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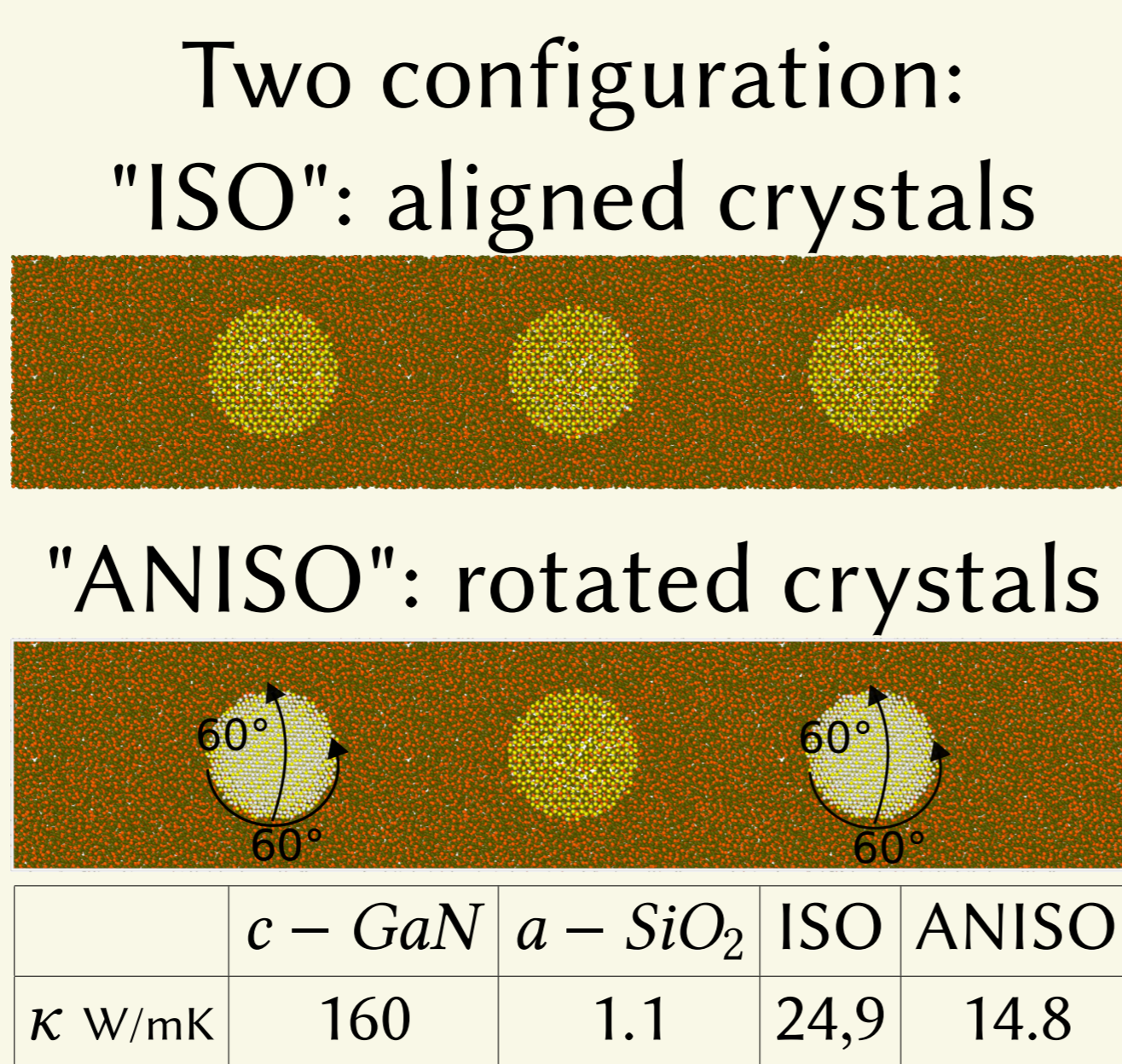
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1 Introduction and Configurations

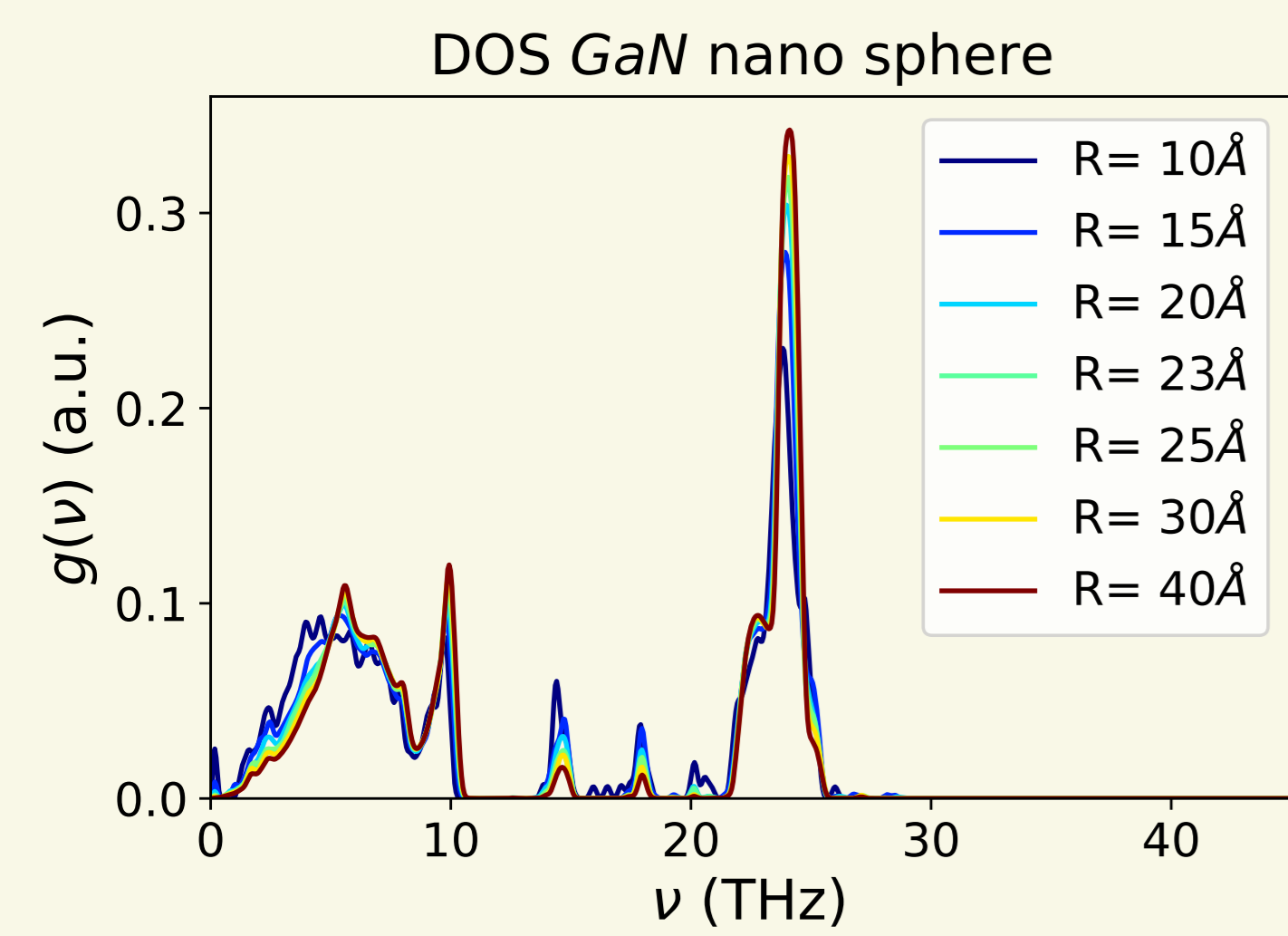
With the increasing demand of efficiency in electronic devices, a good thermal management starts to be crucial. In this regard nanocomposite can be a good solution to tune the conductivity of materials. Here we further investigate previous results [5], that shows that the thermal conductivity can depend significantly on the relative orientation of *c*-GaN inclusion in a *a*-SiO₂ matrix. Which is not taken into account in the Effective Medium Approach. We try to understand how this percolation can take place through molecular dynamics simulation.



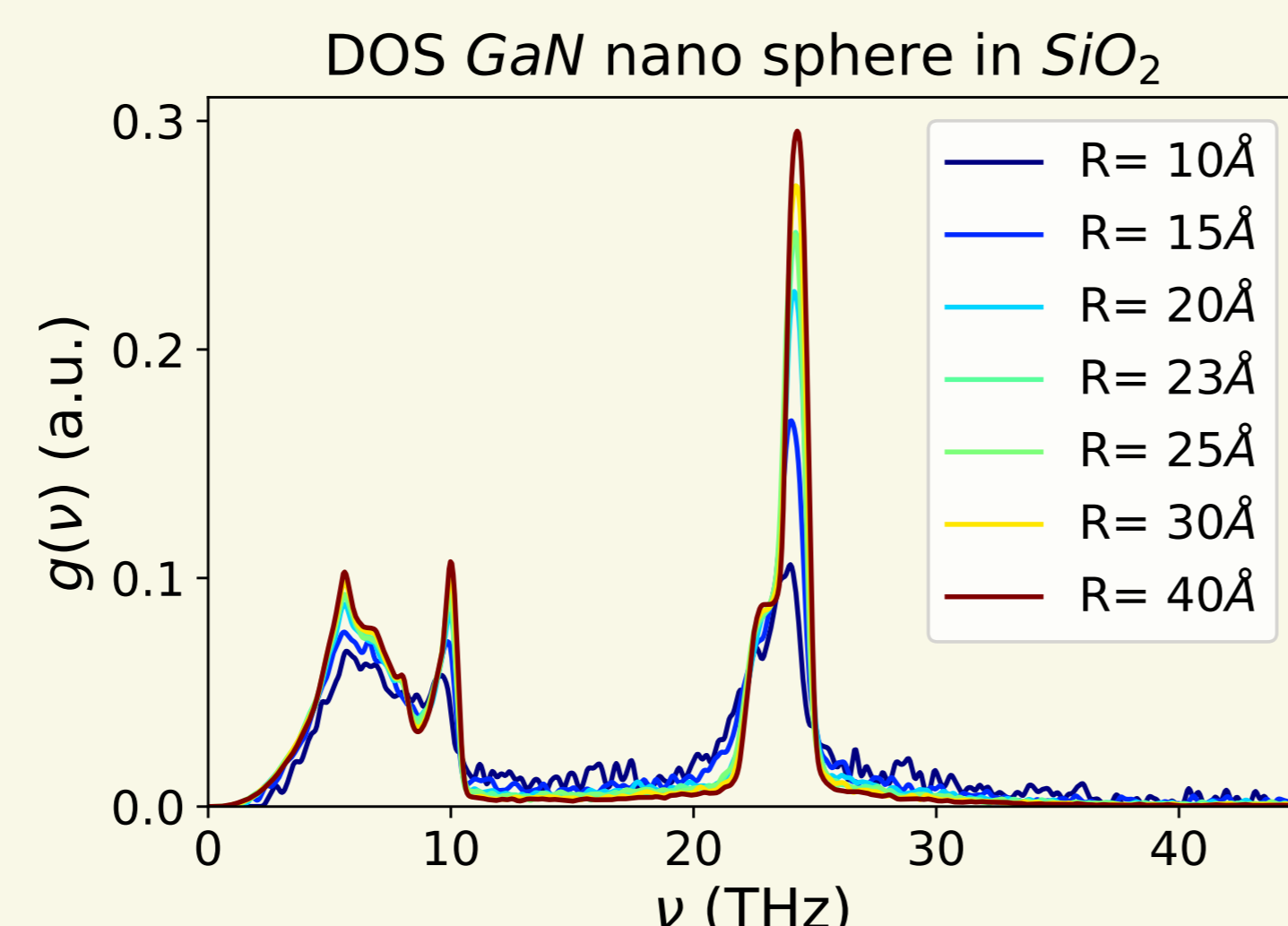
4 VDOS nano sphere Composites

The VDOS is influenced by the size of the nano inclusion

Inclusions Size



Matrix Interface



Red Shift of the acoustic peak

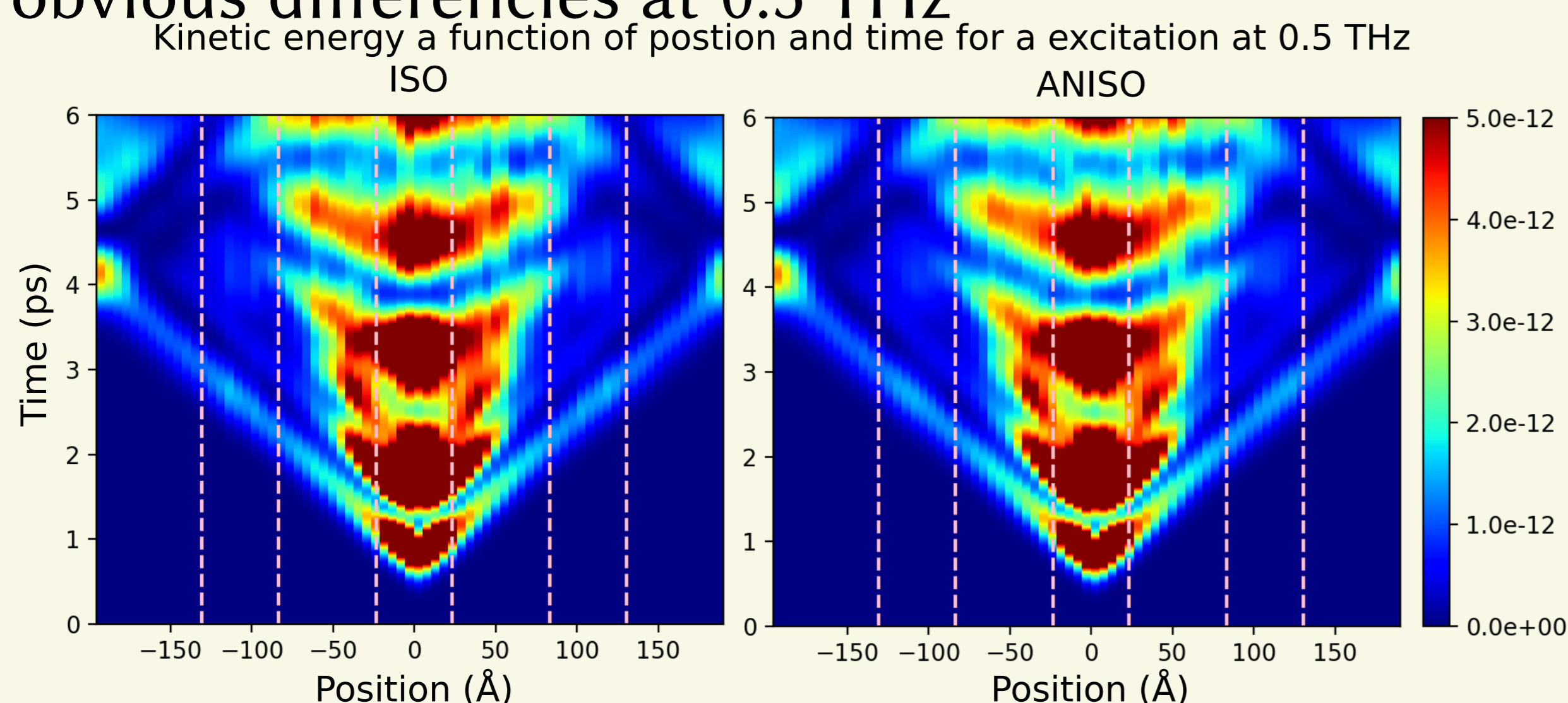
More high frequencies modes

- Modes relative importance [4]
- little to no existing studies
- In both case with the reduction of the radius
 - filling of the band gap
 - reduction of the sharpness of the main peaks
- Influence on the thermal conductivity
 - tailoring of the EMA

6 Wave packet propagation

Comparison of the propagation of an excitation from the inclusion in the middle

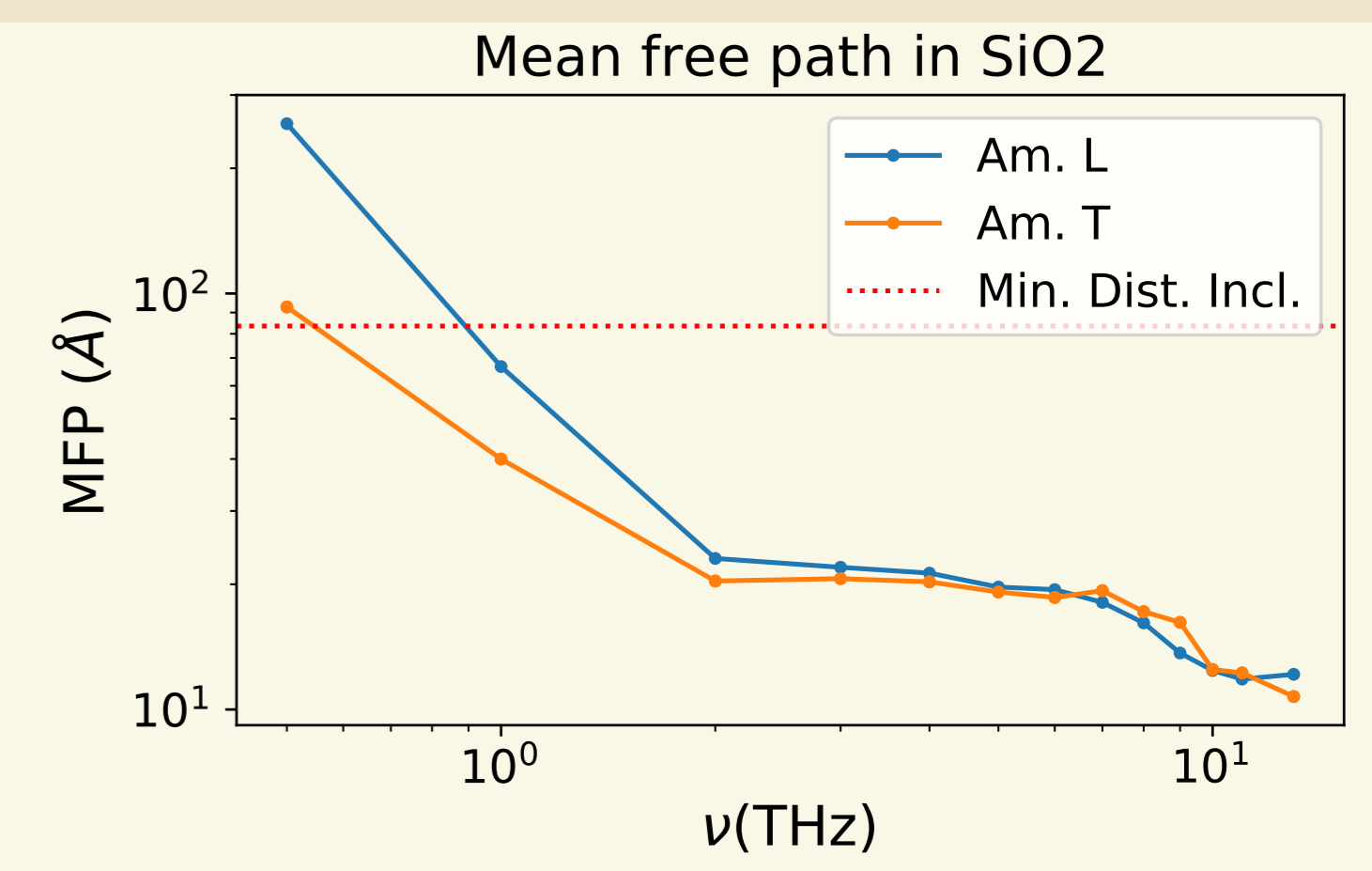
No obvious differences at 0.5 THz



2 Energie transport

Orientation dependant thermal conductivity

- Coherent wave transmission between inclusions
- Possible if Mean Free Path in SiO₂ $\sim l_{incl}$
- If possible at low frequency for longitudinal waves
- Coherent with experimental results [7, 6]



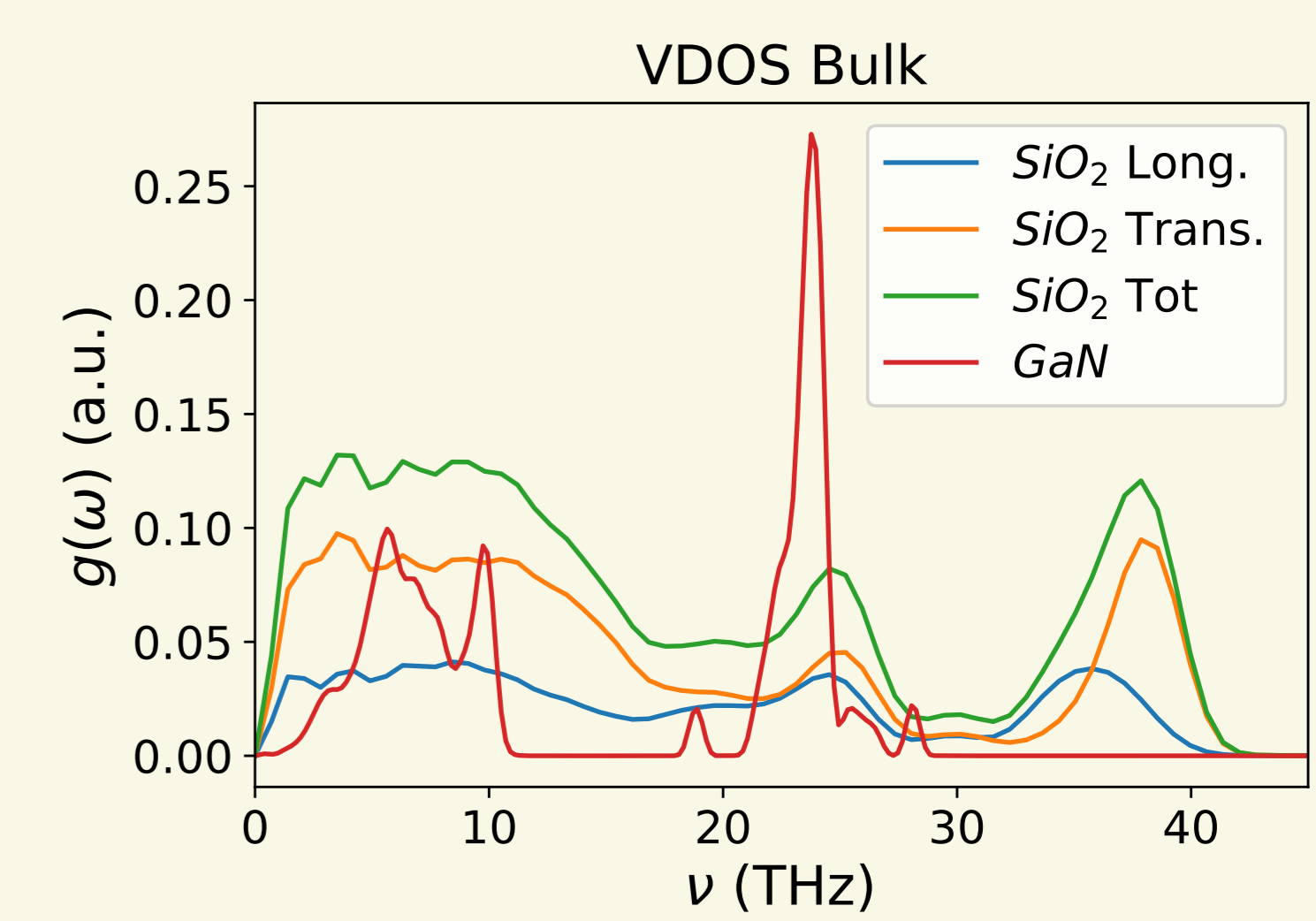
Mean Free Path in SiO₂ from wave packet attenuation [1]

3 Vibrational Density of State

To be transmitted mode of the frequency that travels should be allowed in both matrix and inclusion

Overlap between the DOS at low frequency

- in DOS of the disjunct materials



Transverse as non compressive [2]

5 Dynamical Structure Factor

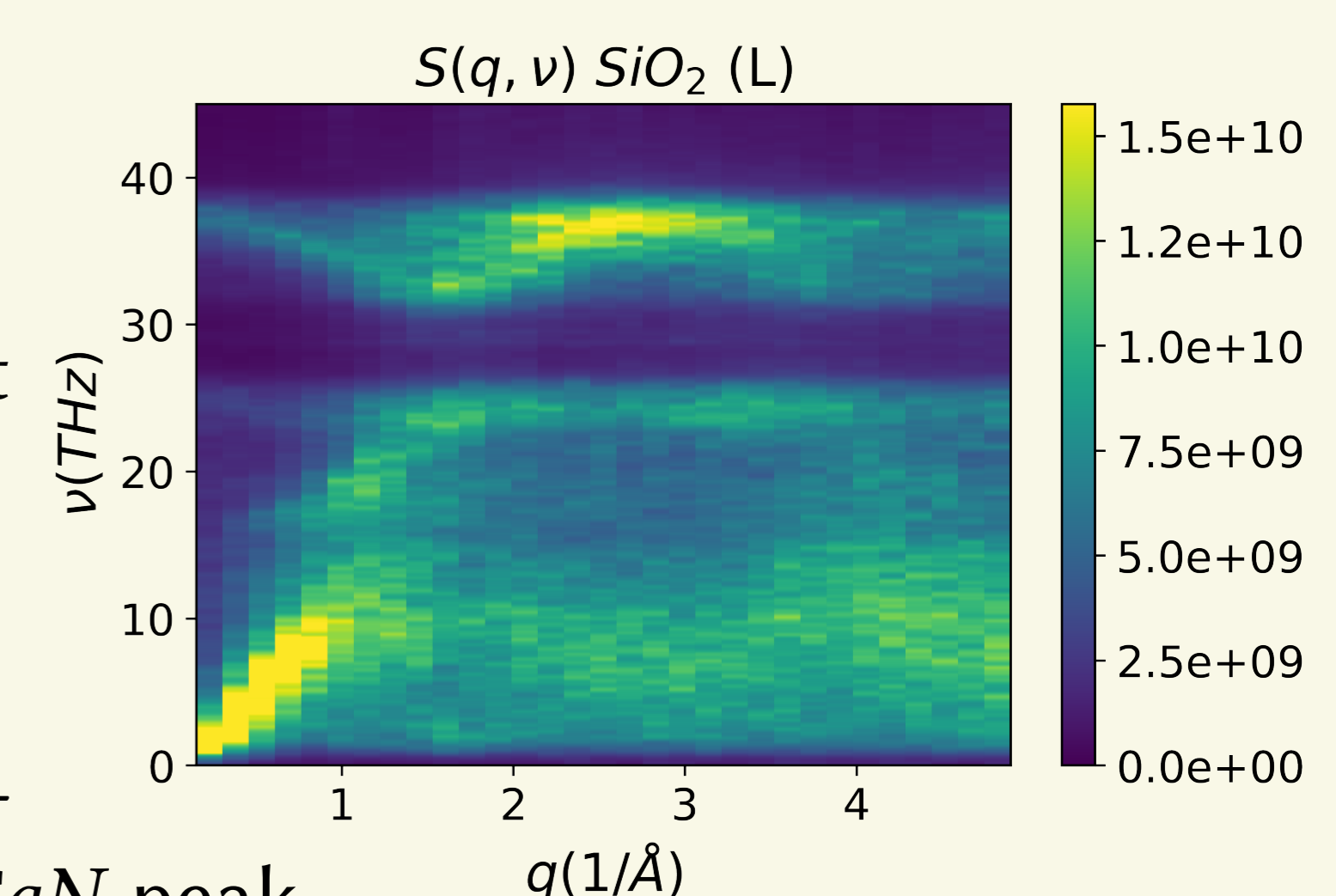
We use the mode resolved dynamical structure [3]

for Bulk *a*-SiO₂

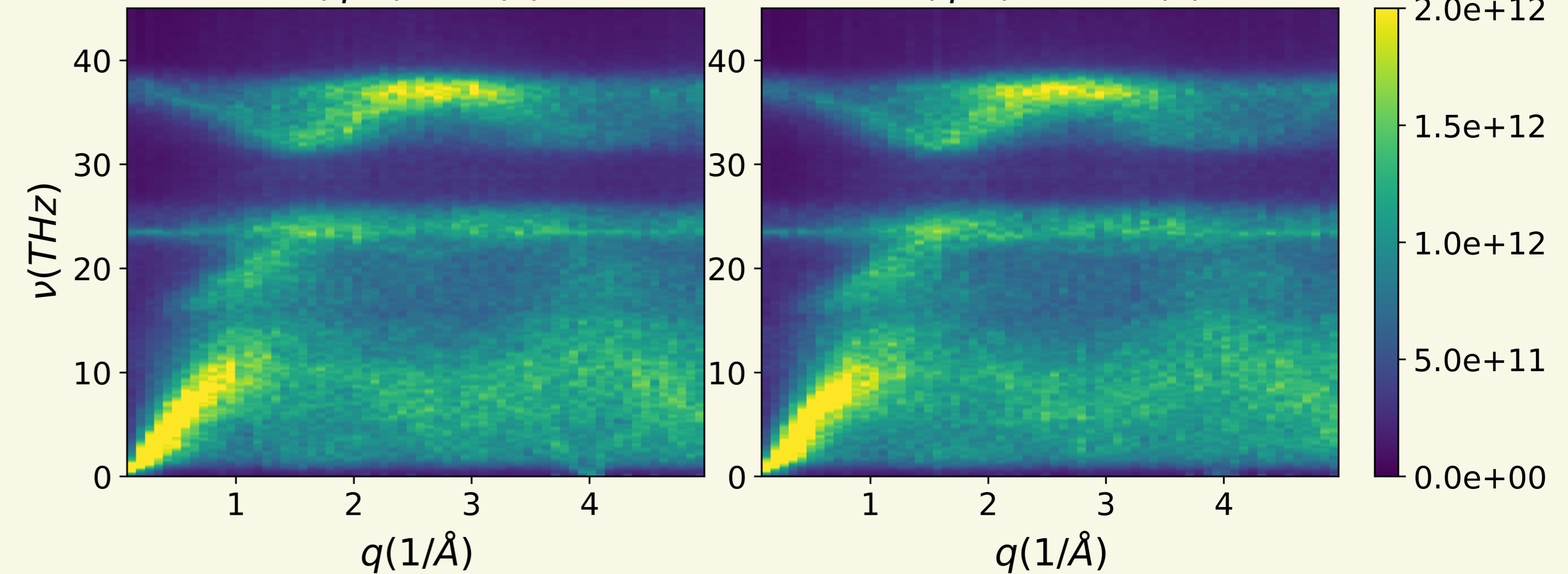
- From the slope of the first phonons
- $v_L(\nu) > v_T(\nu)$

ISO/ANISO

- Apparition of a new band frequency corresponding to the GaN peak
- no obvious differences



$S(q, \nu)$ ISO (L)



Summary and prospective

- Non trivial effect of size / interface to the VDOS
- No obvious difference one the propagative part
 - no supplementary channel in $S(q, \omega)$
- Prospective
 - Computation of κ via another method (NEMD)
 - Test of the propagation at characteristic frequencies
 - Size of the inclusions
 - Distance between inclusion

References

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