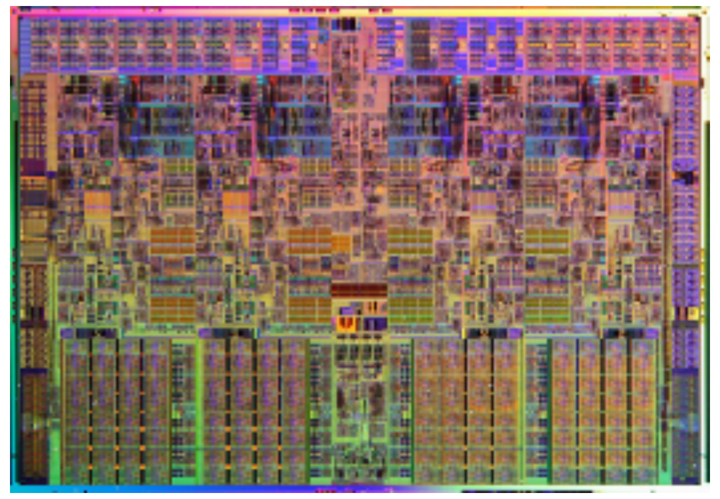



Extrapolation procedure yields satisfactory results!

# APPLICATION TO SILICON AND ZIRCONIA

C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).



Accurate computation of the thermal conductivities in solids achievable from first principles.

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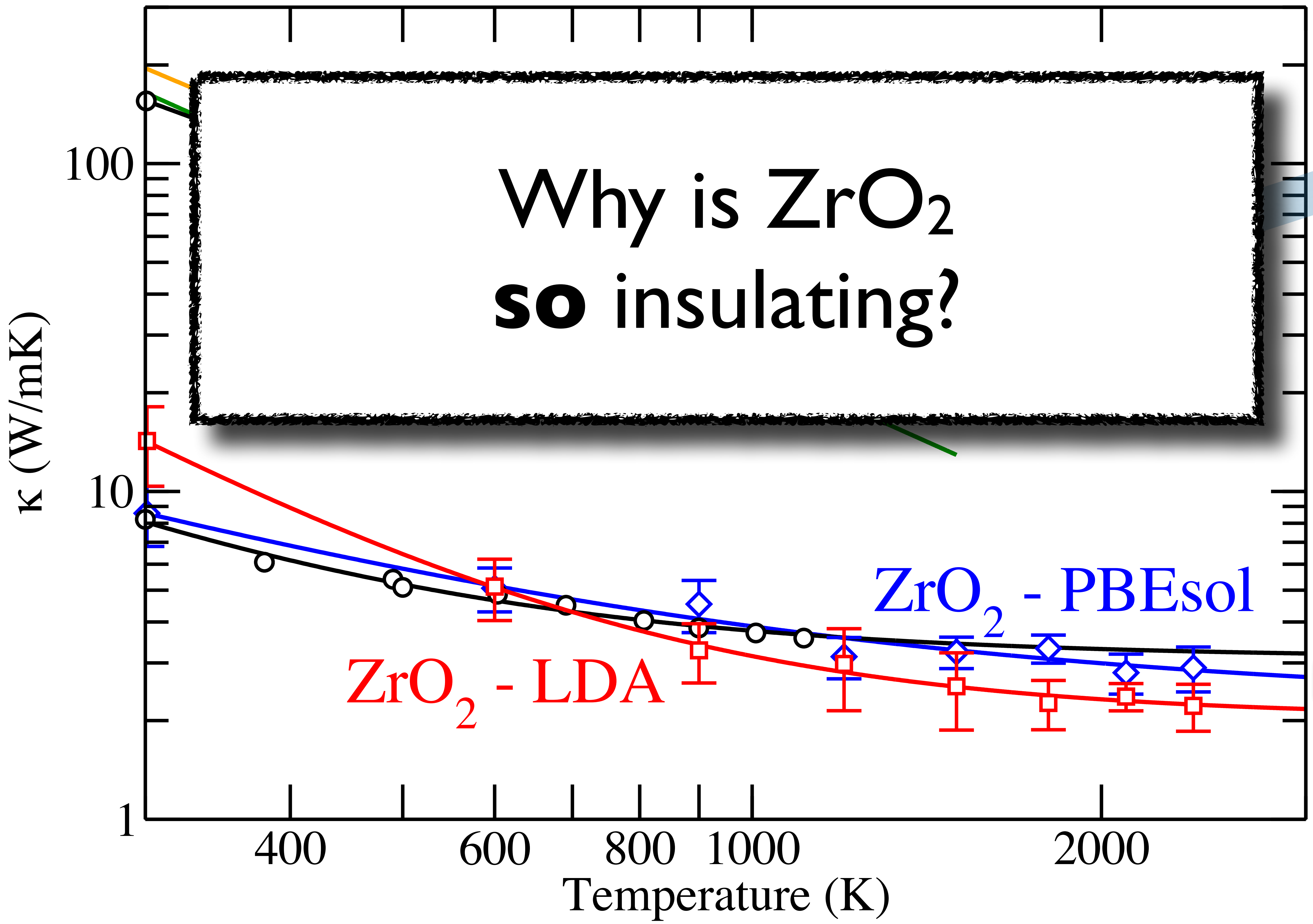


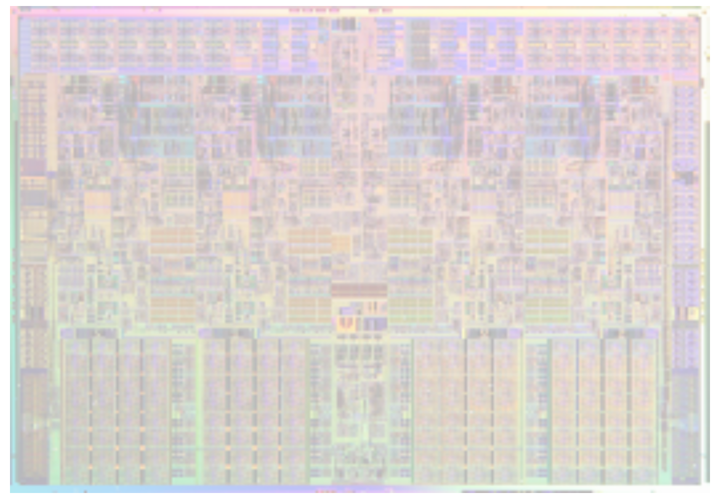

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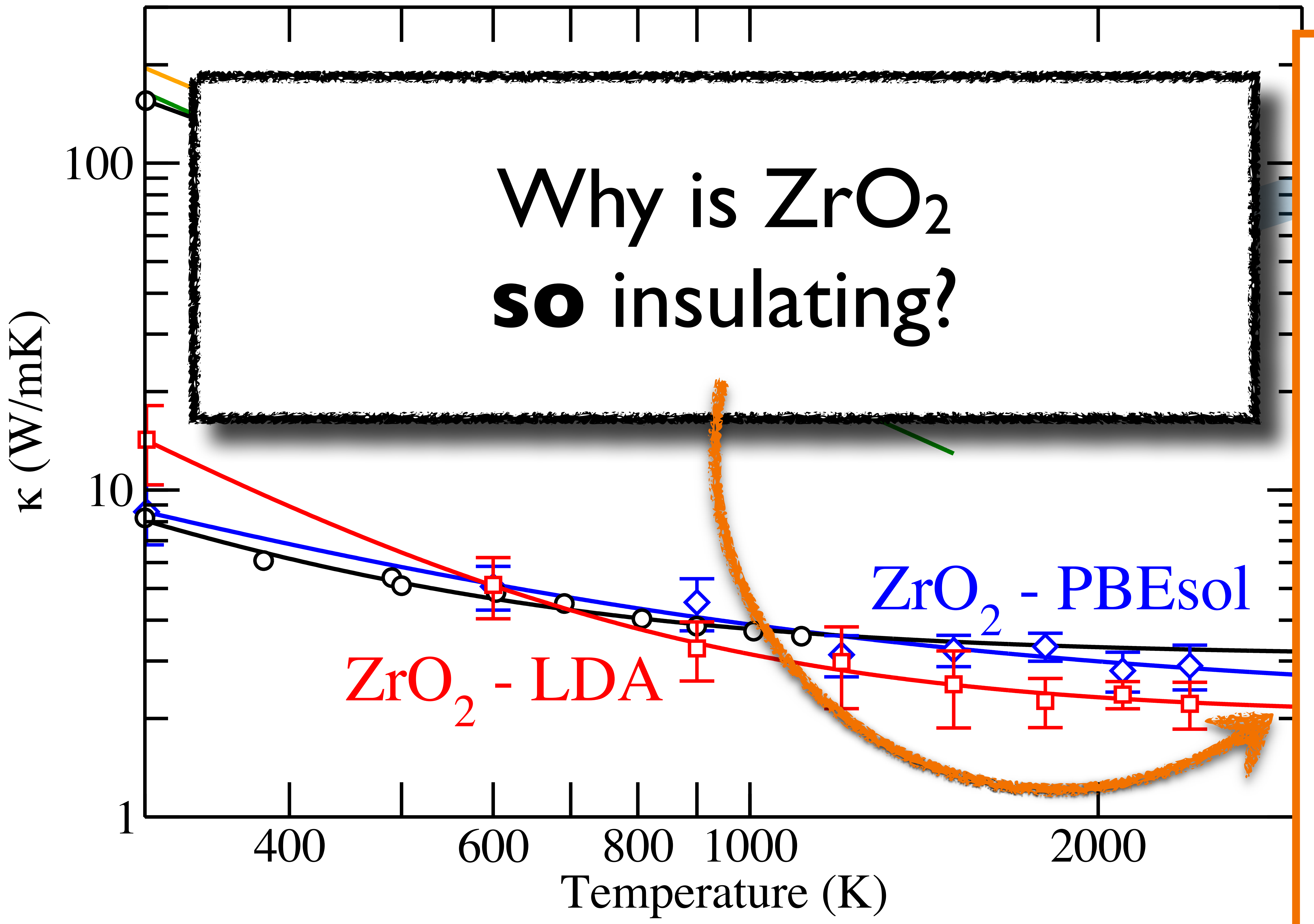
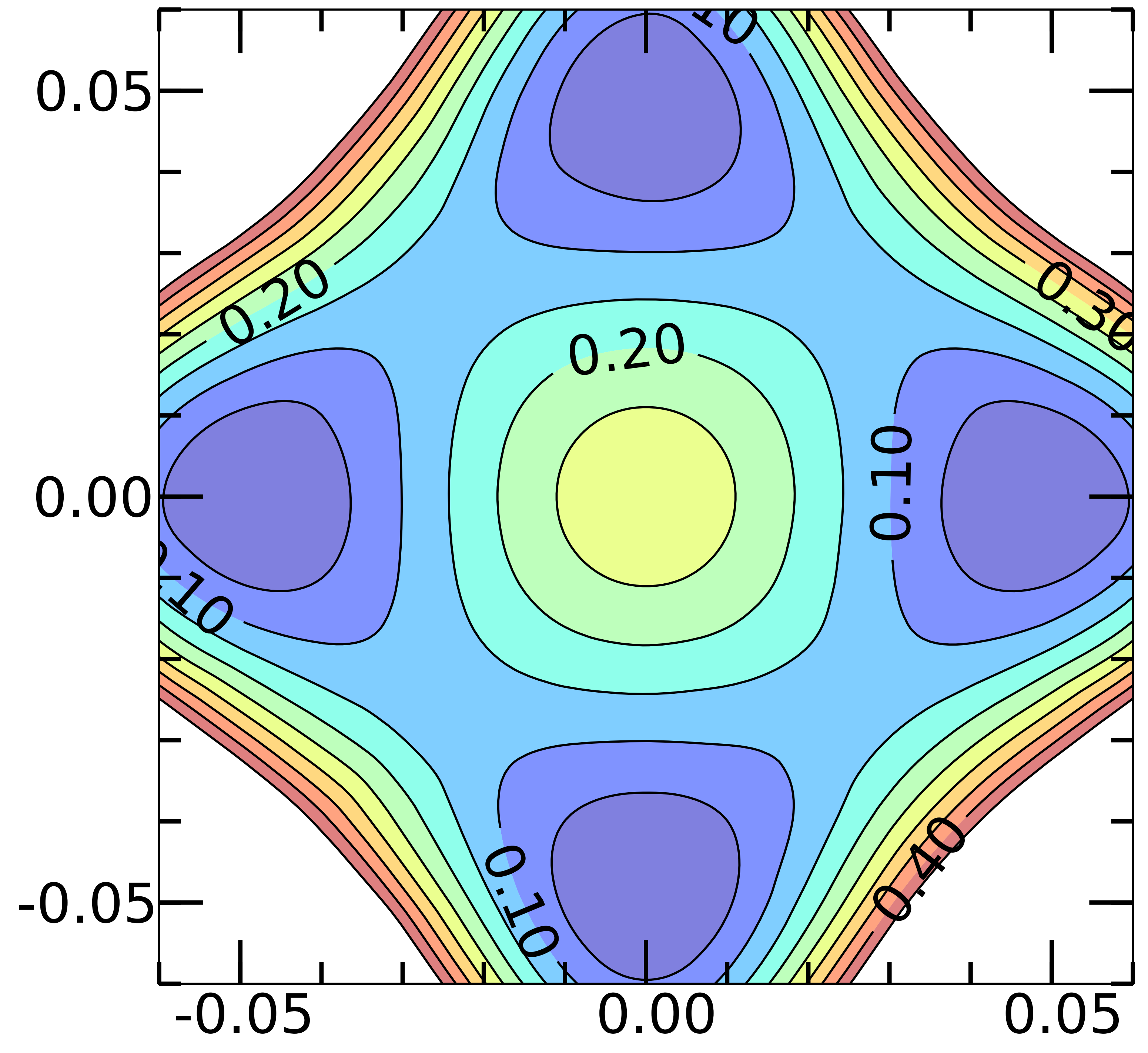



Why is $ZrO_2$
**so** insulating?

Potential Energy Surface of $ZrO_2$

C. Carbogno, C. G. Levi, C. G. Van de Walle, and M. Scheffler, PRB **90**, 144109 (2014).




Accurate computation of the thermal

in solids achievable from first pr

# Take-Home Messages

1) *Ab-initio* Green-Kubo method **quantitatively** describes the **lattice thermal conductivity** both for **very harmonic** and for **strongly anharmonic** systems.

C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

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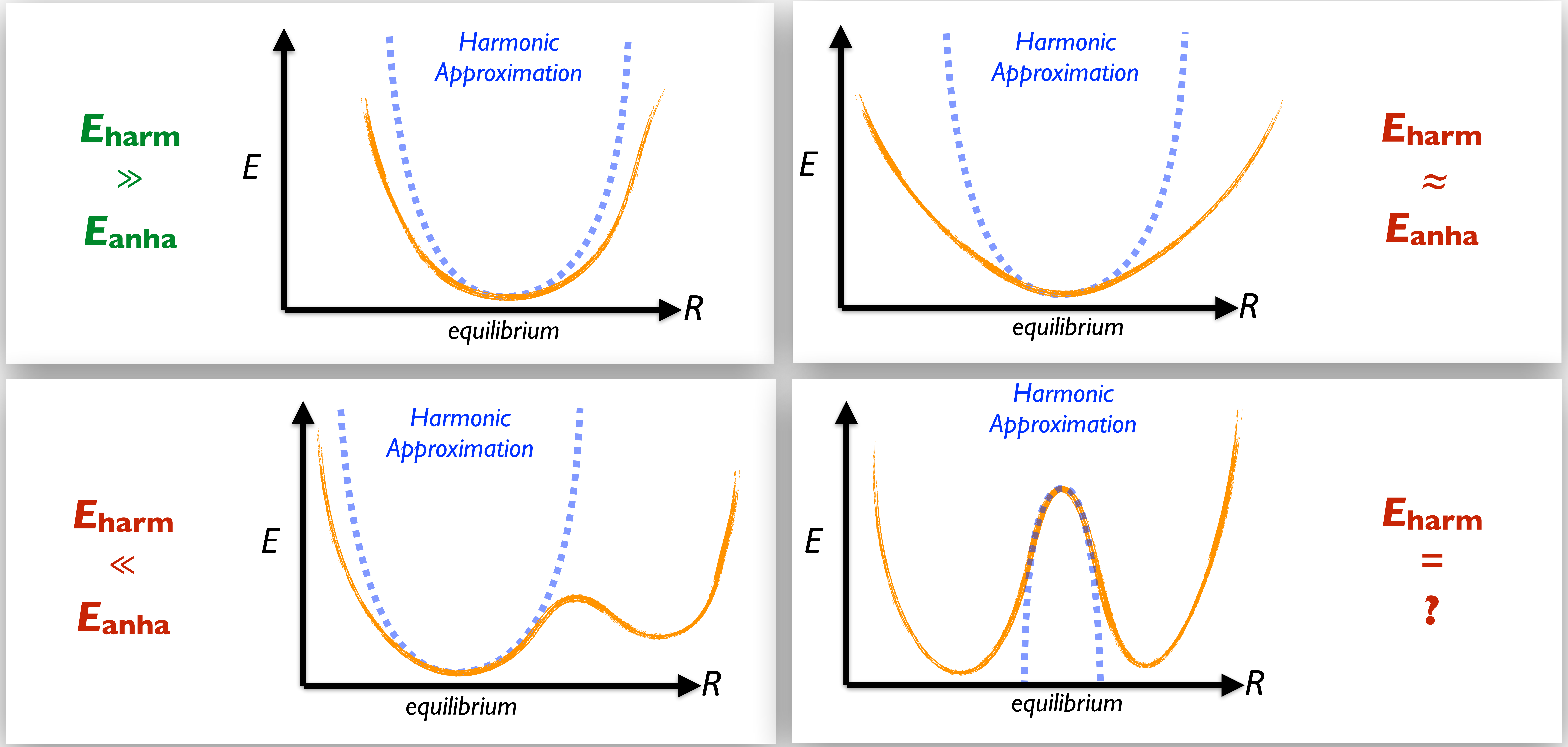
However, the *ab-initio* Green-Kubo method can be **computationally excruciatingly expensive**, especially for **good** heat conductors (long lifetimes, large mean free paths).

# What is Anharmonicity?



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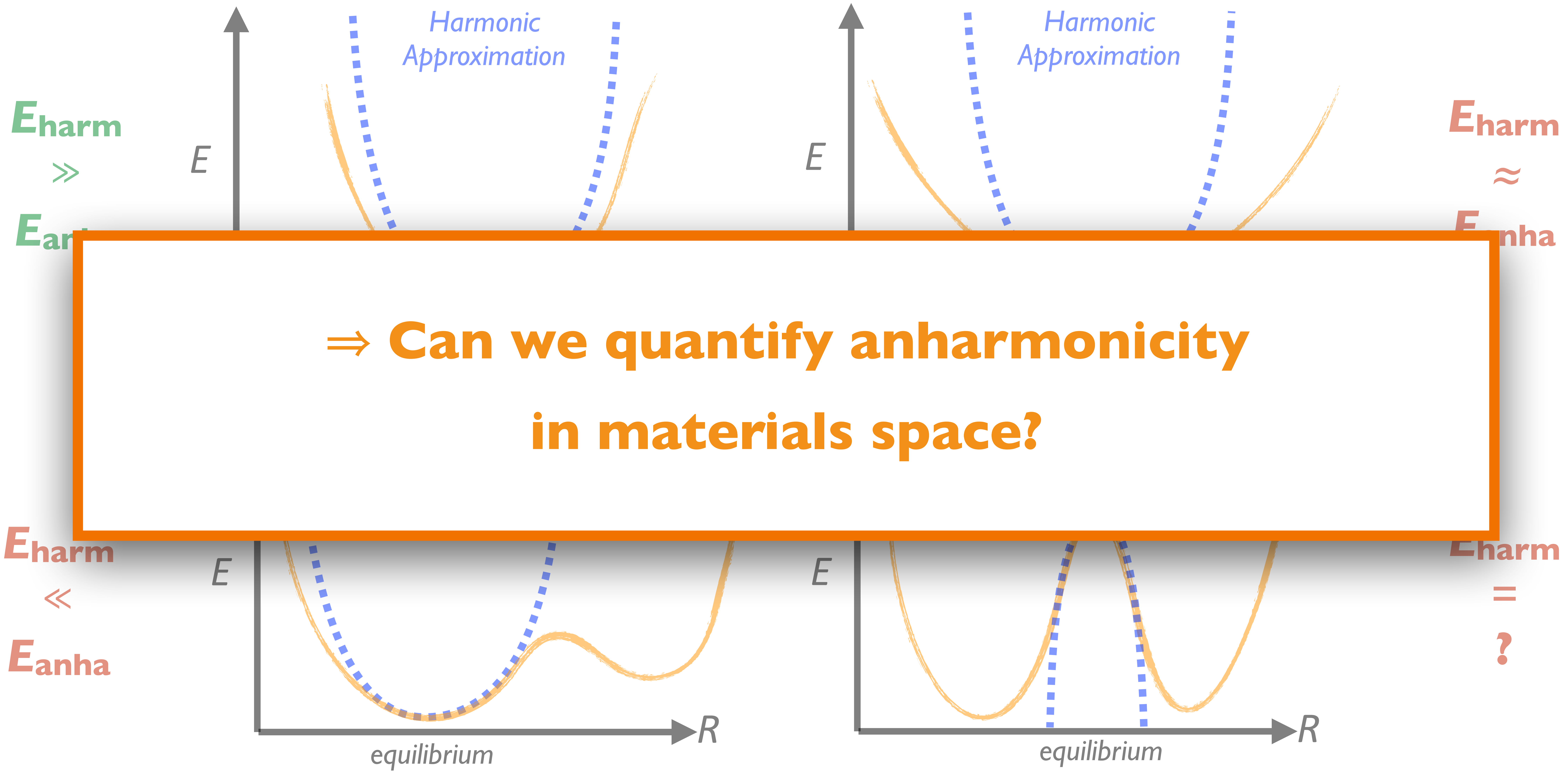
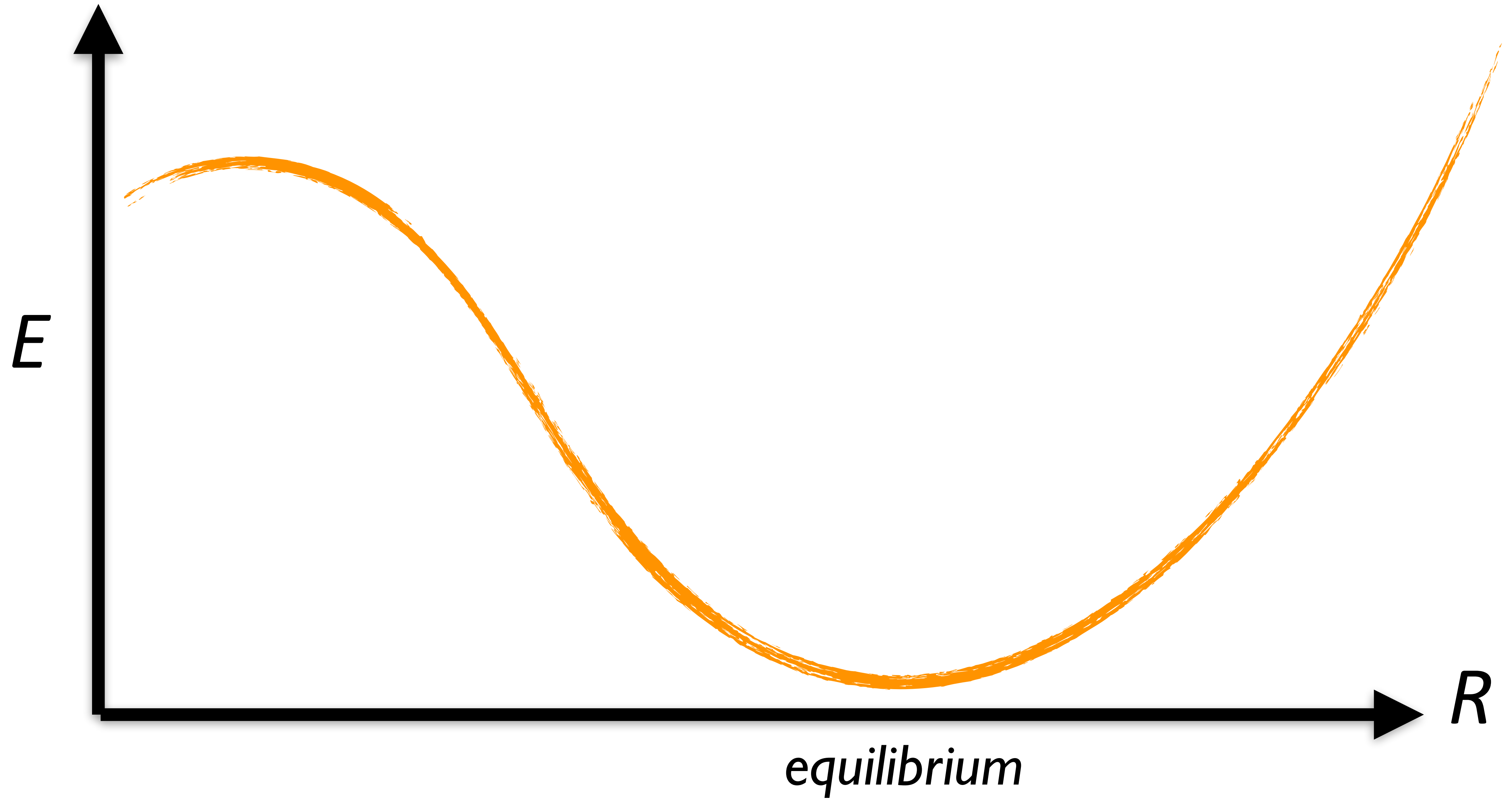



**⇒ Can we quantify anharmonicity in materials space?**

# Anharmonicity Quantification

How do $\boldsymbol{E}_{\mathbf{harm}}$ and $\boldsymbol{E}_{\mathbf{anha}} = \boldsymbol{E}_{\boldsymbol{DFT}}$ compare in different materials?

F. Knoop, T. A. R. Purcell, M. Scheffler, and C. Carbogno, *Phys. Rev. Mater.* **4**, 083809 (2020).



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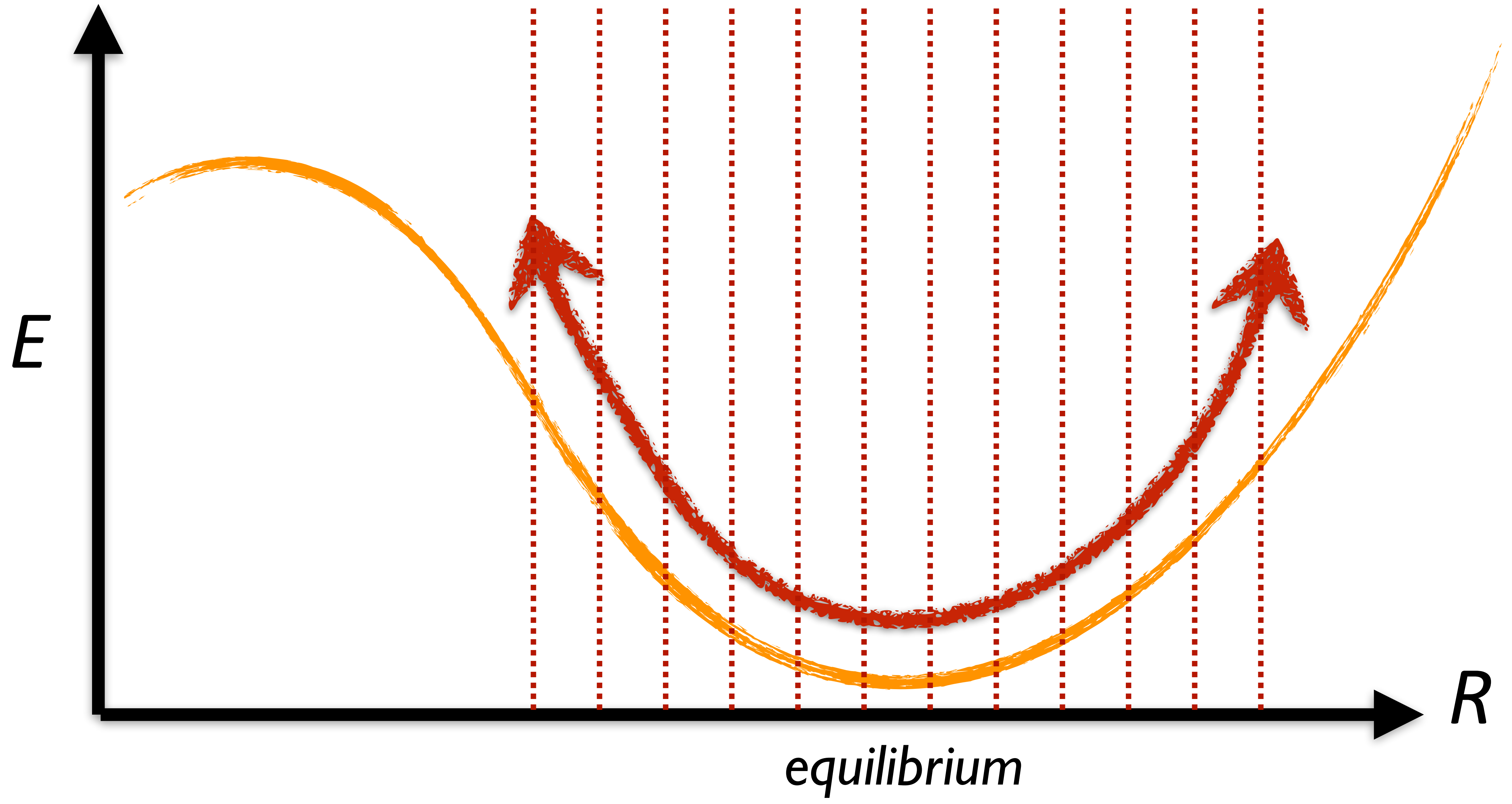
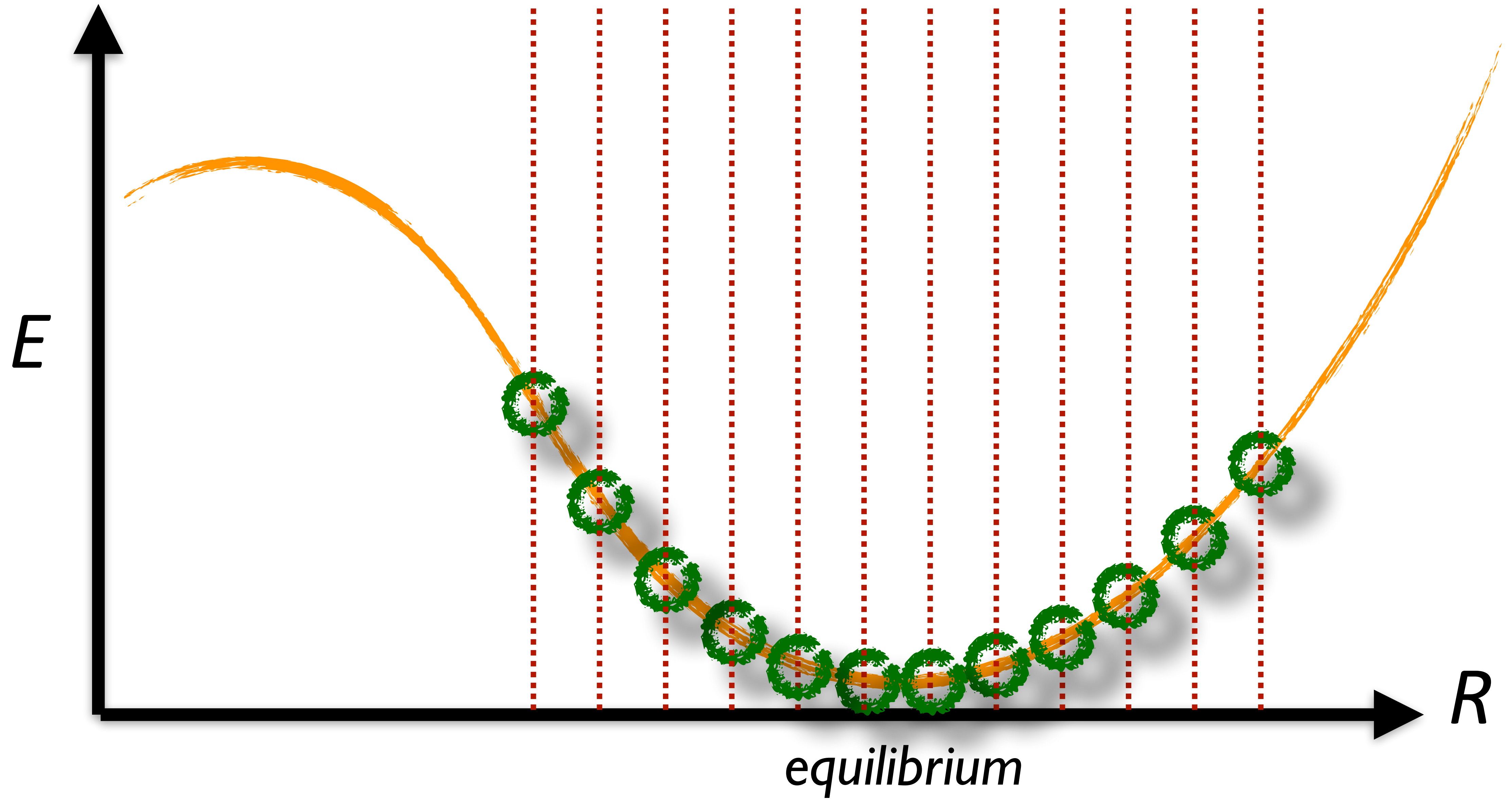



1) Run *ab initio* MD simulations to obtain anharmonic trajectories $\boldsymbol{R}_I^{\mathrm{DFT}}(t)$.

# Anharmonicity Quantification

How do $\boldsymbol{E}_{\mathbf{harm}}$ and $\boldsymbol{E}_{\mathbf{anha}} = \boldsymbol{E}_{\boldsymbol{DFT}}$ compare in different materials?

F. Knoop, T. A. R. Purcell, M. Scheffler, and C. Carbogno, *Phys. Rev. Mater.* **4**, 083809 (2020).




1) Run *ab initio* MD simulations to obtain anharmonic trajectories $\boldsymbol{R}_I^{\mathrm{DFT}}(t)$.

2) Store the potential energies $E^{\mathrm{DFT}}(t)$ observed along $\boldsymbol{R}_I^{\mathrm{DFT}}(t)$.

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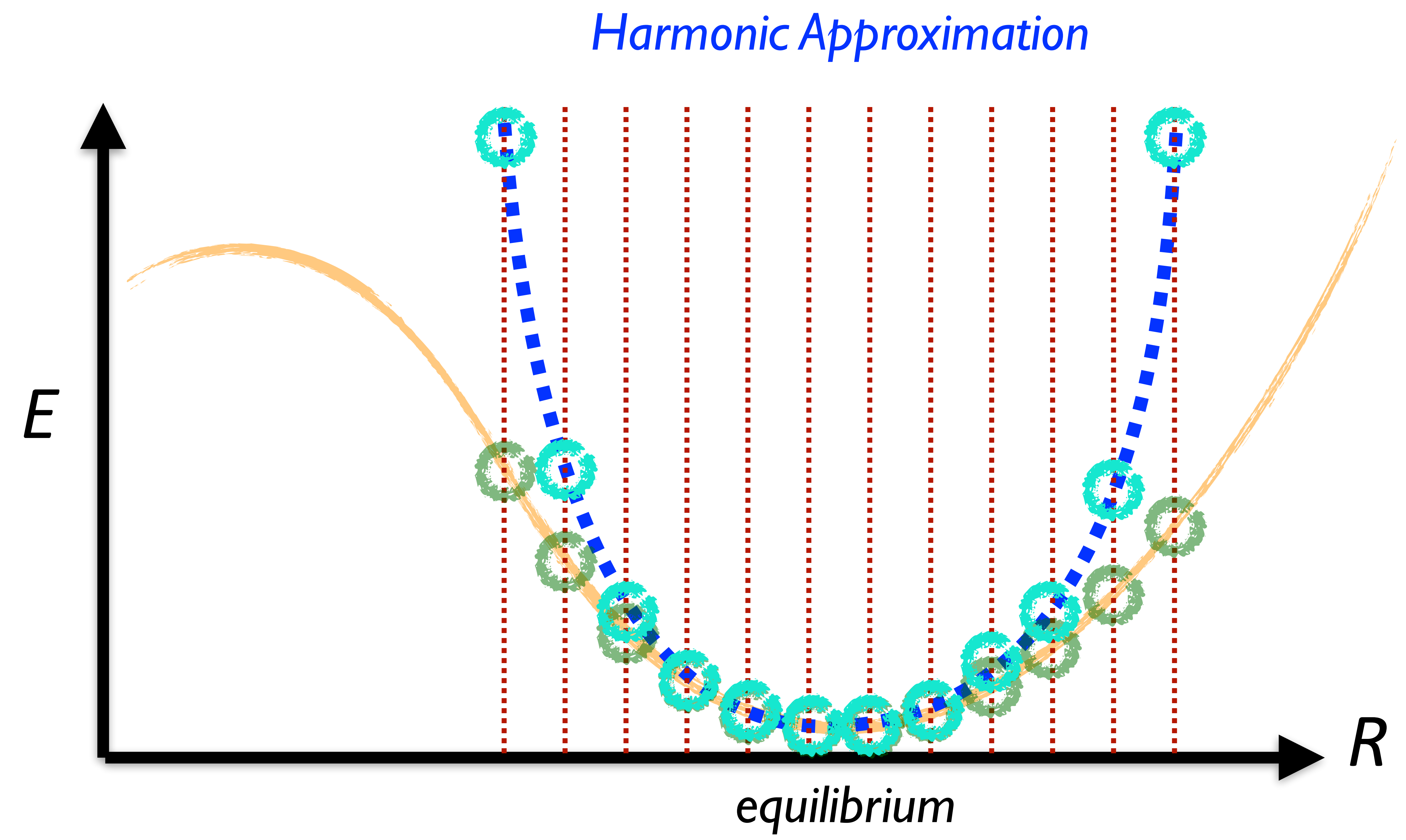


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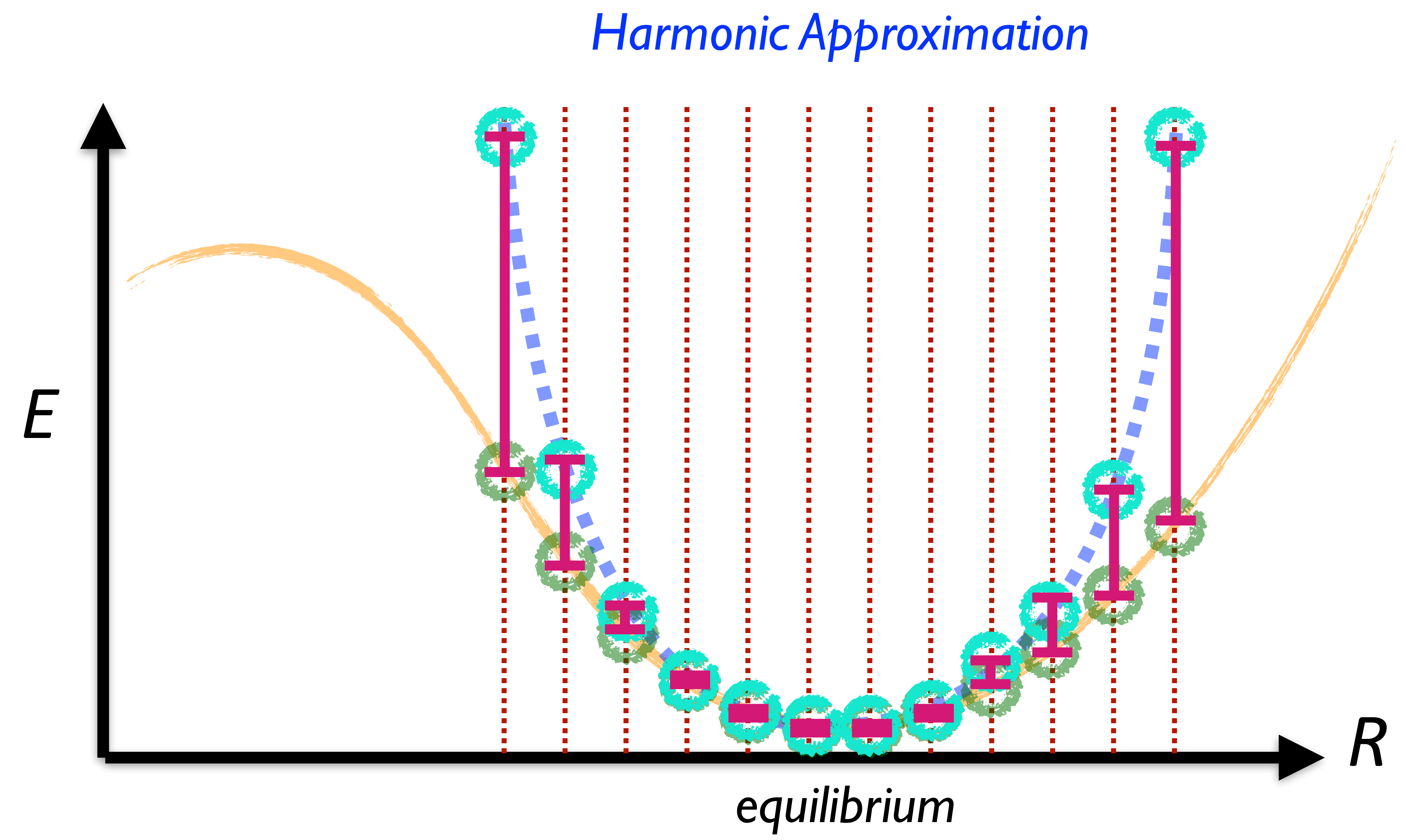


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3) Evaluate which potential energies $E^{harm}(t)$ the *harmonic approximation* would predict along $\boldsymbol{R}_I^{\mathrm{DFT}}(t)$.
4) The difference $E^{harm}(t)$ - $E^{\mathrm{DFT}}(t)$ quantifies the strength of anharmonic effects.

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In practice,
it is beneficial to work with
harmonic $\mathbf{F}_I^{harm}(t)$ and
anharmonic forces $\mathbf{F}_I^{DFT}(t)$,
since this allows for
an atom-specific resolution
of anharmonic effects.

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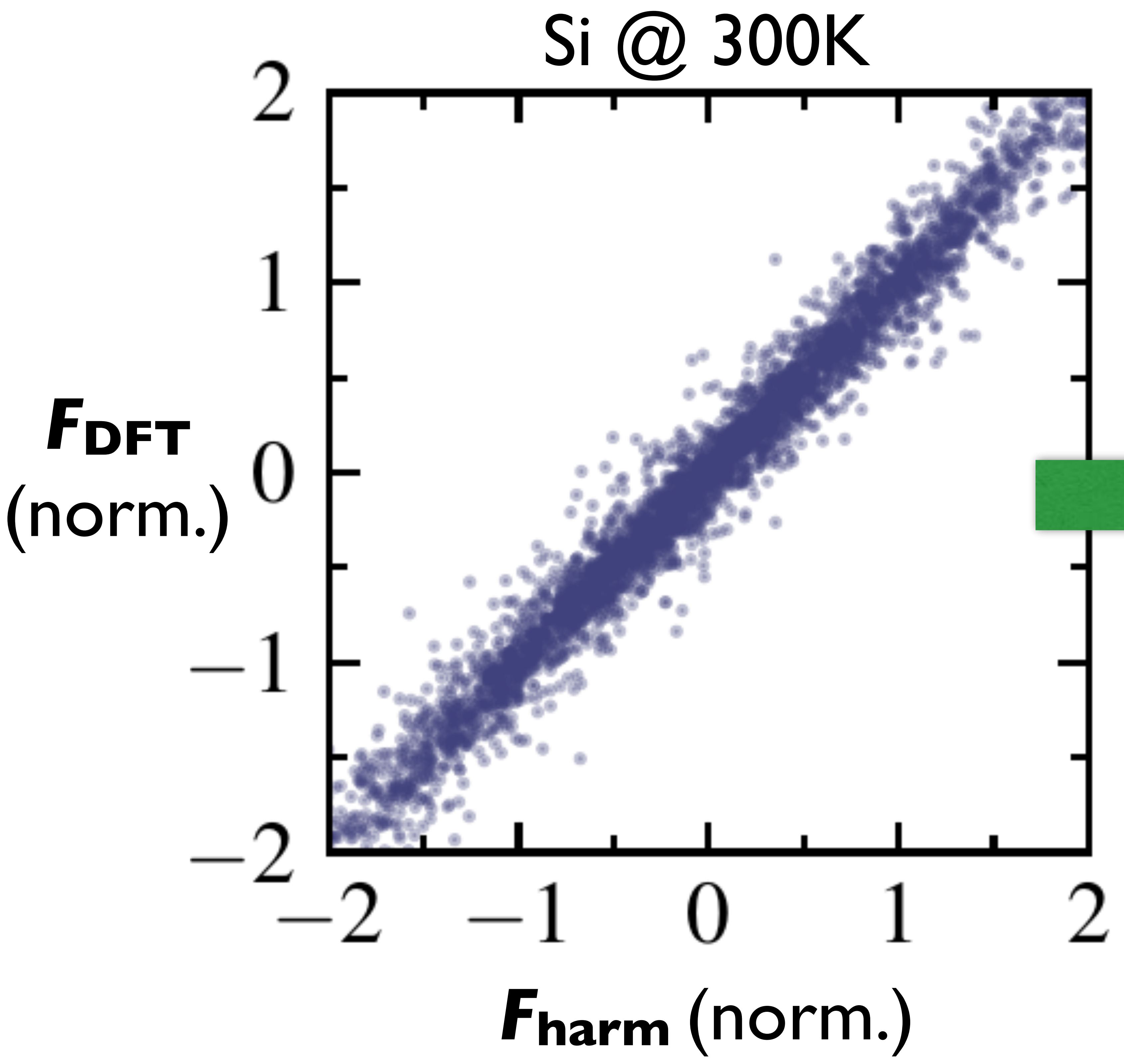


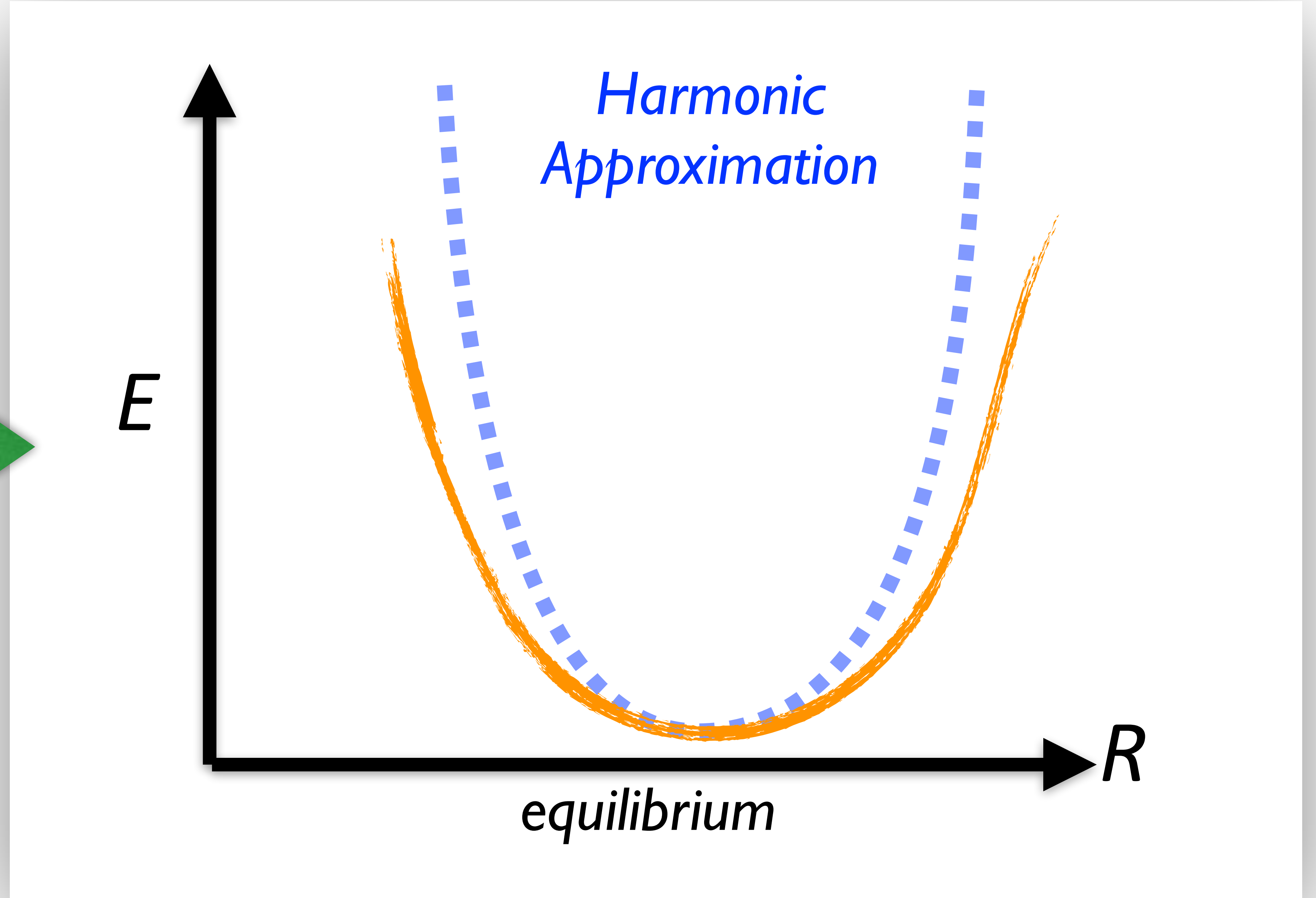


$\boldsymbol{E}_{\mathbf{harm}} \gg \boldsymbol{E}_{\mathbf{anha}}$

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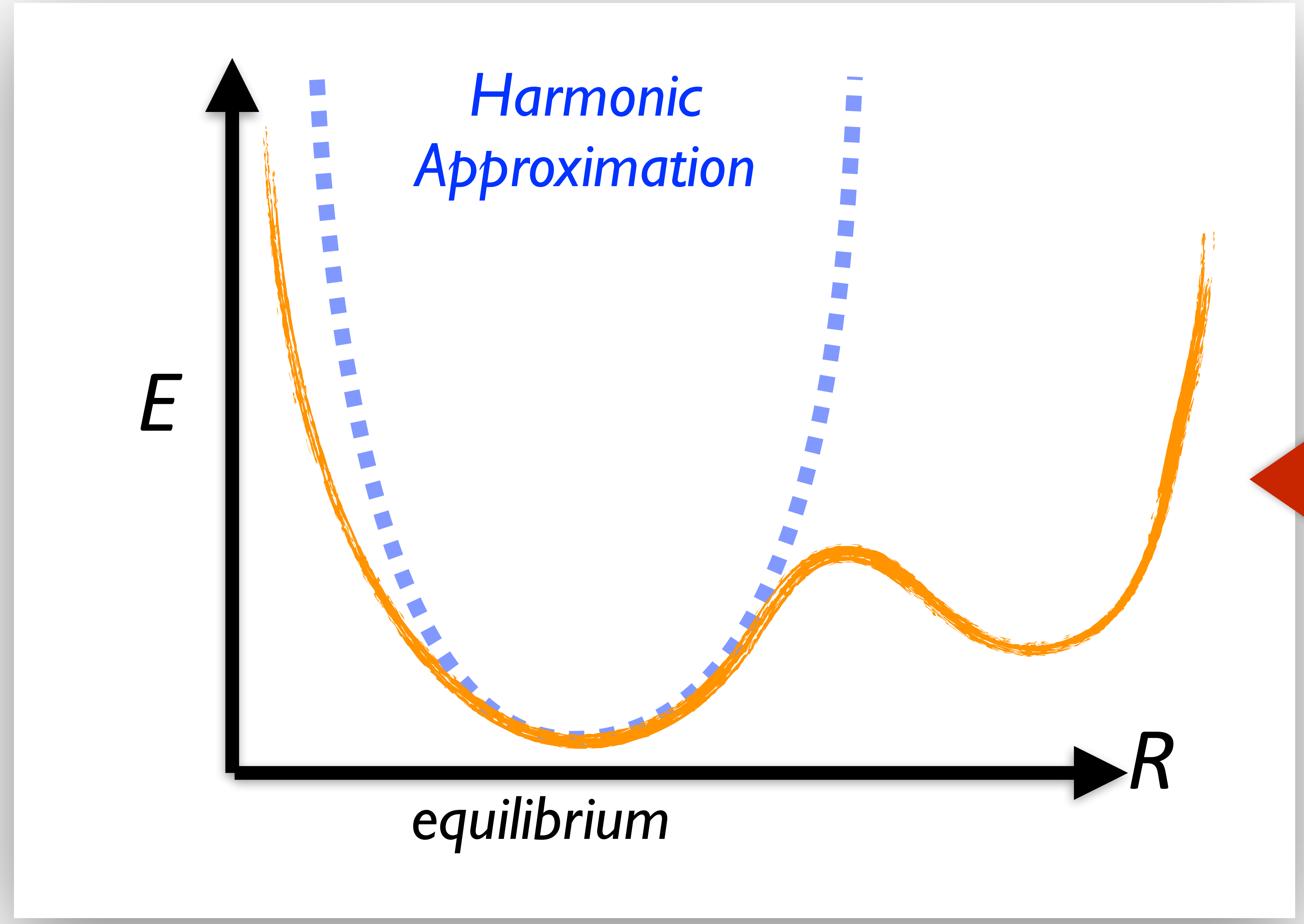
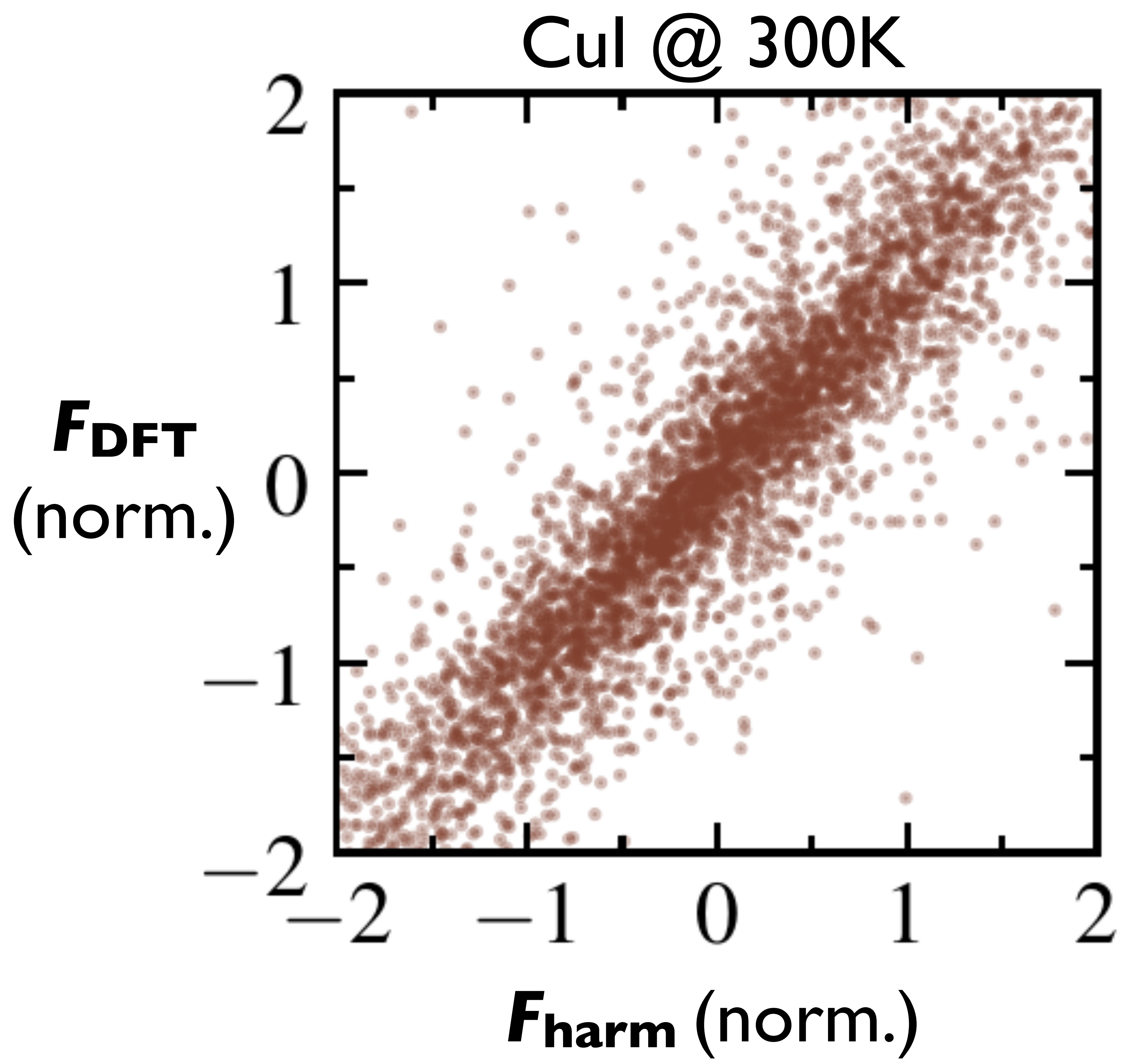



$\boldsymbol{E}_{\mathbf{harm}} \ll \boldsymbol{E}_{\mathbf{anha}}$



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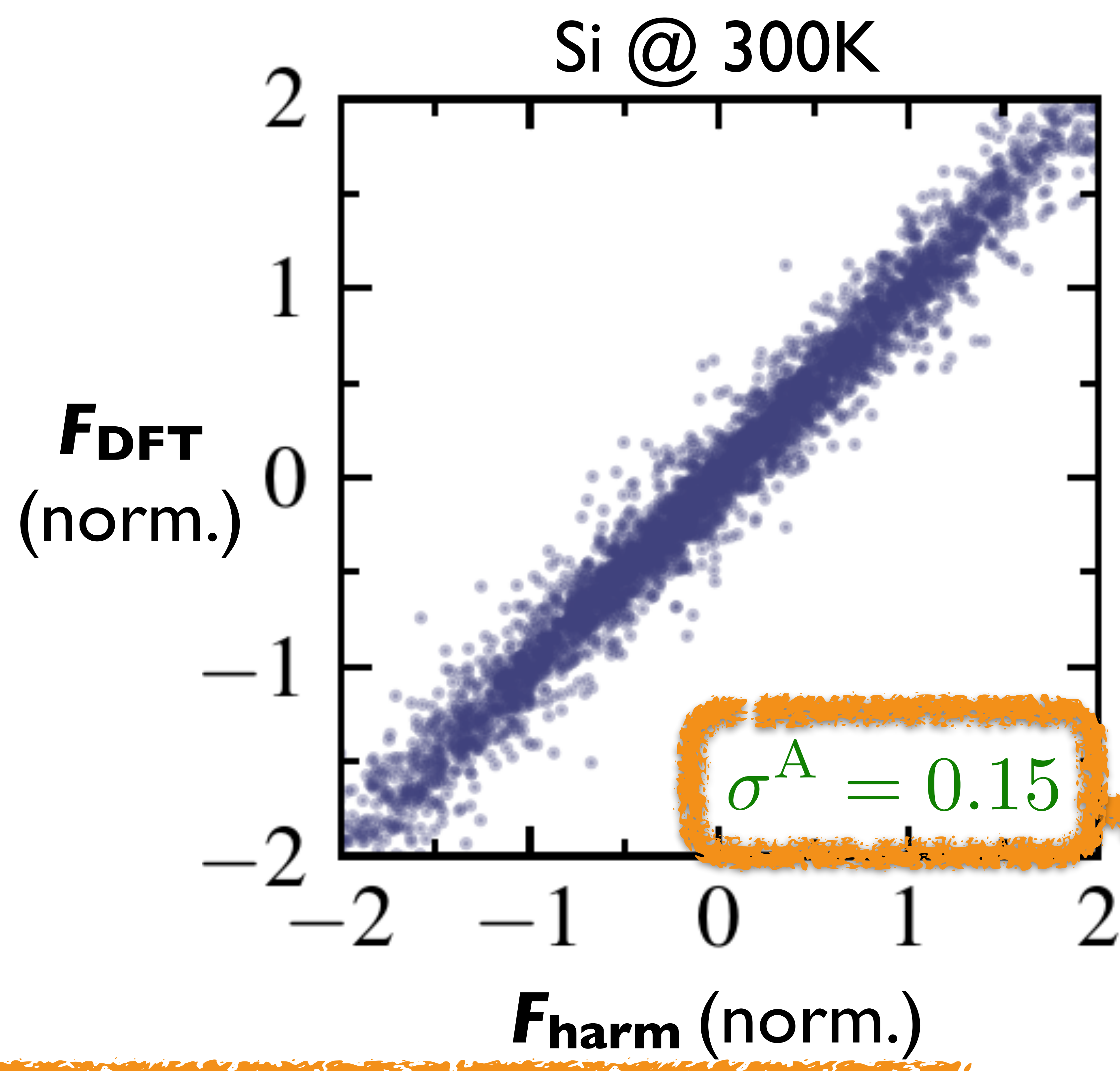


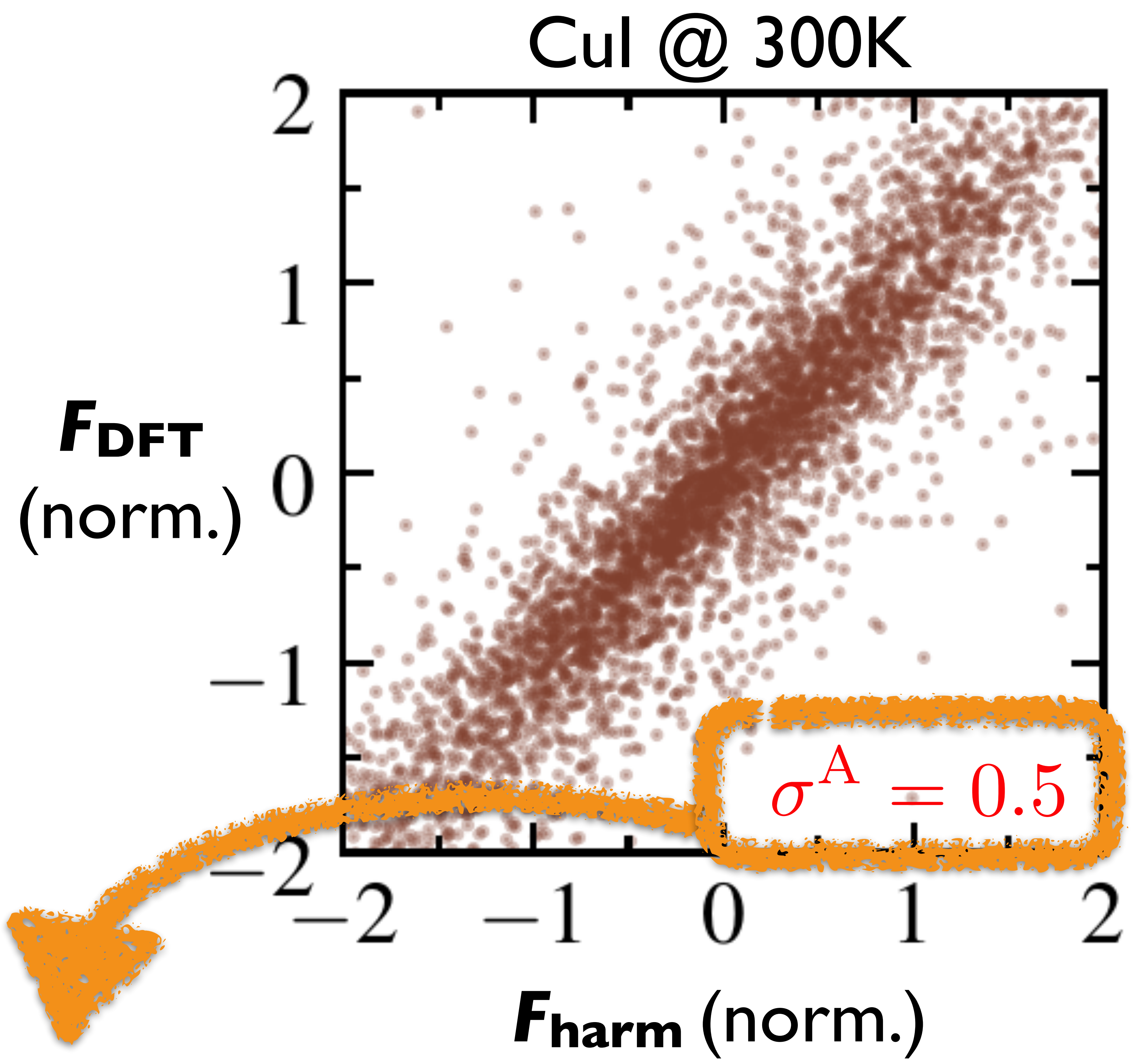


**In Simpler Words:**

*How much do anharmonic effects contribute to the forces on average?*

$$\sigma^{A}(T) = \sqrt{\frac{\sum_{I,\alpha} \left\langle \left( F_{I,\alpha}^{\mathrm{DFT}} - F_{I,\alpha}^{\mathrm{harm}} \right)^2 \right\rangle_T}{\sum_{I,\alpha} \left\langle \left( F_{I,\alpha}^{\mathrm{DFT}} \right)^2 \right\rangle_T}}$$

# Anharmonicity Quantification across Material Space

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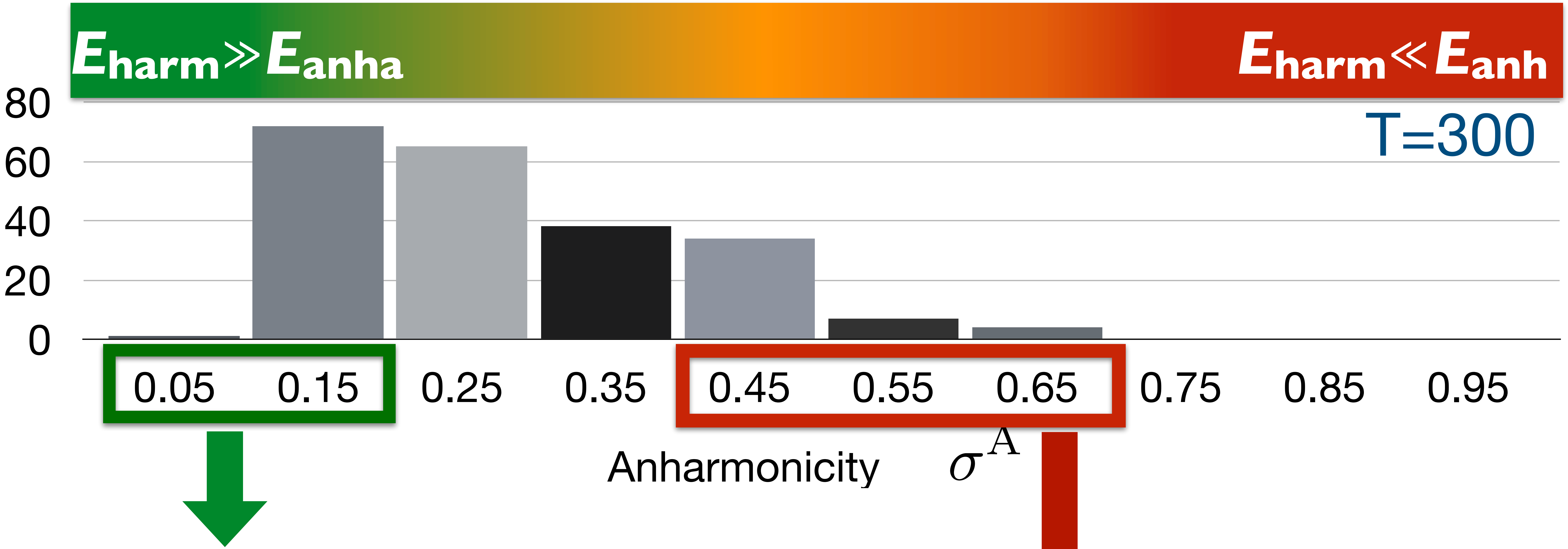


At **300K**, many materials indeed behave **almost perfectly harmonically**.

But even at **300K**, there are systems that exhibit a **strongly anharmonic** dynamics.

**200+ Material Test Set**:
- 97 Rock salt
- 67 Zincblende
- 45 Wurtzite
- 10 Perovskites

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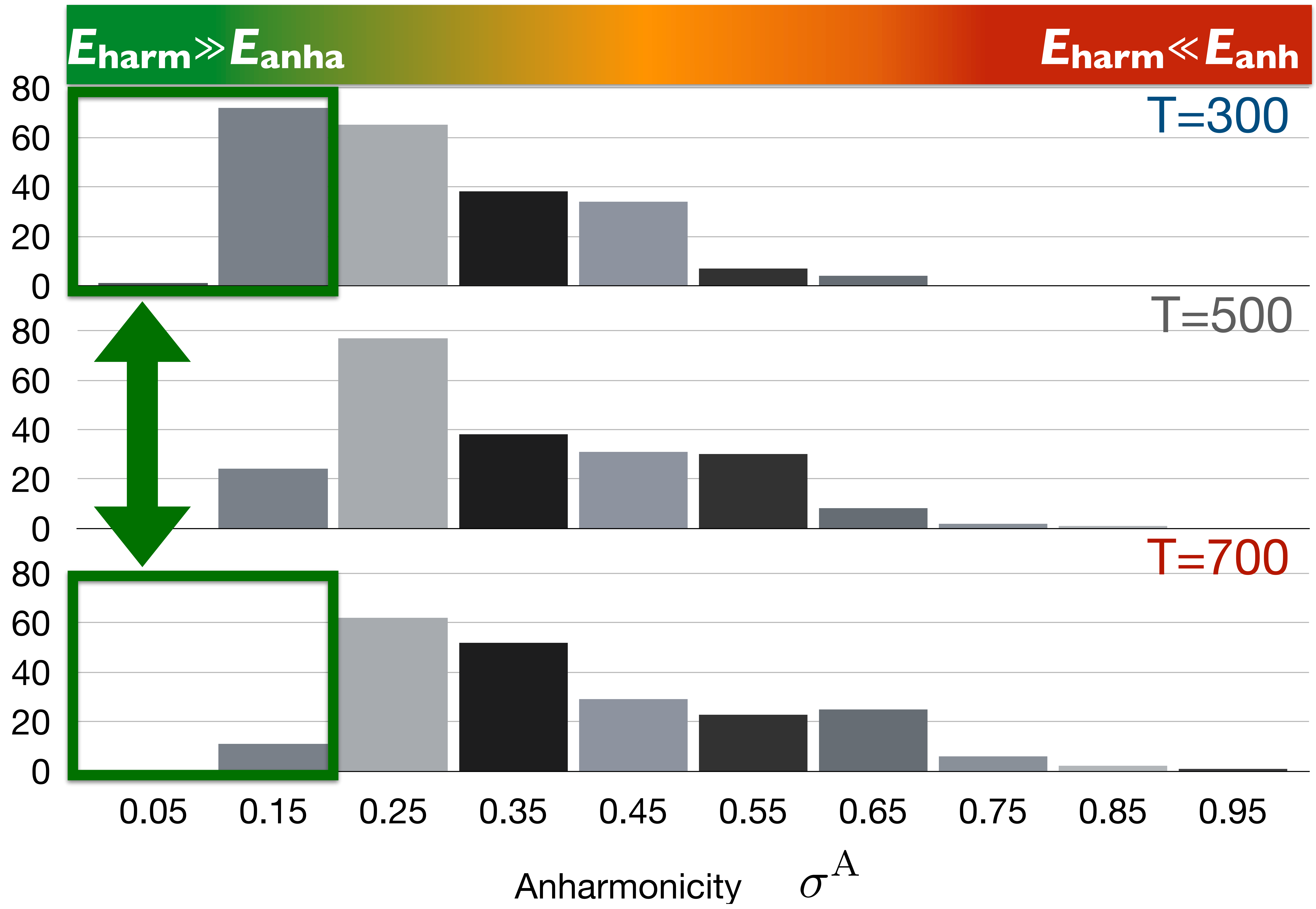


At 700K, only <35% of the materials are **almost perfectly harmonic.**

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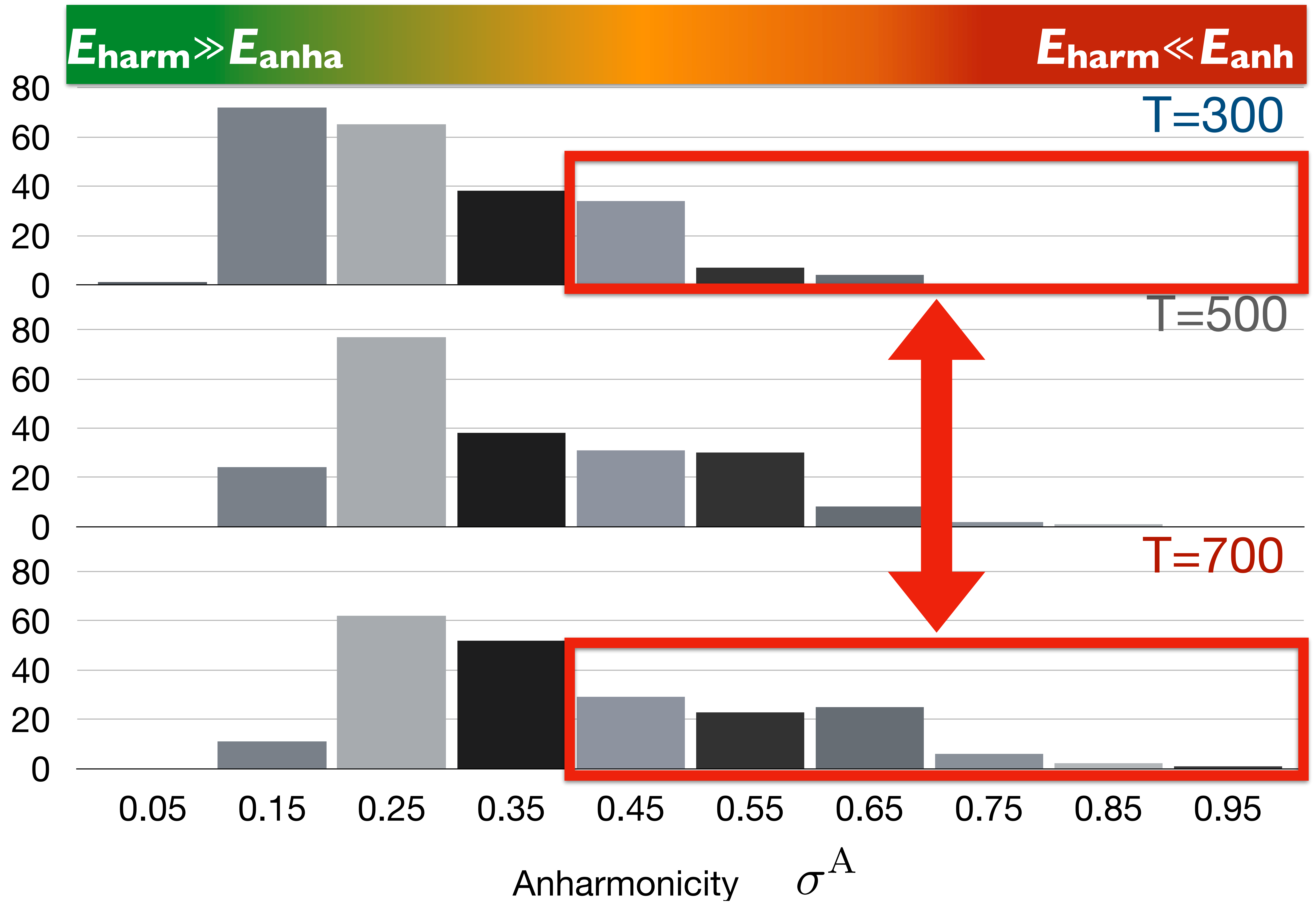


At **700K**, already **>40%** of the materials exhibit **strong anharmonic effects.**

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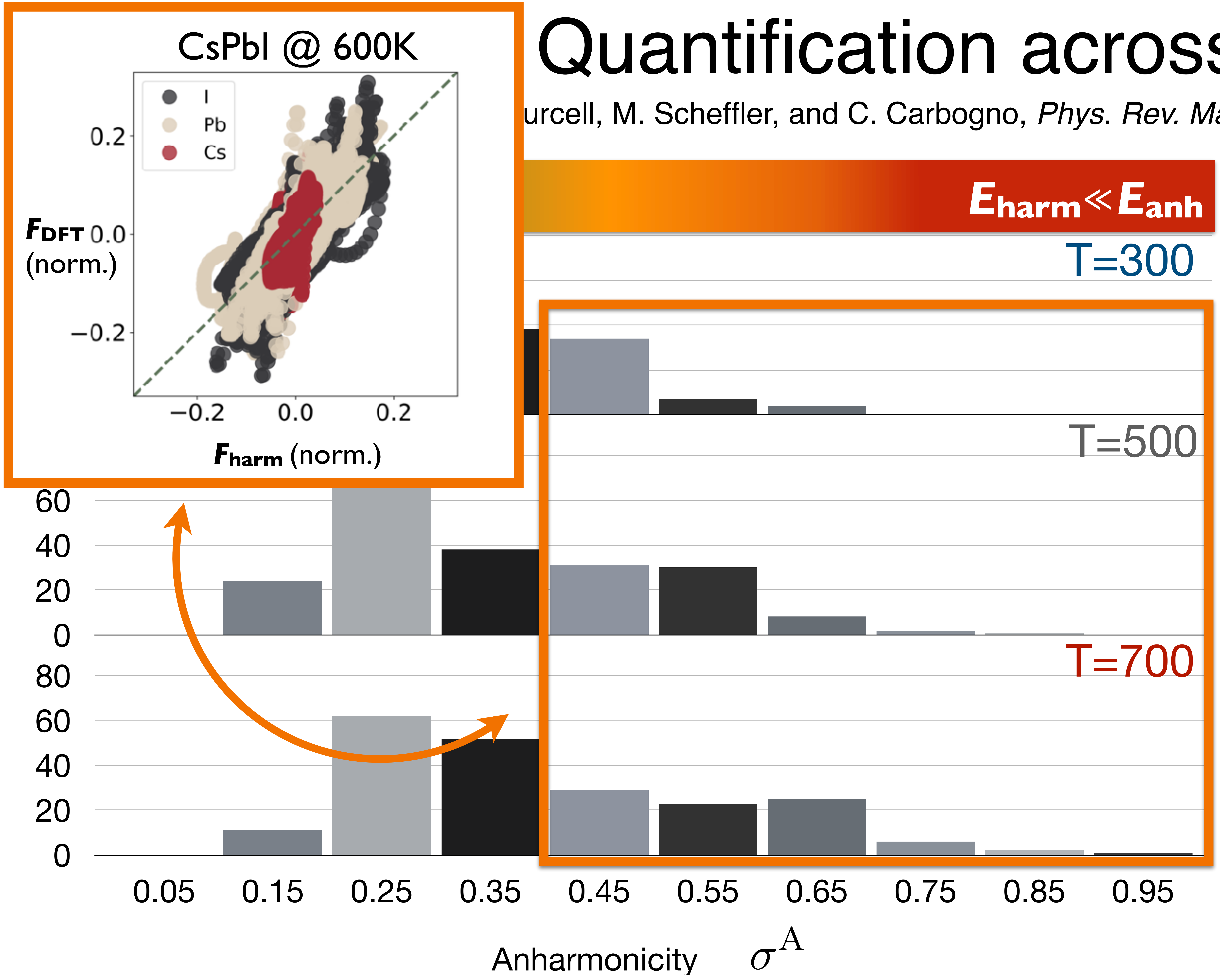
# Quantification across Material Space

urcell, M. Scheffler, and C. Carbogno, *Phys. Rev. Mater.* **4**, 083809 (2020).




At **all** temperatures, **complex materials** exhibit **stronger anharmonic effects.**

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# Take-Home Messages

1) *Ab-initio* Green-Kubo method **quantitatively** describes the **lattice thermal conductivity** both for **very harmonic** and for **strongly anharmonic** systems.

C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

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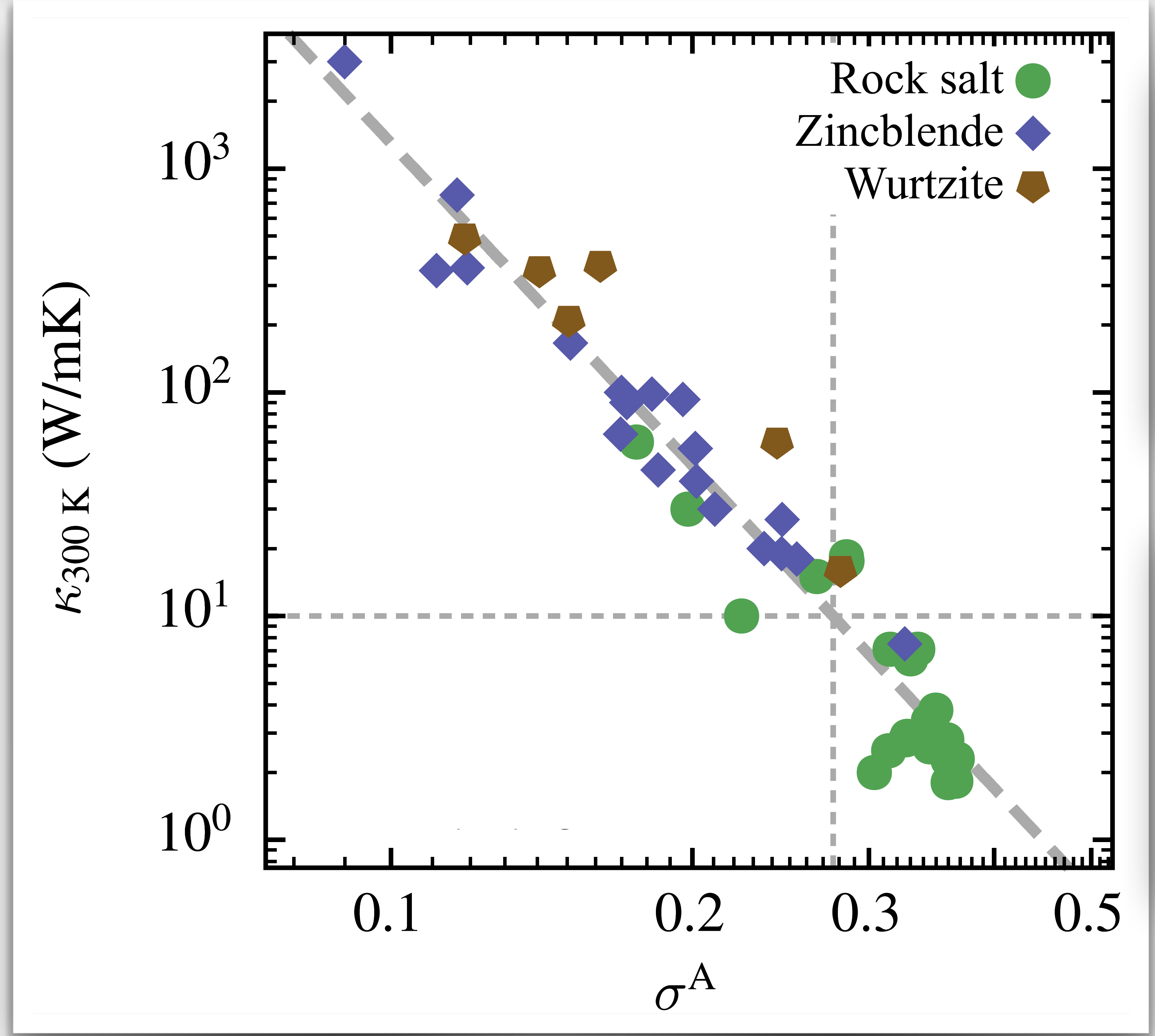


Our *anharmonicity measure* shows a **promising correlation** with *experimental thermal conductivities.*

**Accuracy** is **on par** (if not superior) compared to existing ***machine-learning*** **models** for $\kappa$.

S. A. Miller, *et al.*, *Chem. Mater.* **29**, 2494 (2017).
L. Chen, *et al.*, *Comput. Mater. Sci.* **170**, 109155 (2019).

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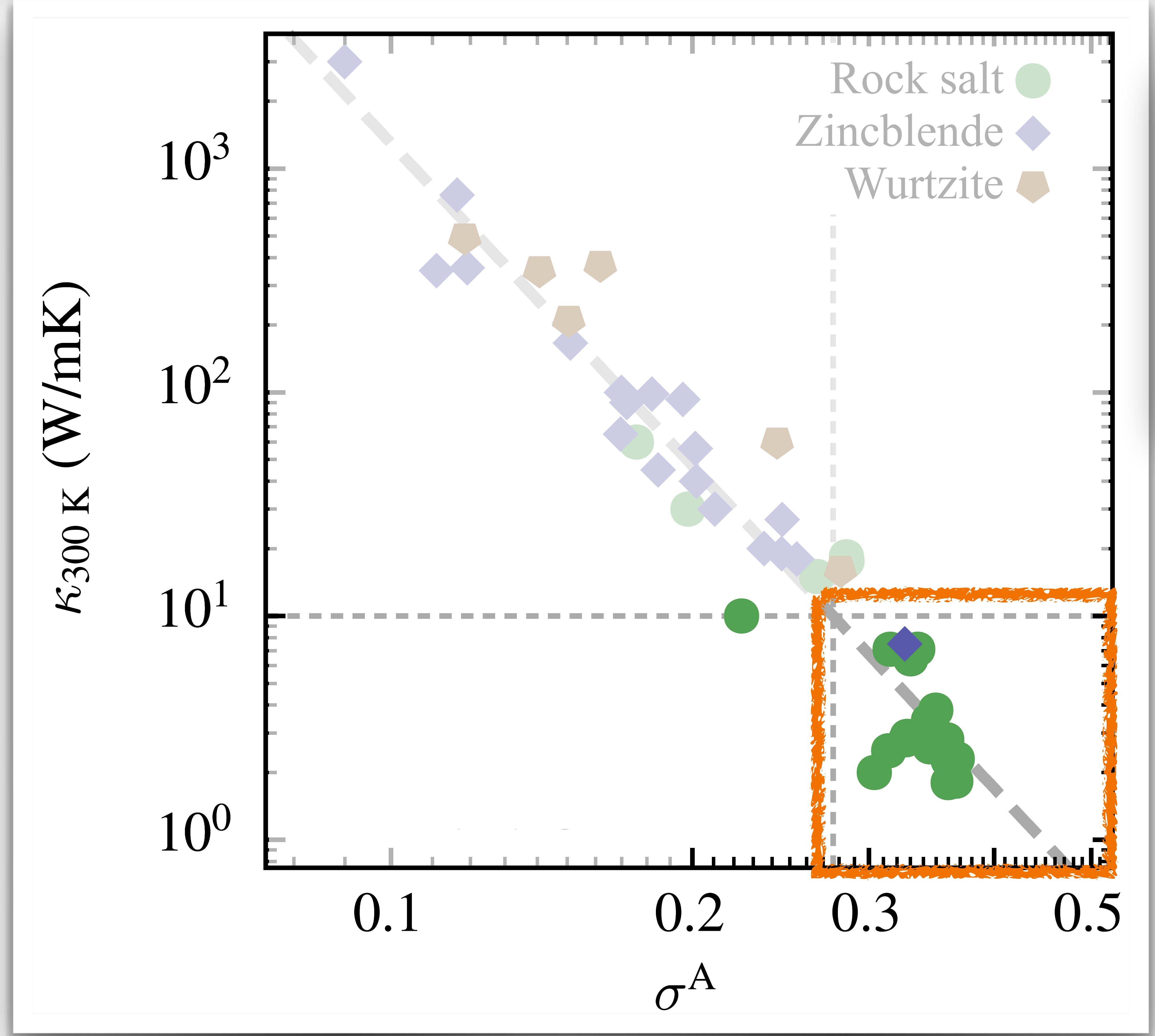
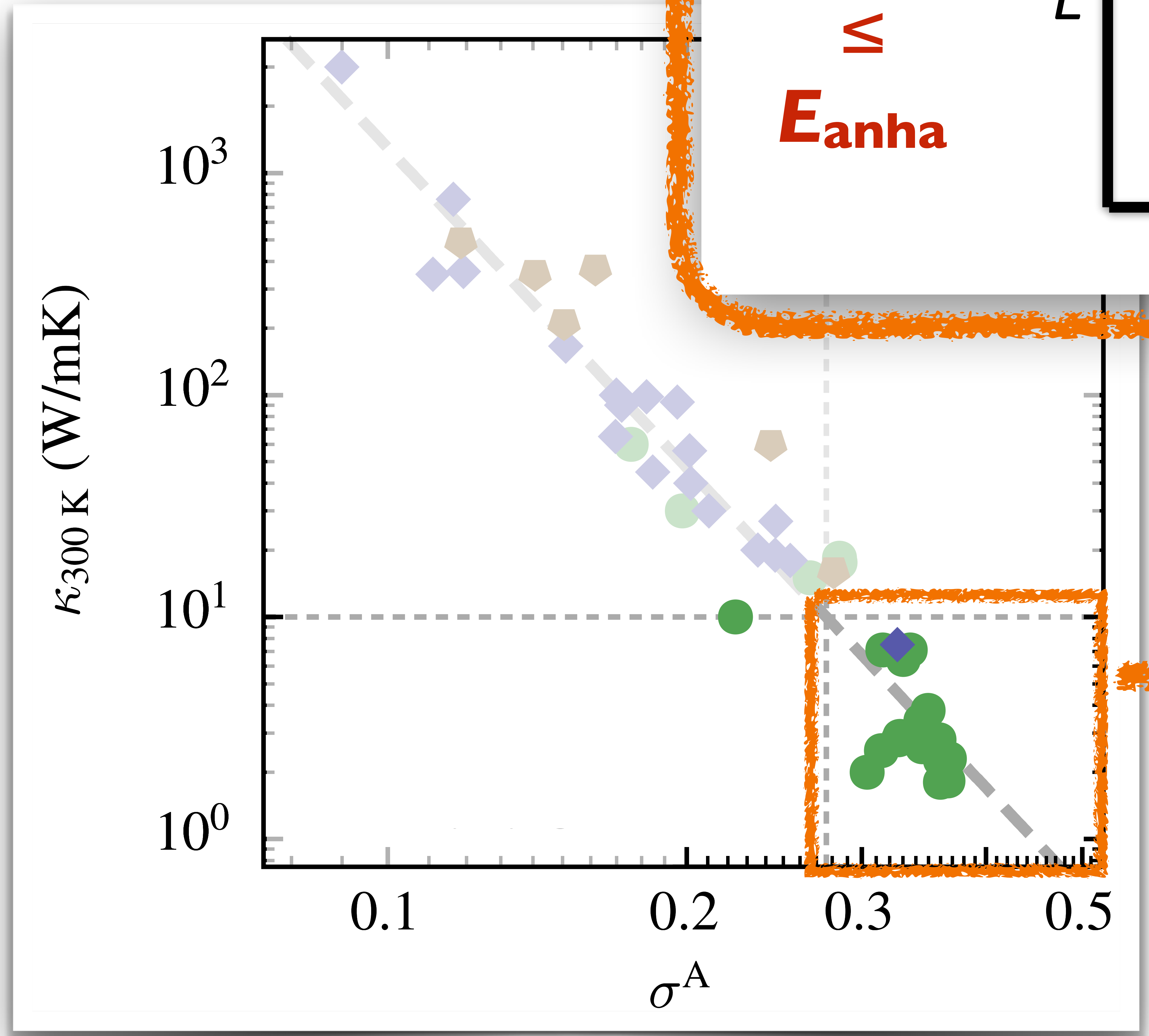
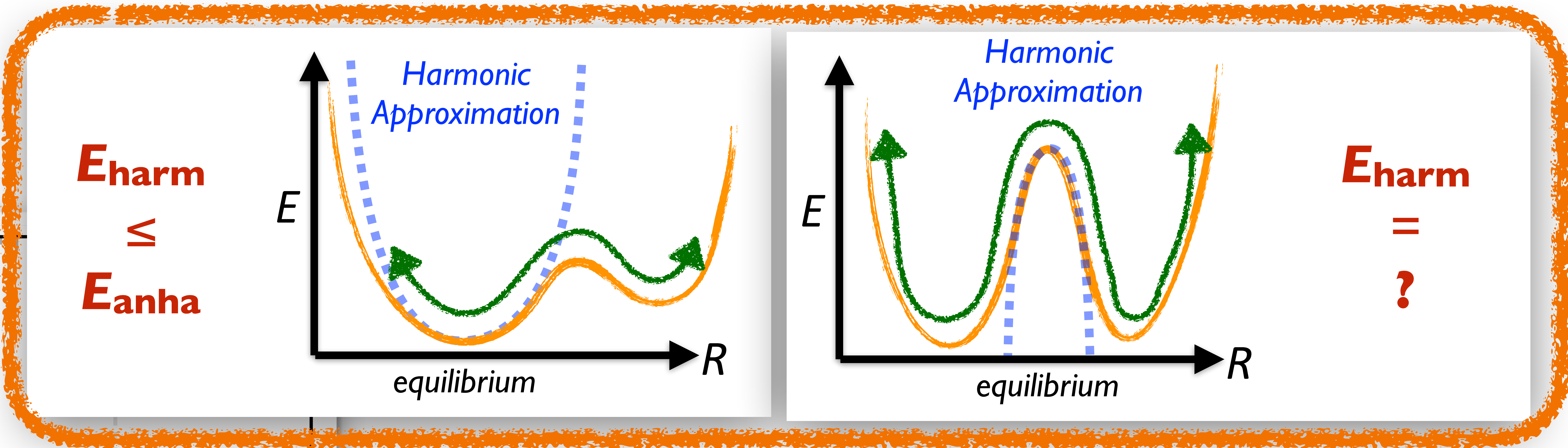



Our *anharmonicity measure* shows a **promising correlation** with *experimental thermal conductivities*.

**Thermal Insulators** typically exhibit **strong anharmonic effects**.

# Take-Home Messages




**In this regime, perturbation theory becomes unreliable, since**

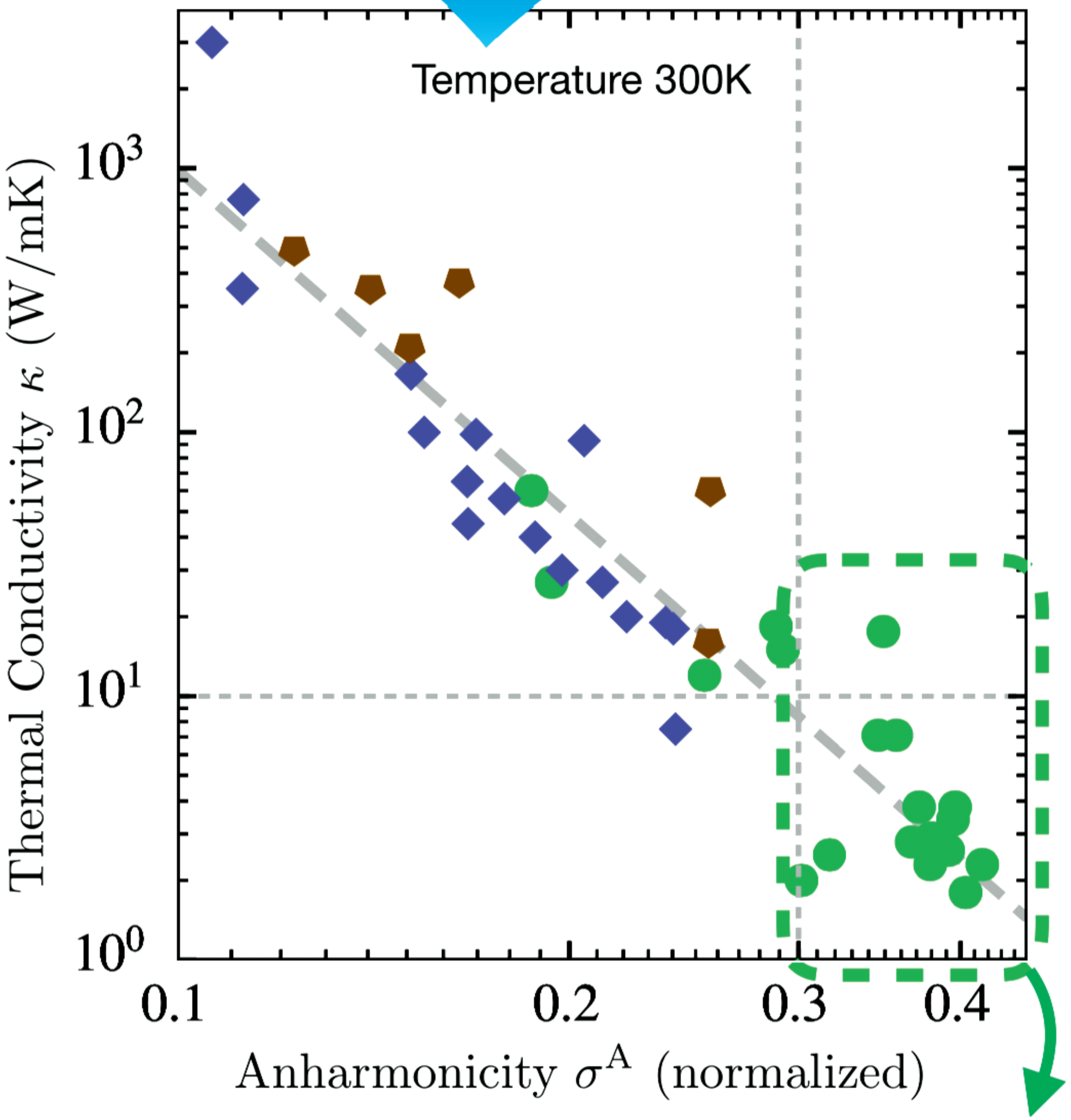
$E_{\mathrm{harm}} \gg E_{\mathrm{anha}}$

**is no longer fulfilled.**

# HIGH-THROUGHPUT SEARCH FOR THERMAL INSULATORS

F. Knoop, M. Scheffler, and C. Carbogno (*to be submitted*).

High-Throughput Scan of Materials Space




*Ab initio* Green-Kubo Calculations for Potentially Ultra-Insulating Materials.

**Step 1:** *(computationally extremely cheap)*
Scan material space for high-$\sigma^A$ materials

**Step 2:** *(computationally heavy)*
Calculate $\kappa$ for those materials with **strong** anharmonic effects with *ab initio* Green-Kubo.

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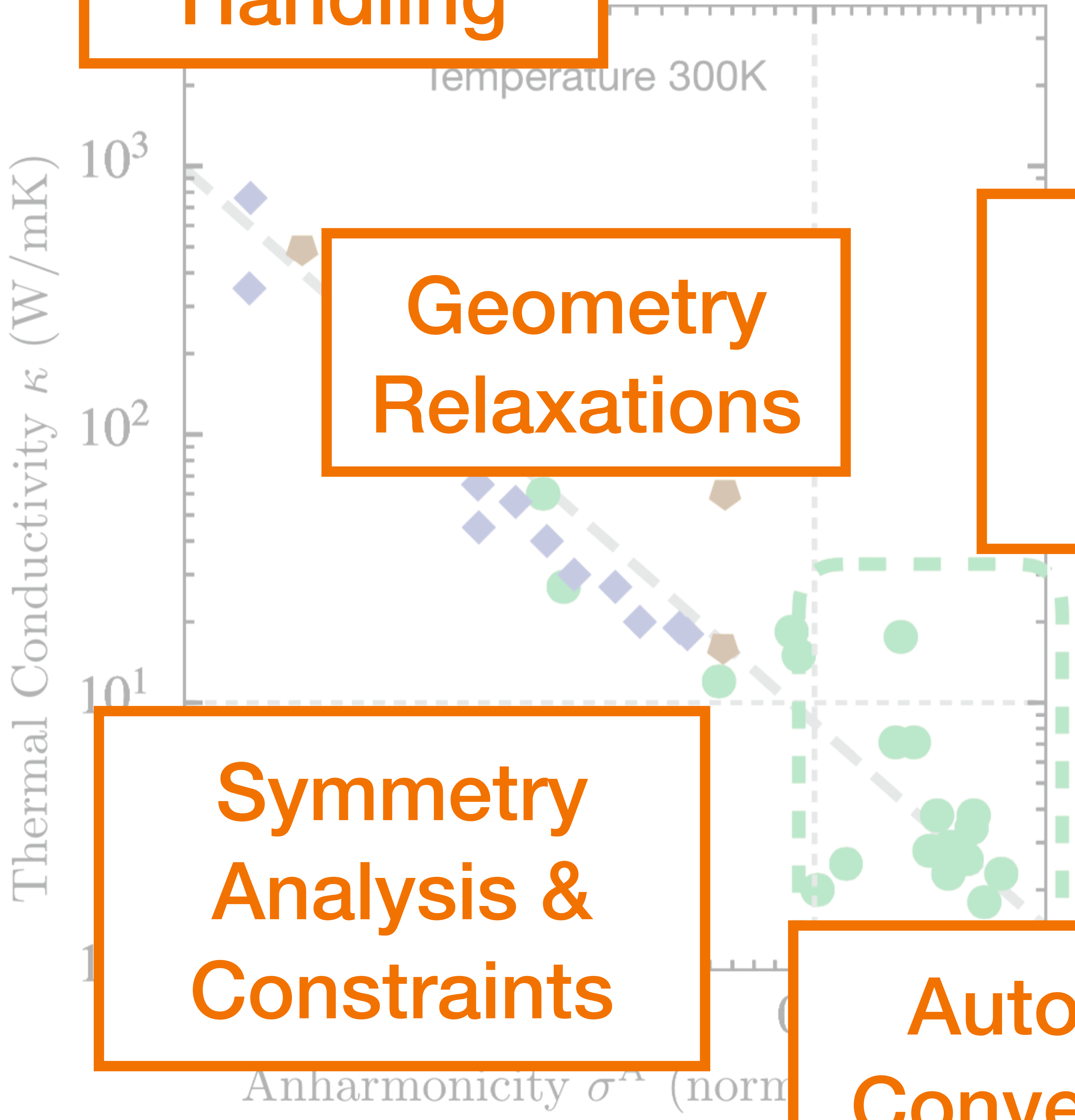
H… of Materials Space

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Potentially Ultra-Insulating M…

…tationally extr…
…erial space fo…

**Step 2:** (computationally heavy)

Calc… …ials with **strong** anha… …o *initio* Green-Kubo.

**Structure Handling**

**Geometry Relaxations**

**Workflow Monitoring**

**Harmonic Phonons**

**Symmetry Analysis & Constraints**

**Automatic Convergence Analysis**

***Ab initio* MD**

**Anharmonicity Metric**

# FHI-vibes

https://vibes.fhi-berlin.mpg.de/

F. Knoop, *et al.*, *JOSS* **5**, 2671 (2020).

Structure Handling

Geometry Relaxations

Workflow Monitoring

TDEP

Harmonic Phonons

Automatic - FLOW for Materials Discovery

Symmetry Analysis & Constraints

*Ab initio* MD

phonopy & phono3py

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F. Knoop, *et al.*, *JOSS* **5**, 2671 (2020).

Structure Handling

***FHI-vibes*** **interfaces between existing codes and frameworks,**
**so to allow for a seamless assessment of vibrational properties at different level of sophistication within a unified user interface.**

phonopy & phono3py

Convergence Analysis

Anharmonicity Metric

# VALIDATION & DATA ANALYSIS

F. Knoop, M. Scheffler, and C. Carbogno (*to be submitted*).

20 materials at 300 K, for which multiple experiments measured comparable values for $\kappa$.

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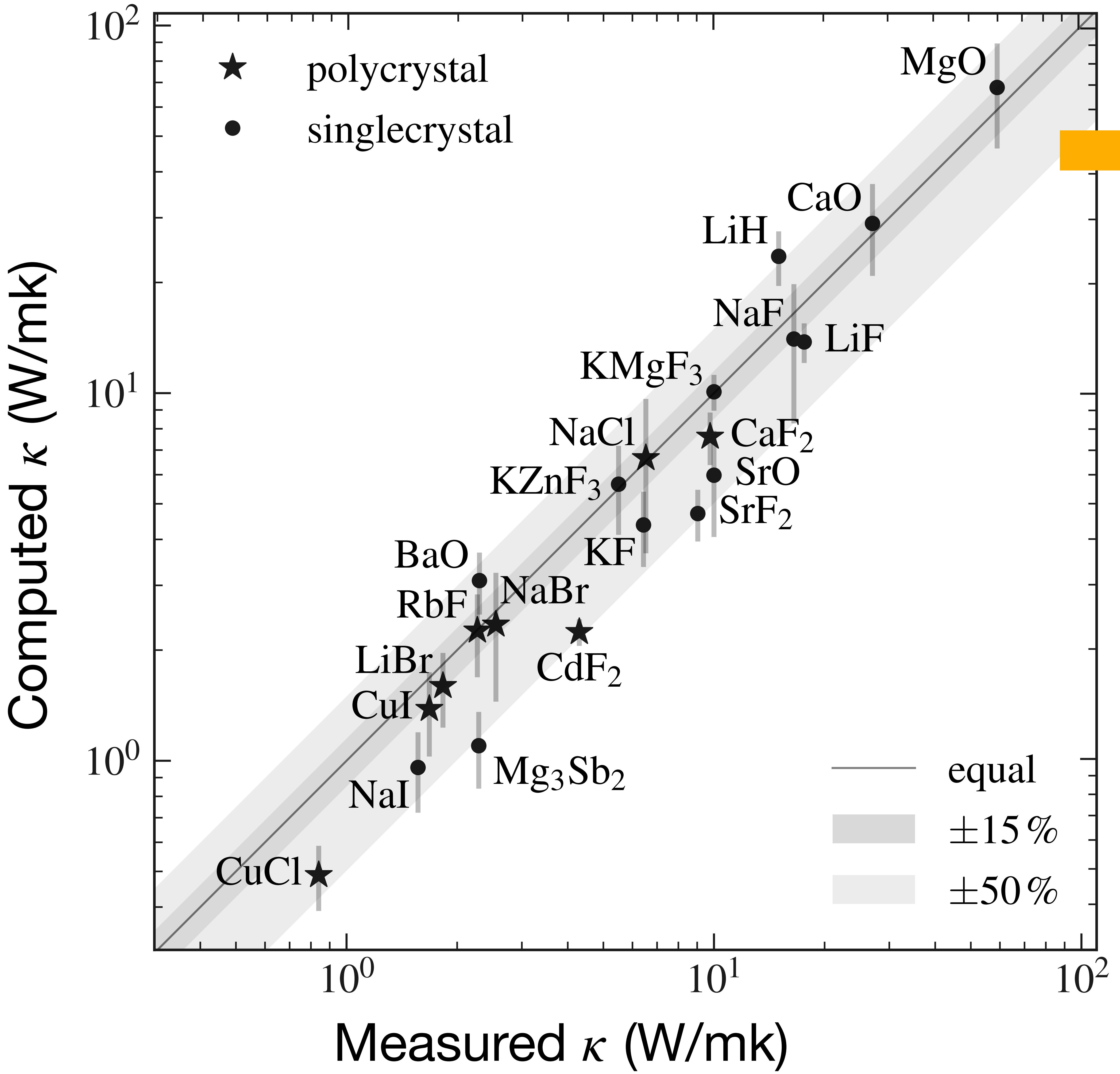


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***Ab initio* Green-Kubo Method** allows for **reliable**, **predictive** calculations for all degrees of **anharmonicity**.

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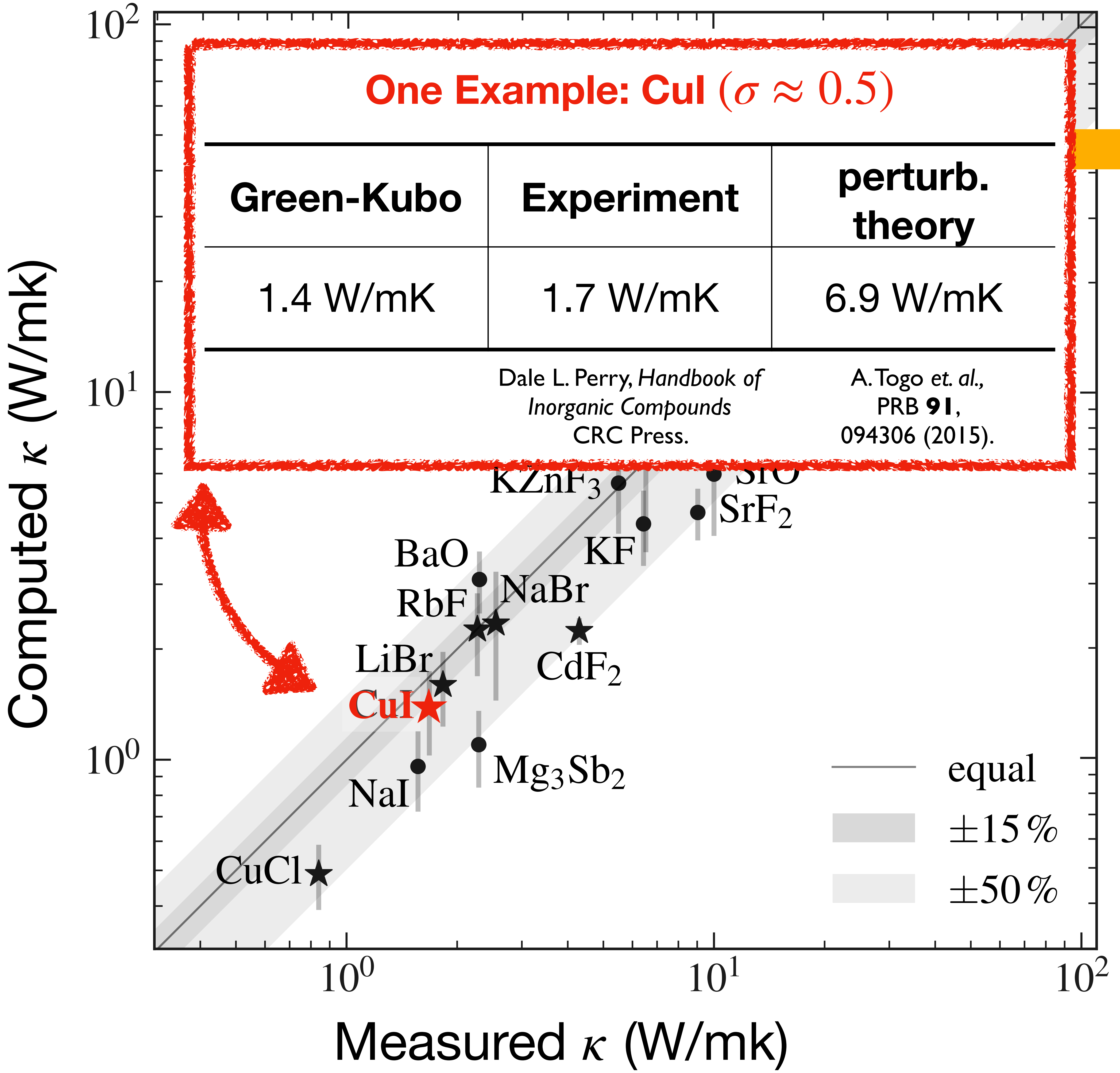


**One Example: CuI** ($\sigma \approx 0.5$)

| Green-Kubo | Experiment | perturb. theory |
|---|---|---|
| 1.4 W/mK | 1.7 W/mK | 6.9 W/mK |
| | Dale L. Perry, *Handbook of Inorganic Compounds* CRC Press. | A. Togo *et. al.*, PRB **91**, 094306 (2015). |

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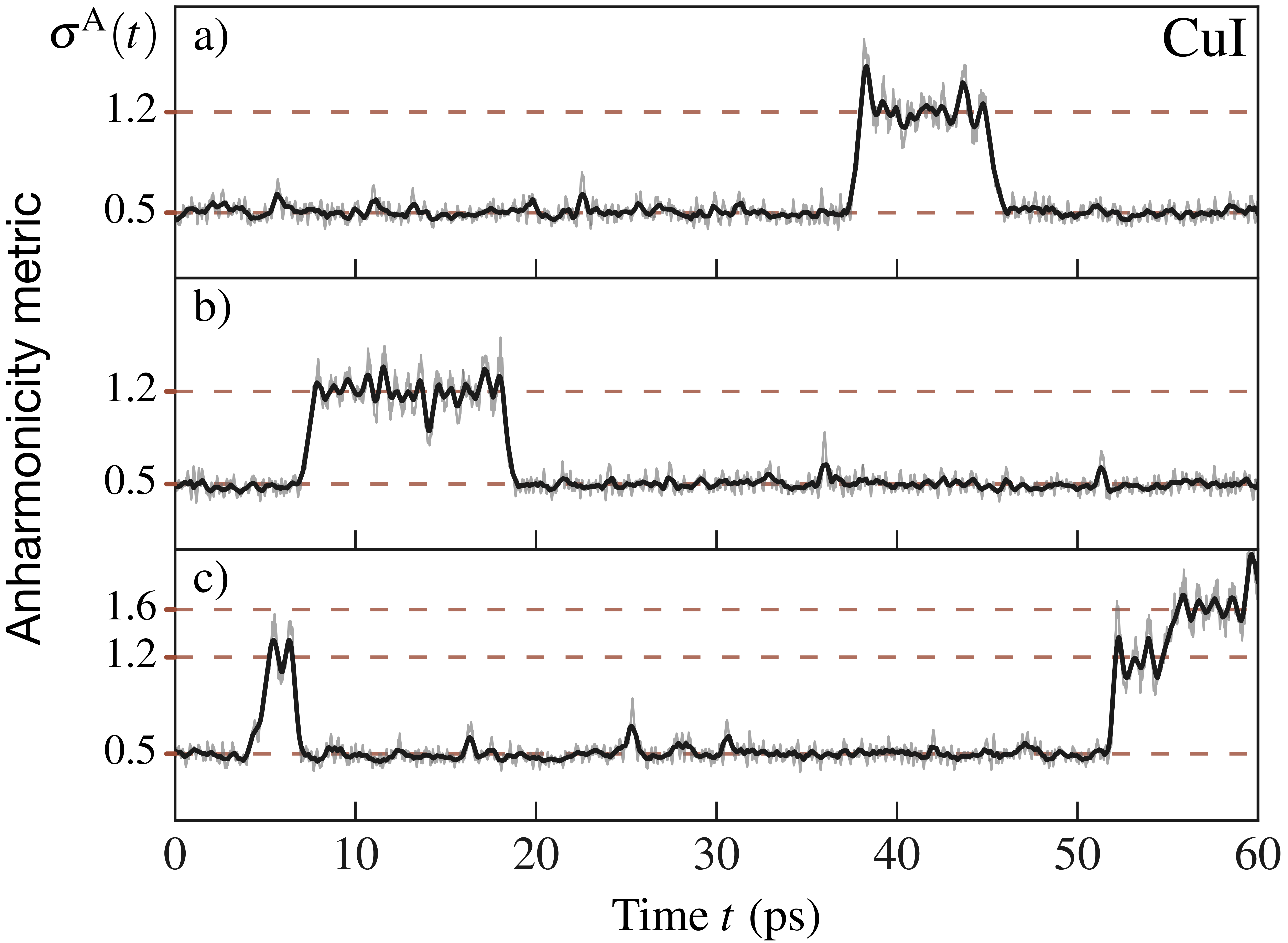

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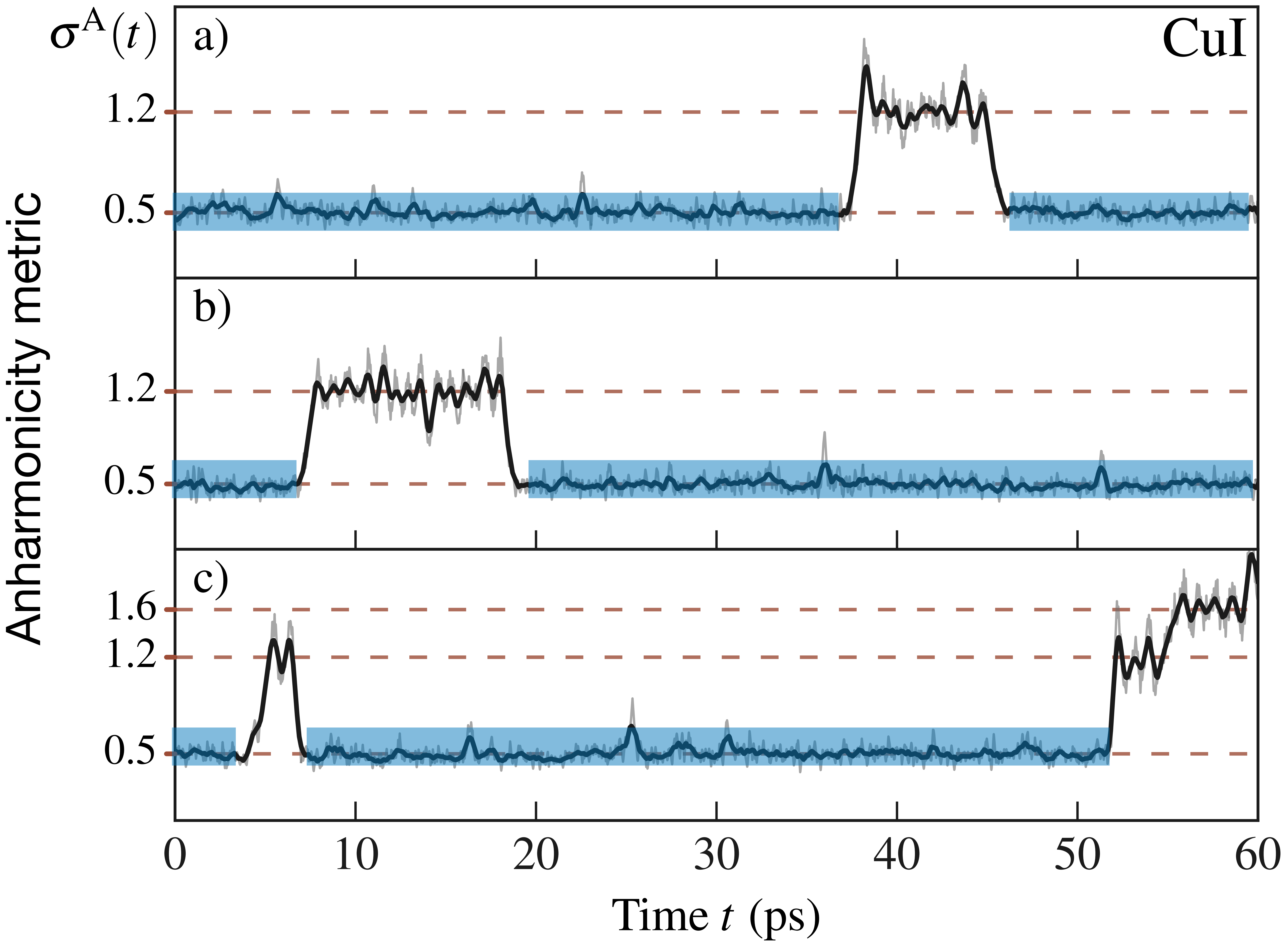


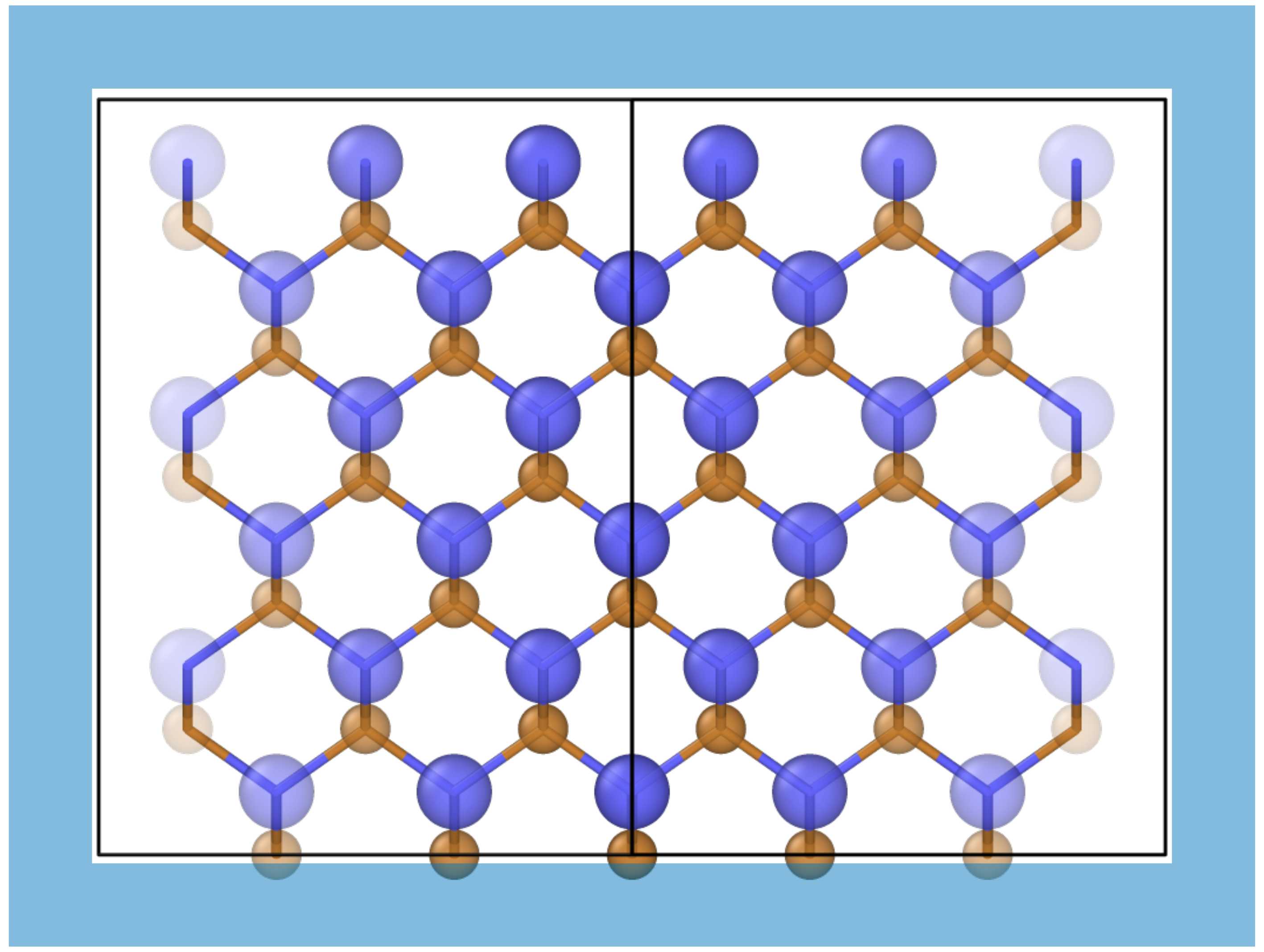

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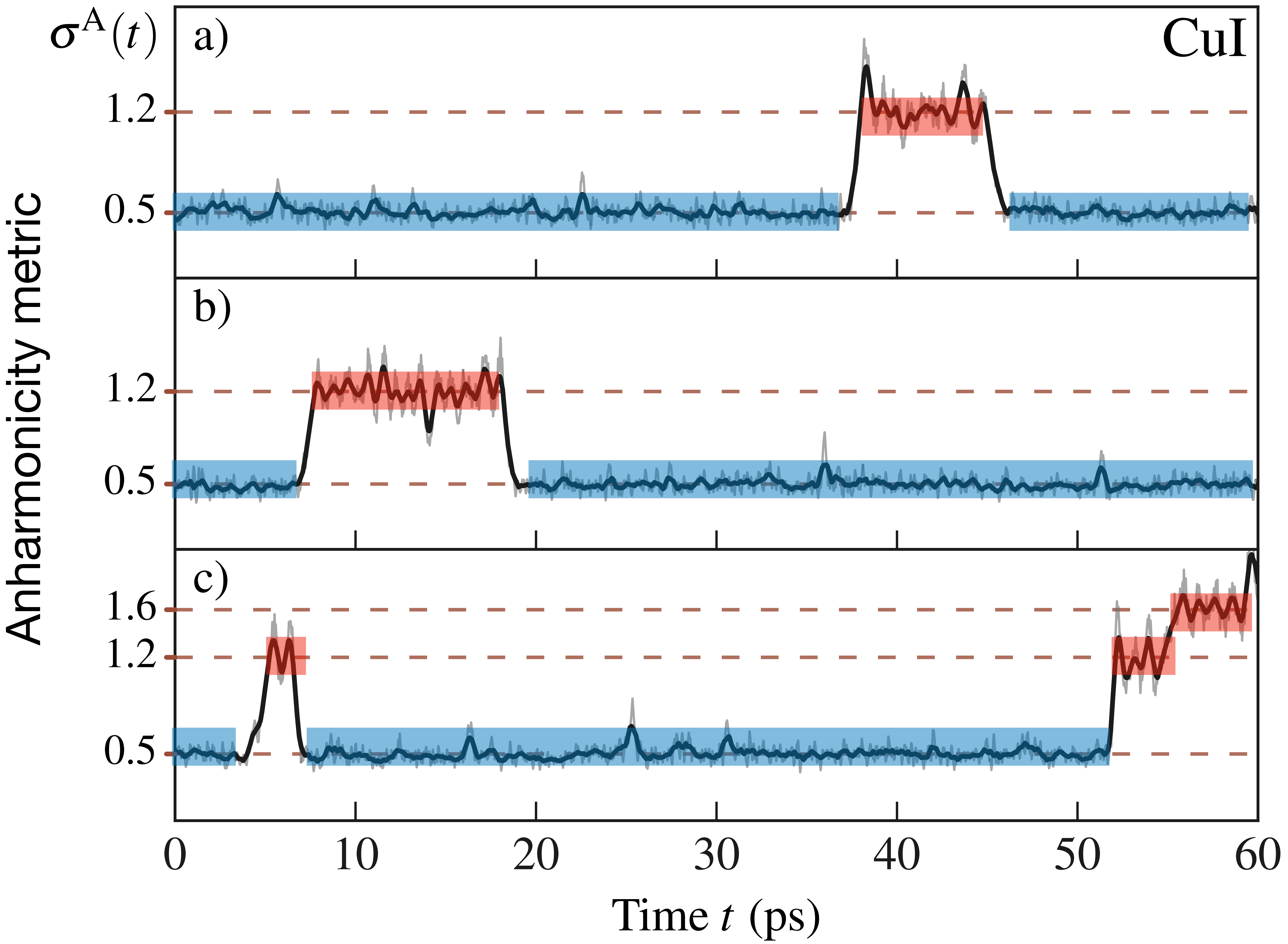


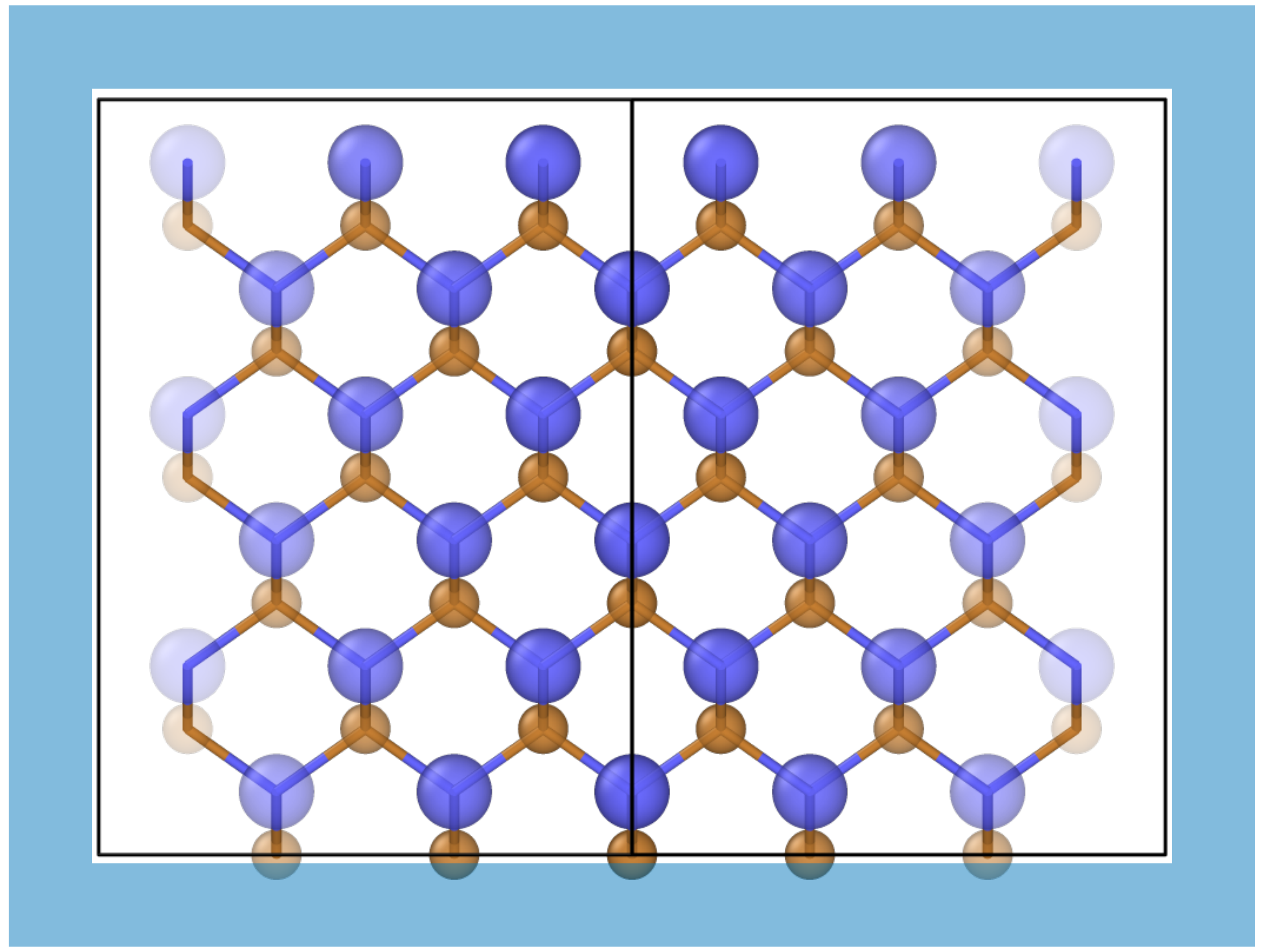

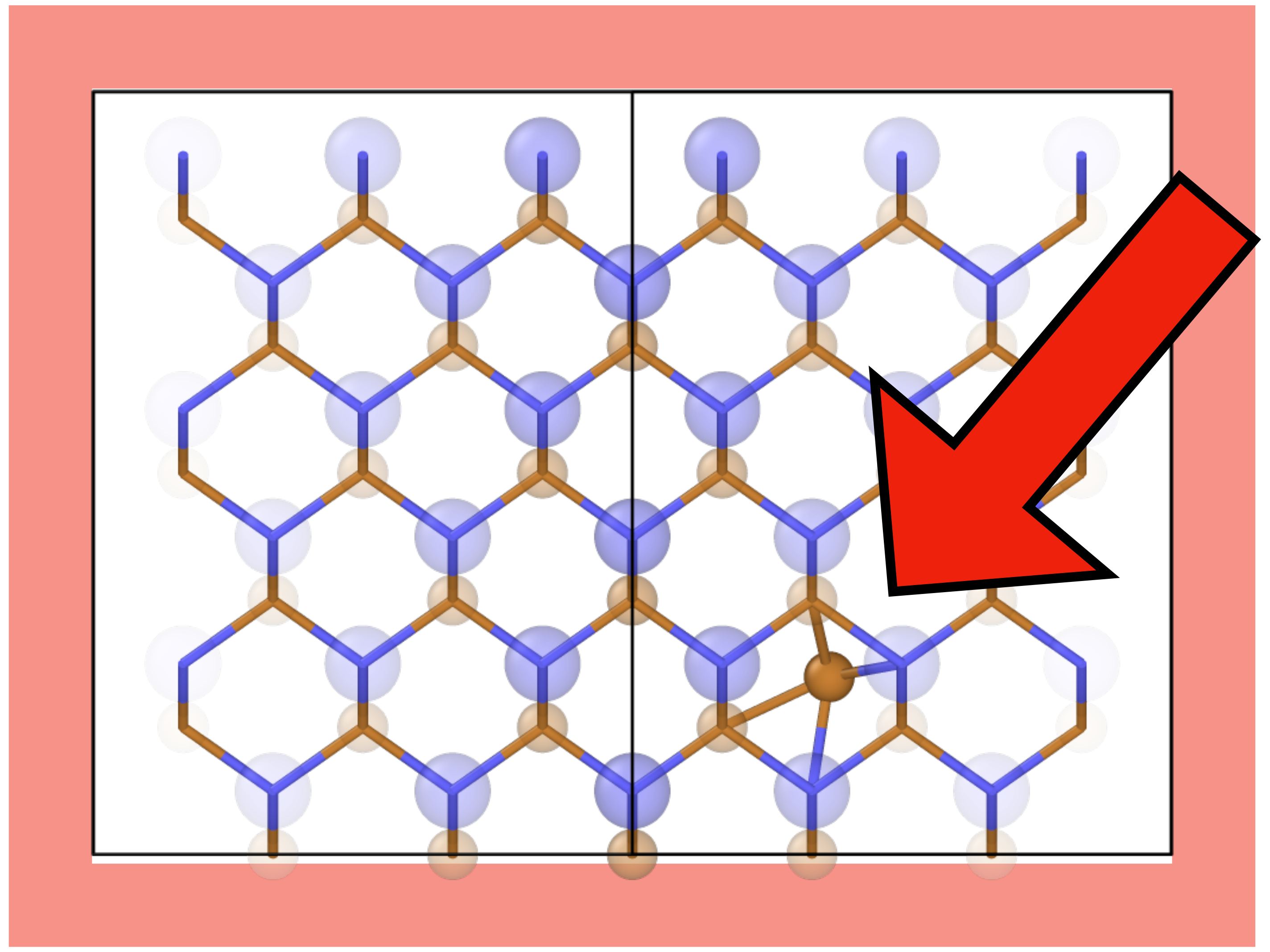

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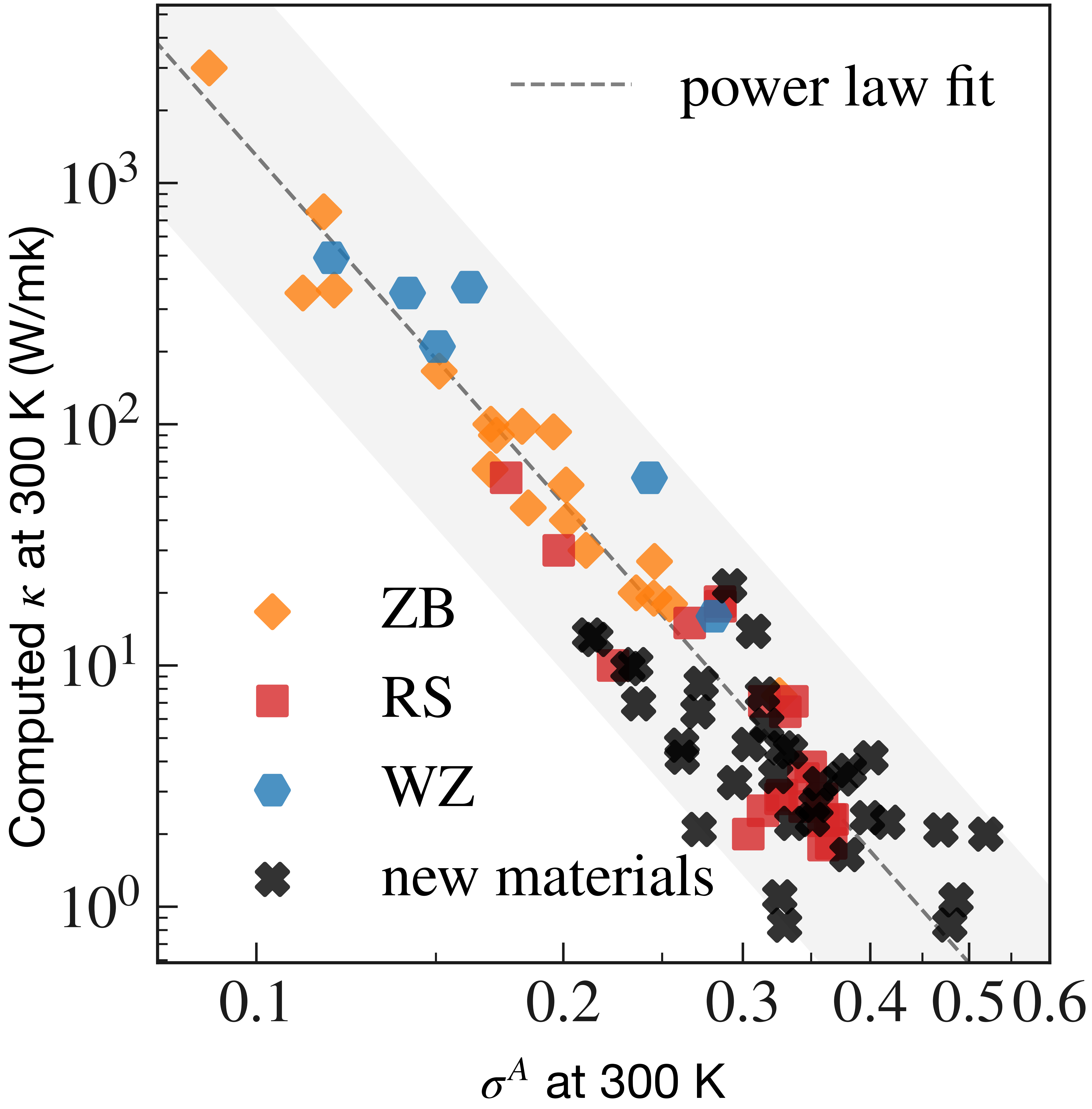


# WHAT ABOUT PREDICTIONS?

F. Knoop, M. Scheffler, and C. Carbogno (*to be submitted*).

**Colored Symbols:**

Materials with measured $\kappa$

**Black Crosses:**

*Known* Materials with *hitherto unknown* $\kappa$

28 materials with $\kappa^{\text{aiGK}}$ < 10 W/mK

24 materials with $\kappa^{\text{aiGK}}$ < 5 W/mK

8 materials with $\kappa^{\text{aiGK}} \leq 2$ W/mK

**5 materials with $\kappa^{\text{aiGK}} \leq 1$ W/mK**

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4) The developed ***high-throughput*** framework reliably identifies **strong thermal insulators.**

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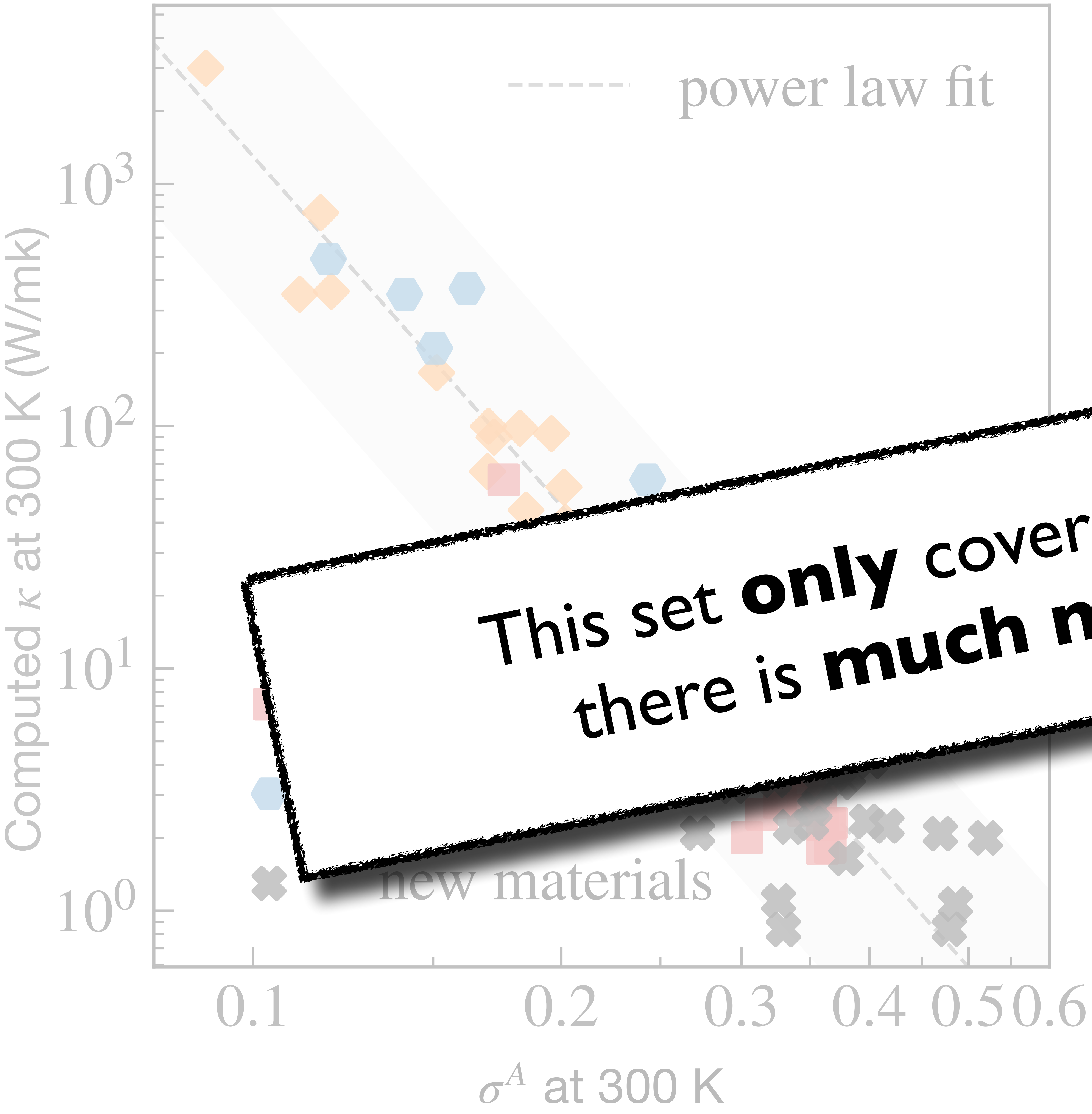


Colored Symbols:

This set **only** covers **100 materials**,
there is **much more** to come…

28 materials with $\kappa^{\mathrm{aiGK}} < 10$ W/mK

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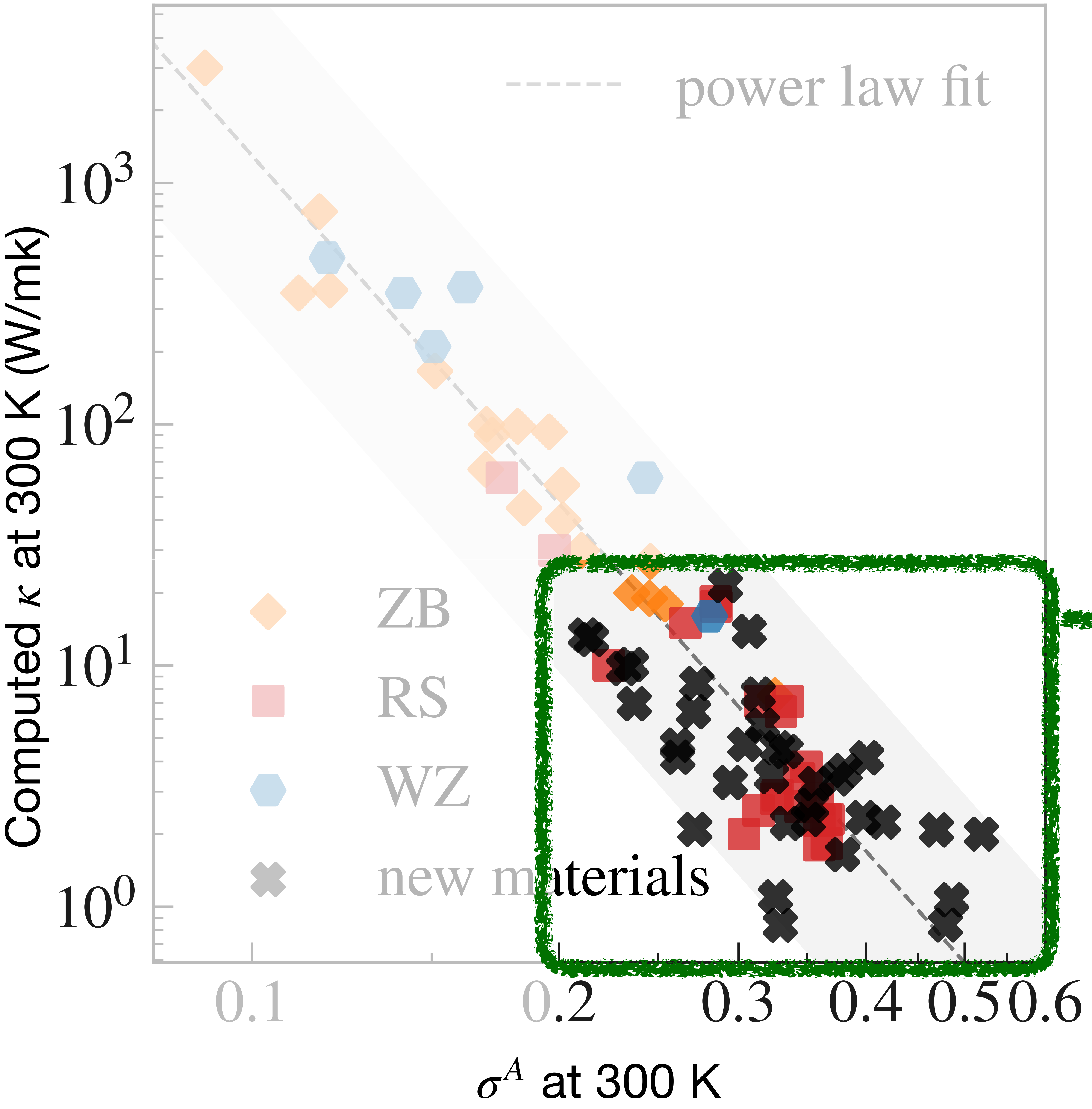


The **anharmonicity metric $\sigma$** reliably identifies **good thermal insulators.** [$\kappa \ll 20$ **W/mK**]

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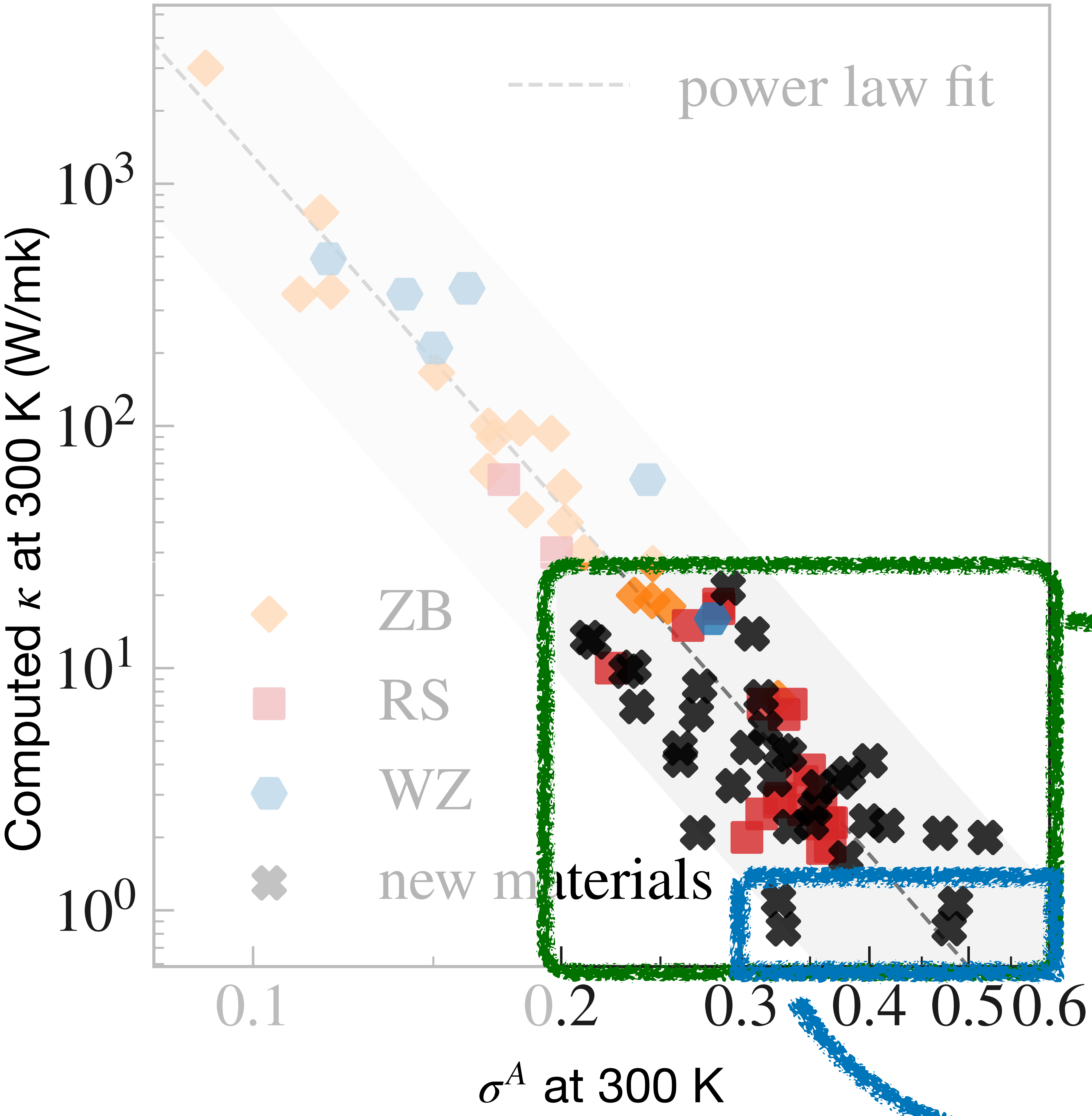


The **anharmonicity metric $\sigma$** reliably identifies **good thermal insulators.** [$\kappa \ll 20$ **W/mK**]

For the **rapid** identification of materials with **ultra-low** $\kappa( \ll 2$ **W/mK**) an even better descriptor is **desirable.**

# ACKNOWLEDGEMENTS


Florian Knoop
now @ Linköping

Dr. Tom Purcell,
FHI

Maja O. Lenz.
FHI

Stefano Curtarolo
Duke U. / FHI

Matthias Scheffler
FHI

erc
European Research Council
Established by the European Commission

NOMAD

DFG

MATERIALS
UC Santa Barbara

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