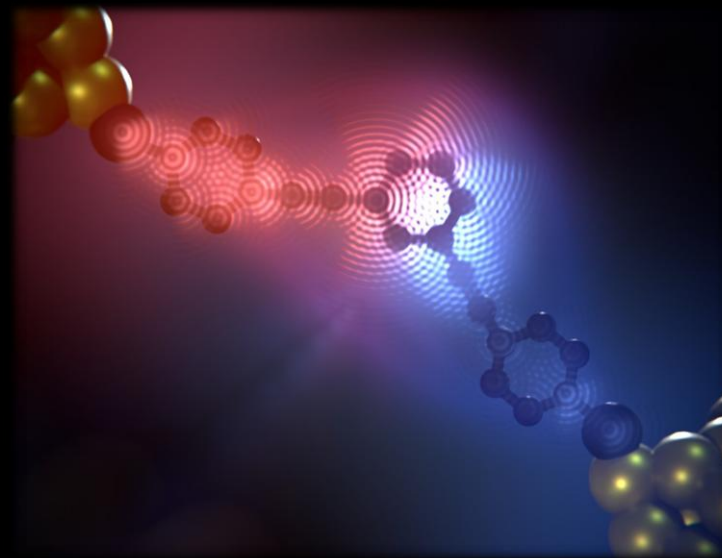
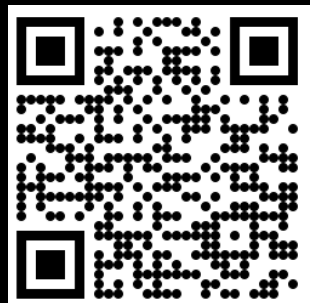
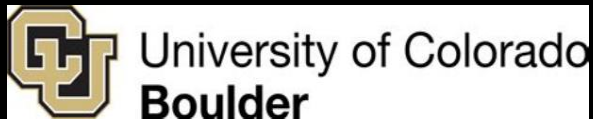


Phonon interference in single-molecule junctions

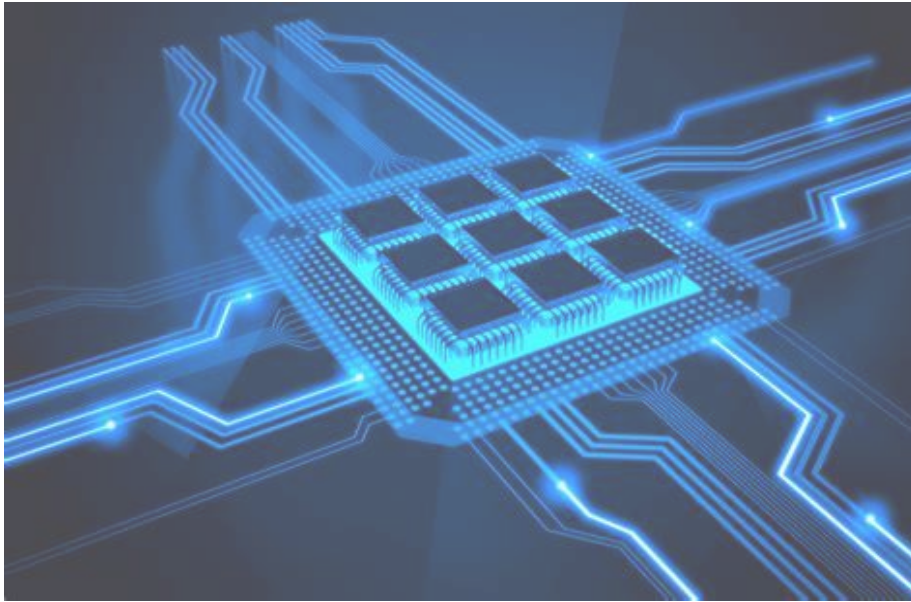
Nat. Mater. **24**, pp. 1258–1264, 2025



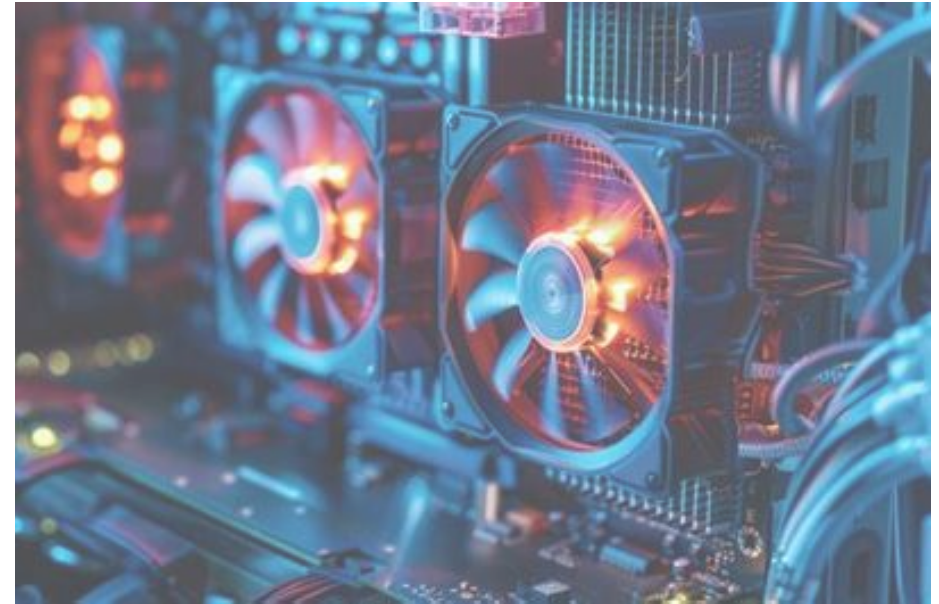
S.C. Yelishala*, Y. Zhu*, P.M. Martinez*, H. Chen, M. Habibi, G. Prampolini, J.C. Cuevas, W. Zhang, J.G. Vilhena[‡], L. Cui[‡]



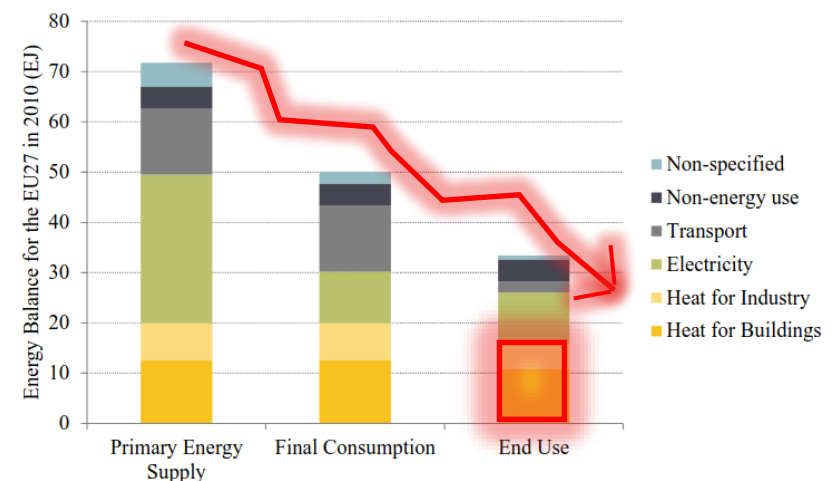
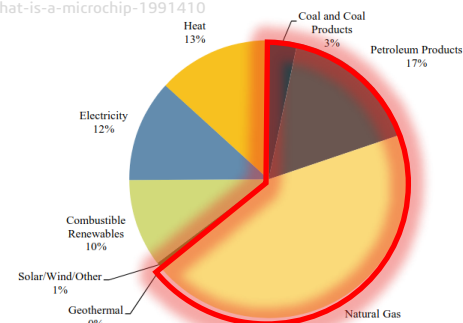
A persistent technological bottleneck



<https://www.thoughtco.com/what-is-a-microchip-1991410>



https://pngtree.com/freebackground/cooling-fan-in-the-computer-system-unit_15538491.html



Influence of tribology on global energy consumption, costs and emissions
 International Journal of Energy Research
 Volume 42, Issue 10, October 2018
 ISSN 0195-9018
 Abstract
 Evaluation of the impact of tribology on energy consumption, emissions, costs, and CO₂ emissions is presented in this paper. This paper reviews the tribology research activities worldwide, considering energy generation, conversion, and distribution. Tribology is a key factor in energy efficiency, and its impact on energy consumption, emissions, and costs is significant. This paper presents a comprehensive review of the tribology research activities worldwide, considering energy generation, conversion, and distribution. Tribology is a key factor in energy efficiency, and its impact on energy consumption, emissions, and costs is significant. This paper presents a comprehensive review of the tribology research activities worldwide, considering energy generation, conversion, and distribution. Tribology is a key factor in energy efficiency, and its impact on energy consumption, emissions, and costs is significant.

~23% (119 EJ) of the world's total energy consumption

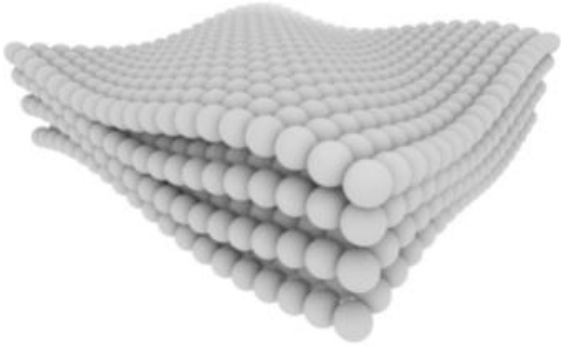
savings would amount to (8.7% of the total energy)

wear could potentially be reduced by 40%

reduce the CO₂ emissions

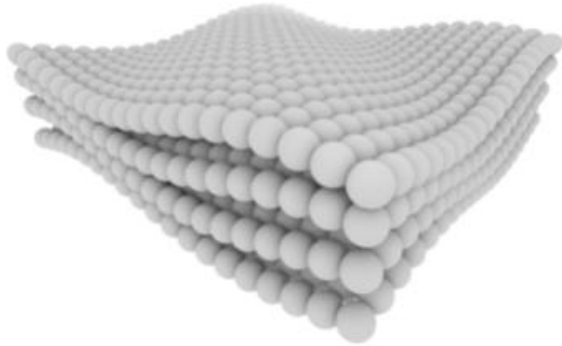
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Heat as a delocalized wave

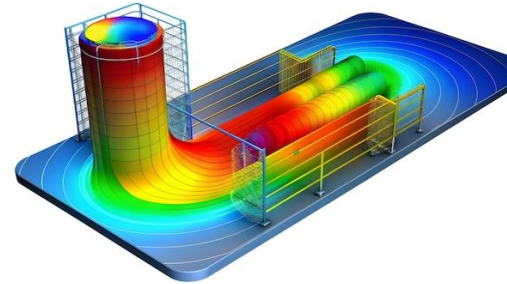


[https://eng.libretexts.org/Bookshelves/Materials_Science/Supplemental_Modules_\(Materials_Science\)/Electronic_Properties/Lattice_Vibrations](https://eng.libretexts.org/Bookshelves/Materials_Science/Supplemental_Modules_(Materials_Science)/Electronic_Properties/Lattice_Vibrations)

Heat as a delocalized wave

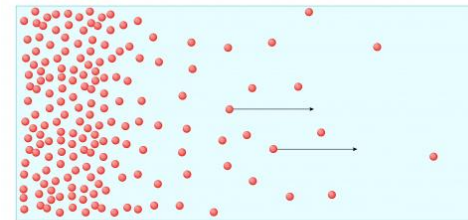


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https://www.freepik.com/premium-ai-image/understanding-temperature-distribution-finite-element-analysis-heat-transfer-fea_200622480.htm

$$\dot{Q} = -\kappa \frac{\partial T}{\partial x}$$

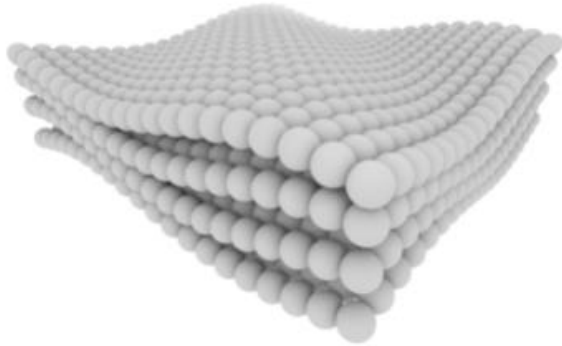


High concentration Low concentration

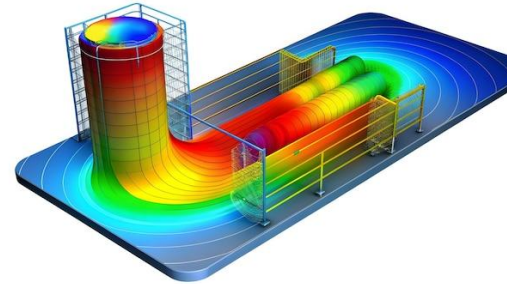
<https://fity.club/lists/suggestions/diffusion/>

$$\dot{N} = -D \frac{\partial \phi}{\partial x}$$

Heat as a delocalized wave

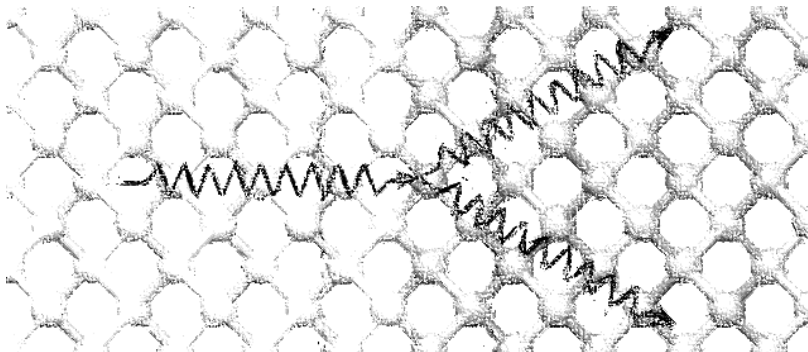


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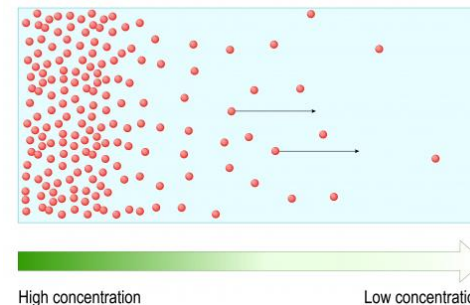


$$\dot{Q} = -\kappa \frac{\partial T}{\partial x}$$

https://www.freepik.com/premium-ai-image/understanding-temperature-distribution-finite-element-analysis-heat-transfer-fea_200622480.htm



Y. Guo et.al. *PRB*. **103**, 174306 (2021)



$$\dot{N} = -D \frac{\partial \phi}{\partial x}$$

<https://fity.club/lists/suggestions/diffusion/>

Methods

Methods: Simulations & Experiments (SThM)

➤ All-atom molecular dynamics simulations



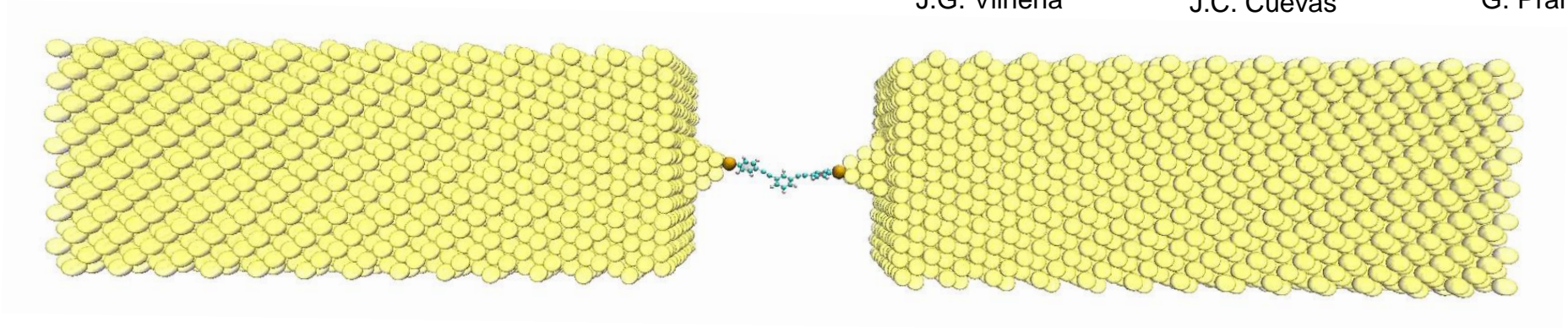
J.G. Vilhena



J.C. Cuevas

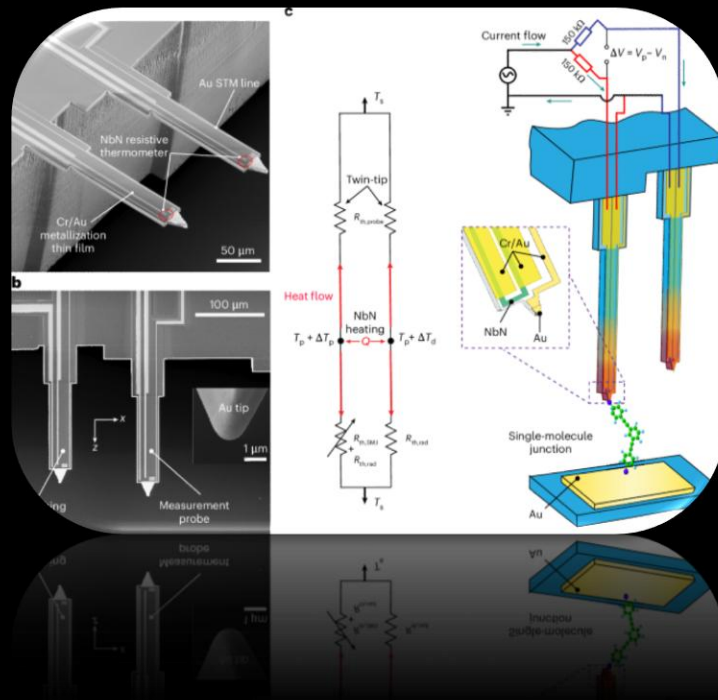


G. Prampolini



Results

Measurements

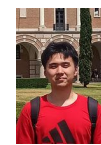


Nat. Mater. 24, pp. 1258–1264, 2025

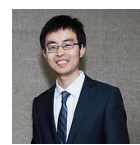
Measurement protocol: single-junction resolution



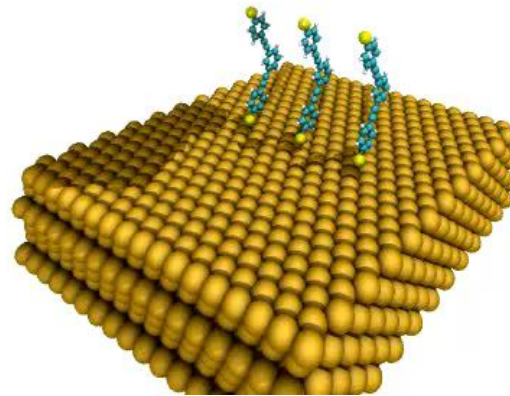
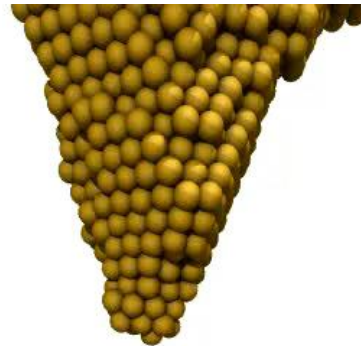
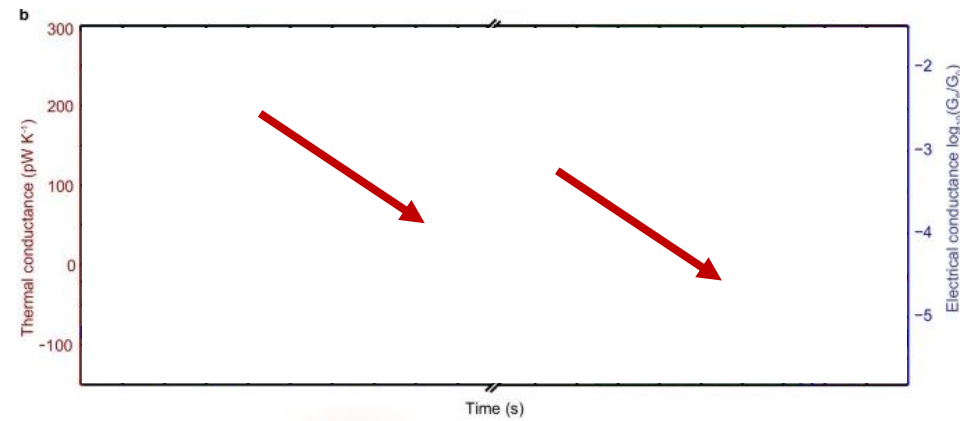
S.C. Yelishala



Y. Zhu



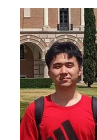
L. Cui



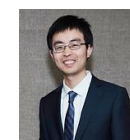
Measurement protocol: single-junction resolution



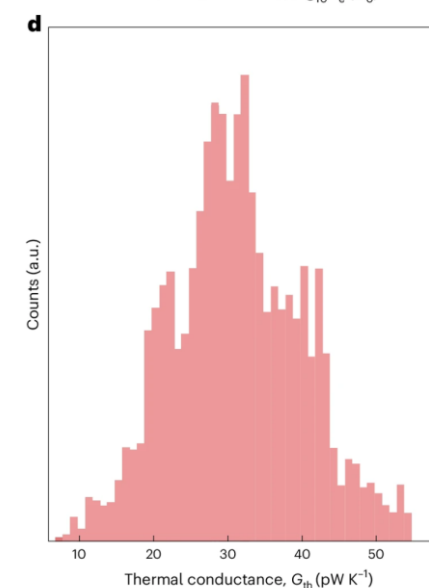
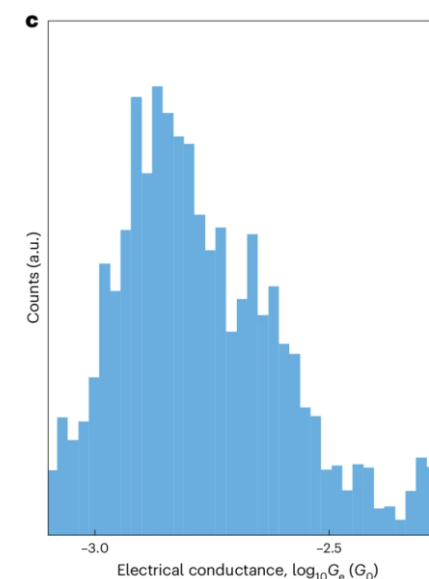
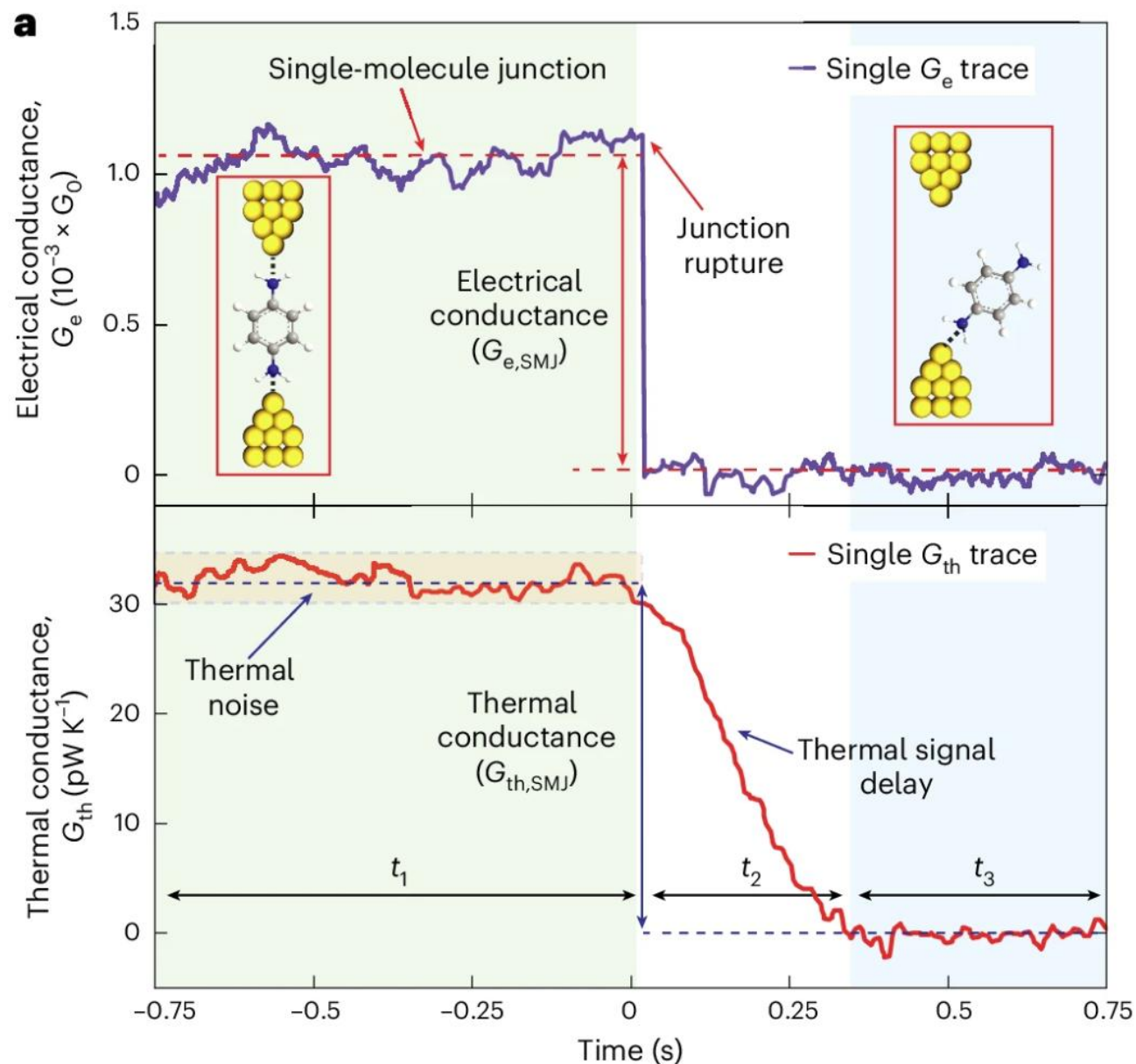
S.C. Yelishala



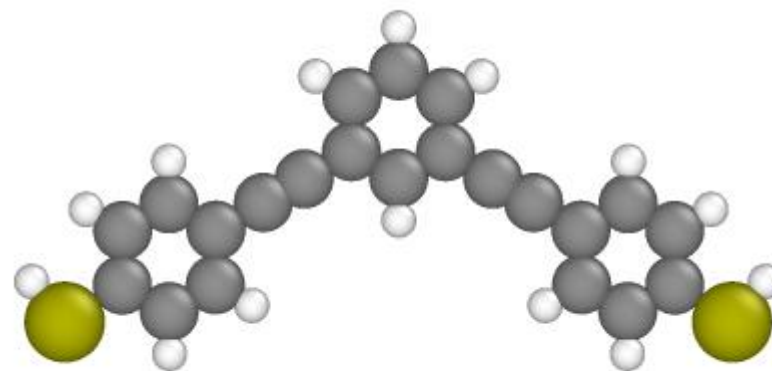
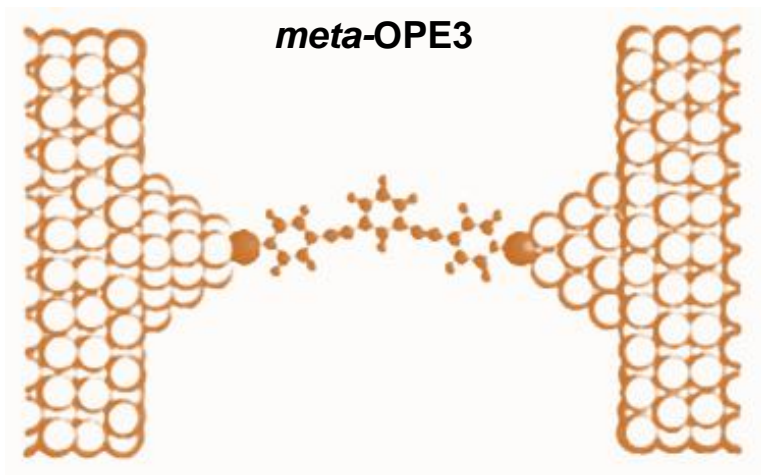
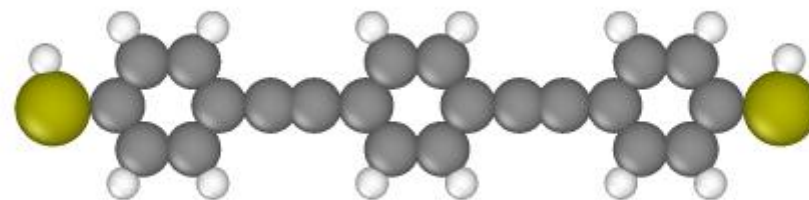
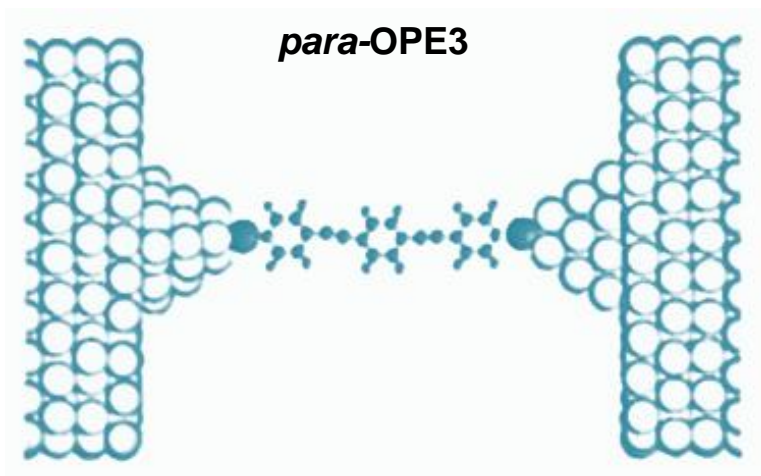
Y. Zhu



L. Cui



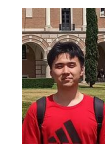
Thermal conductance of *meta*- and *para*-OPE3



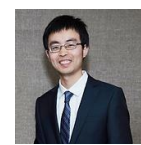
Thermal conductance of *meta*- and *para*-OPE3



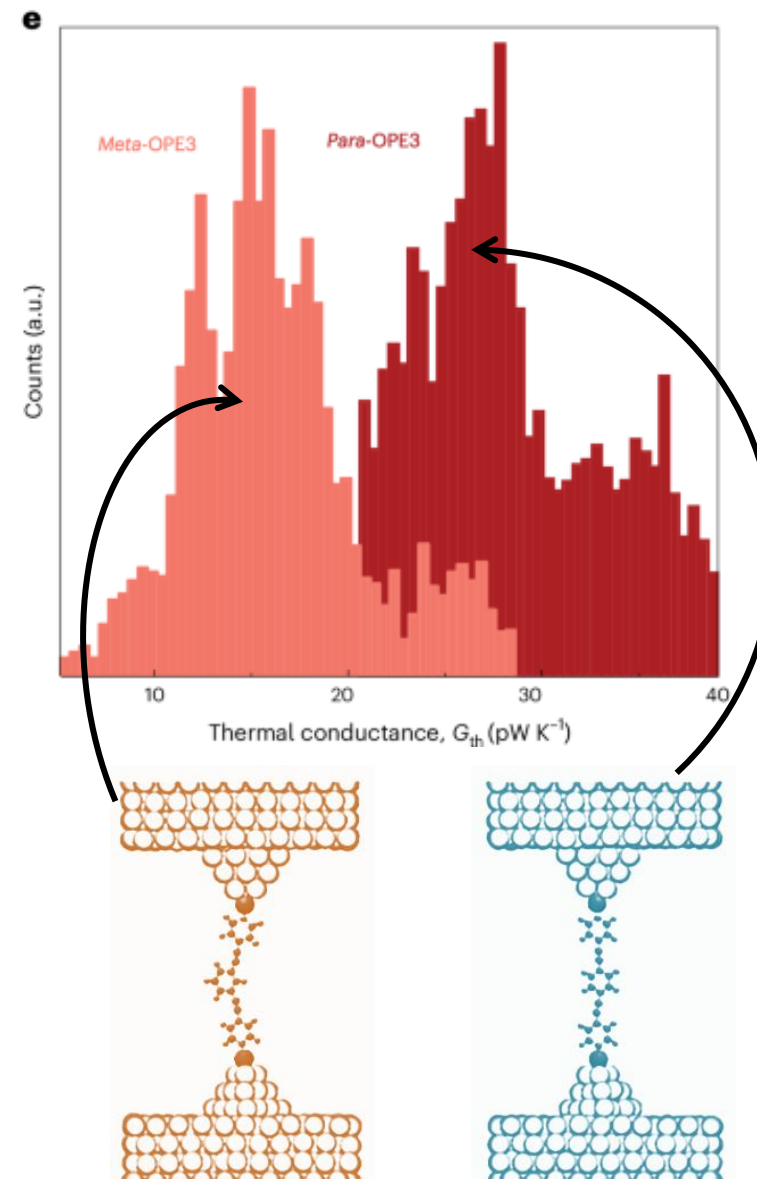
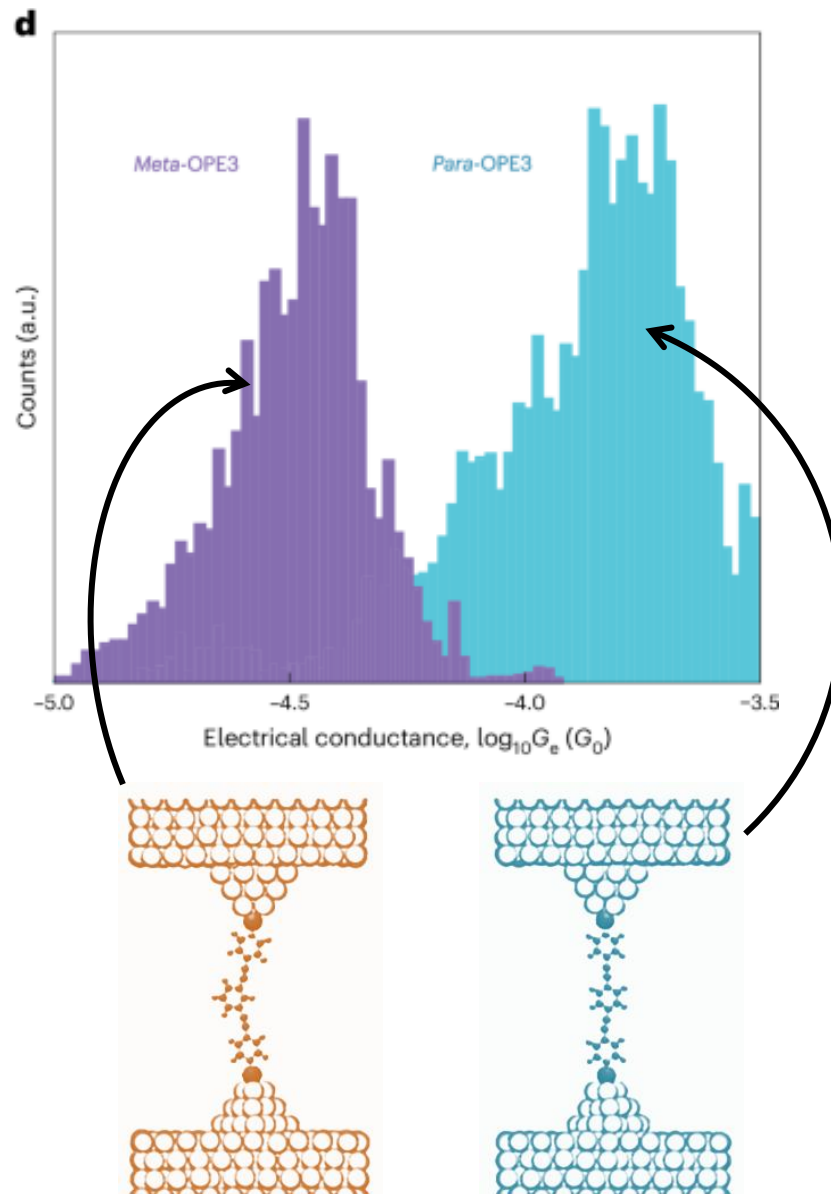
S.C. Yelishala



Y. Zhu

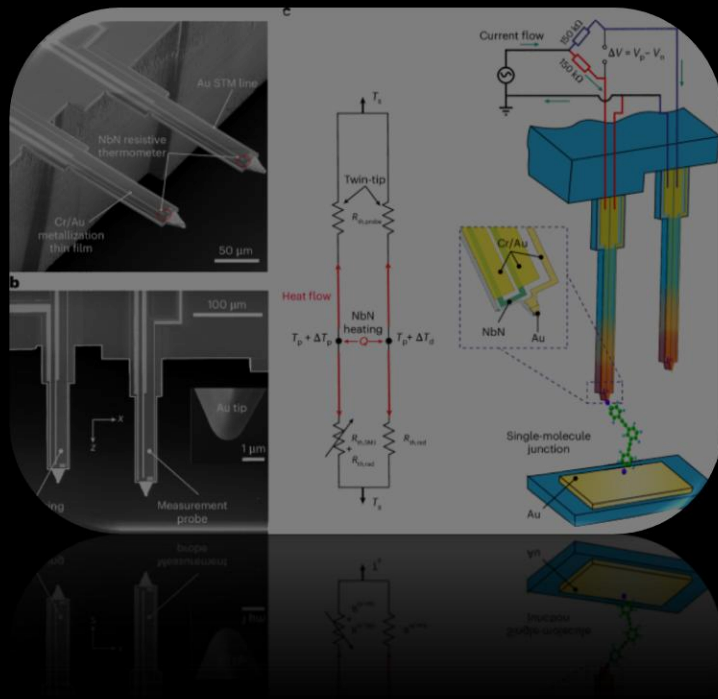


L. Cui

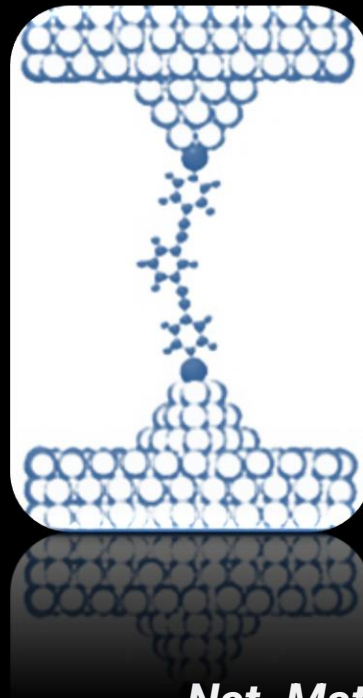


Results

Measurements



MD simulation



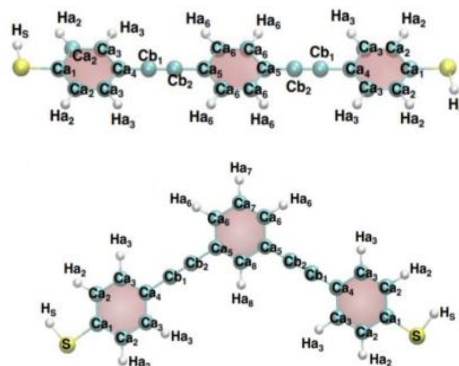
Nat. Mater. 24, pp. 1258–1264, 2025

NEMD simulations with QM-derived force fields

- Intramolecular force field sourced from QM data



G. Prampolini

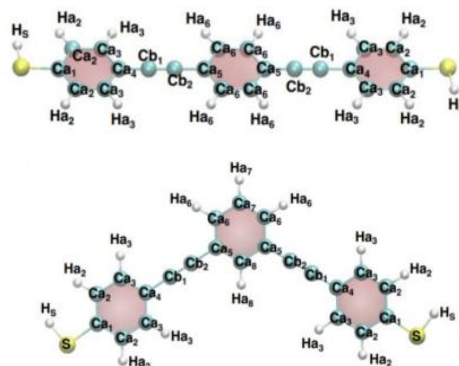


NEMD simulations with QM-derived force fields

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G. Prampolini



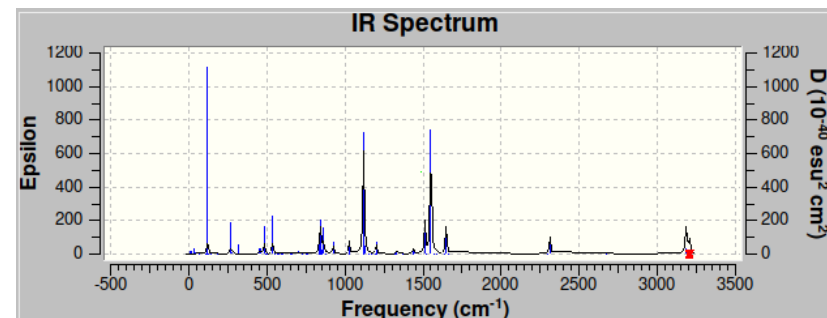
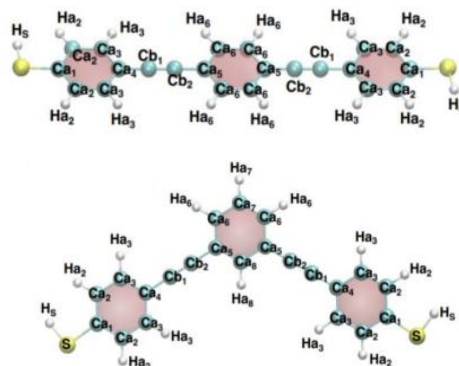
$$\begin{aligned}
 U(\{r_i\}) = & \sum_{bonds} K_r (r - r_0)^2 + \sum_{angles} K_\theta (\theta - \theta_0)^2 + \\
 & + \sum_{dihedrals} \sum_n^4 K_{n\delta} (1 + \cos(n\delta)) + \sum_{i < j} 4\epsilon_{ij} \left(\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right)
 \end{aligned}$$

NEMD simulations with QM-derived force fields

- Intramolecular force field sourced from QM data



G. Prampolini



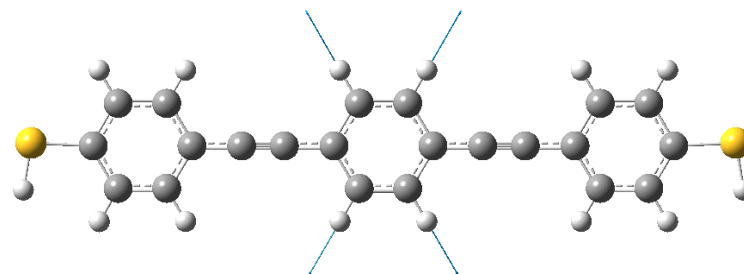
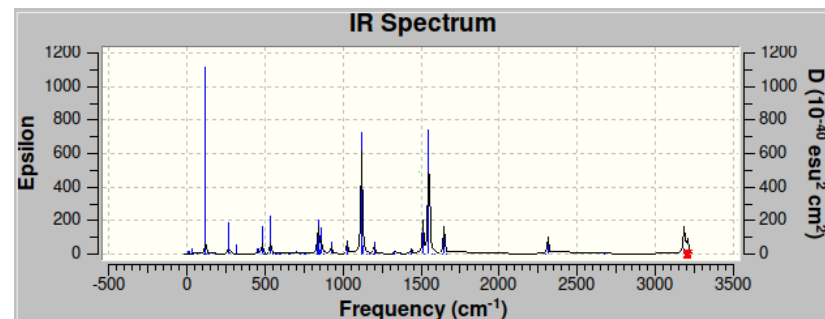
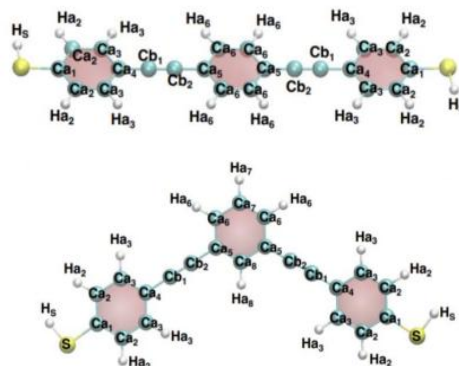
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NEMD simulations with QM-derived force fields

- Intramolecular force field sourced from QM data



G. Prampolini



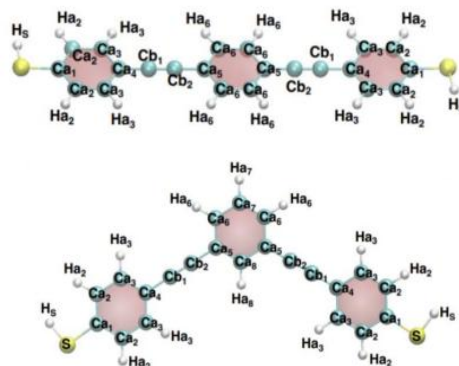
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NEMD simulations with QM-derived force fields

- Intramolecular force field sourced from QM data



G. Prampolini

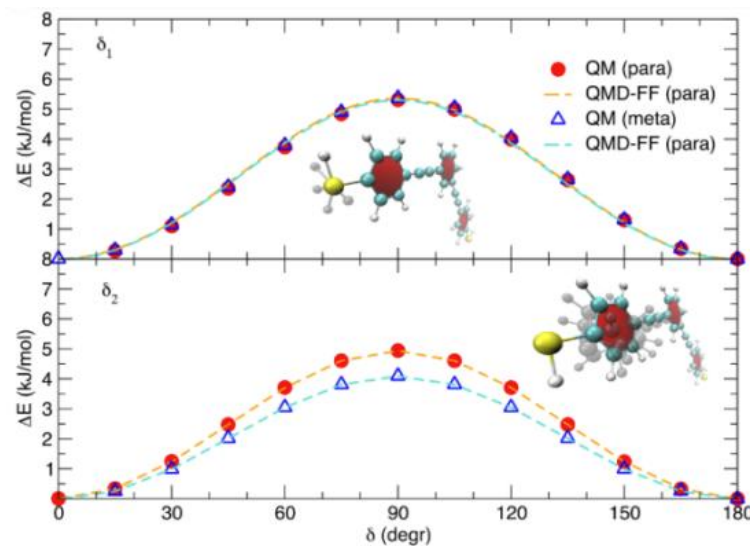
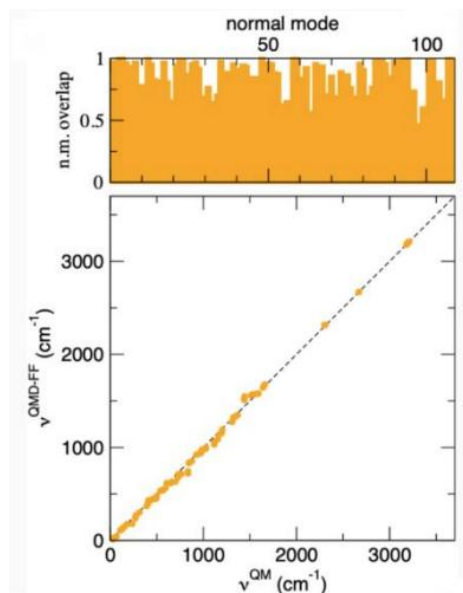
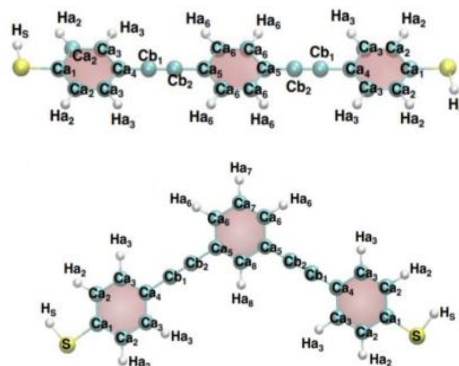


NEMD simulations with QM-derived force fields

- Intramolecular force field sourced from QM data



G. Prampolini

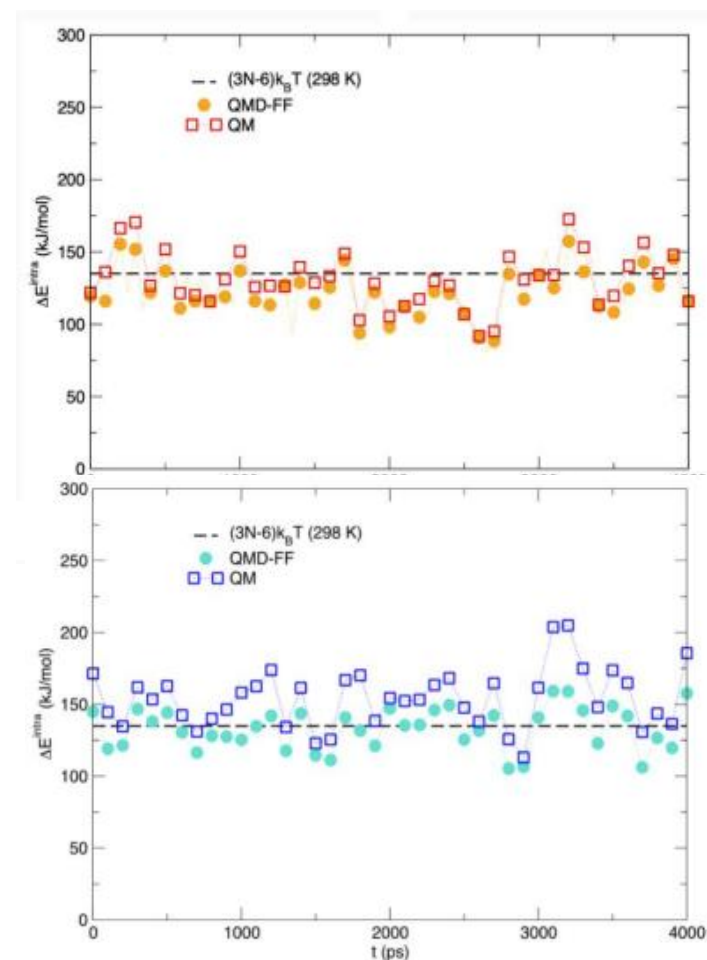
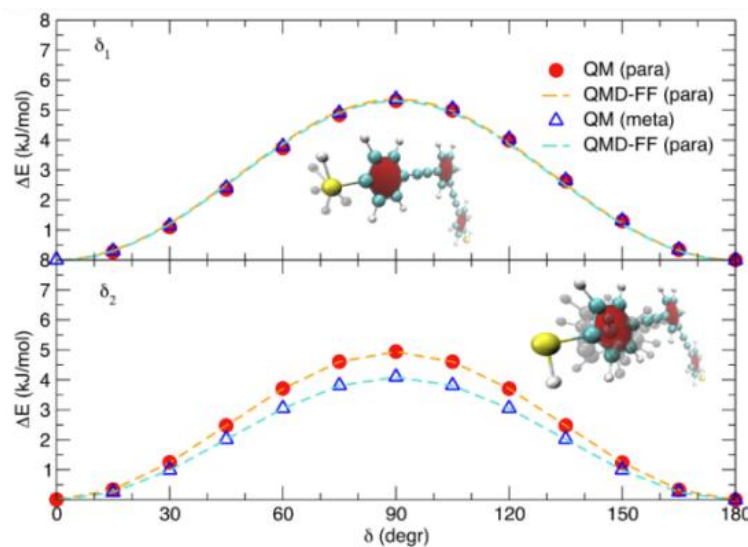
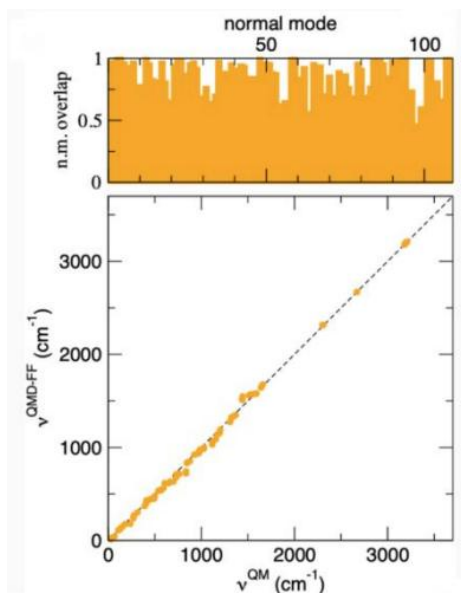
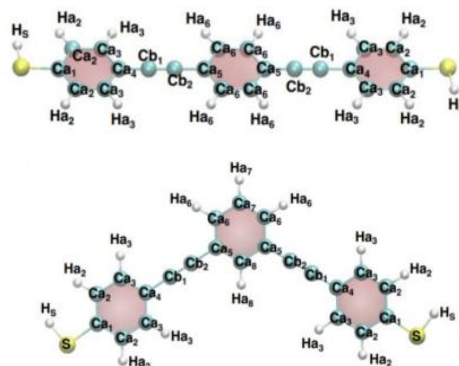


NEMD simulations with QM-derived force fields

➤ Intramolecular force field sourced from QM data



G. Prampolini



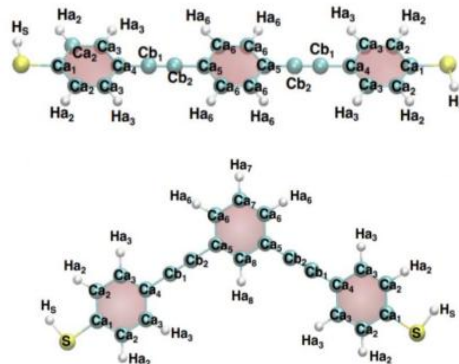


NEMD simulations with QM-derived force fields

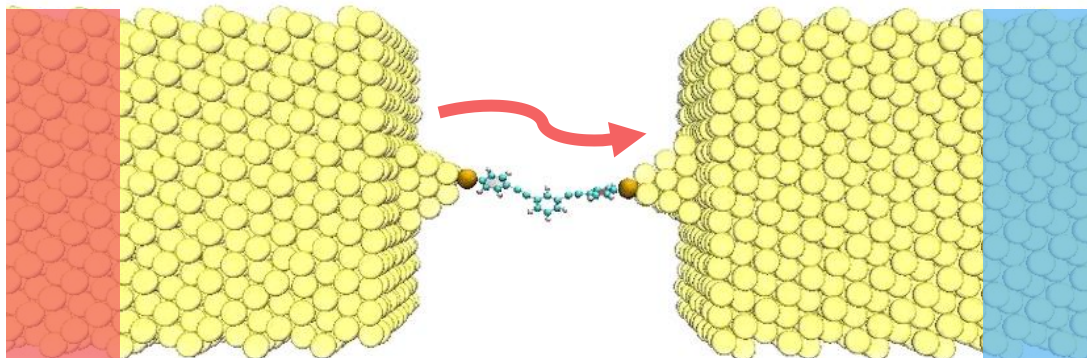
- Intramolecular force field sourced from QM data



G. Prampolini



- How to measure heat in MD?

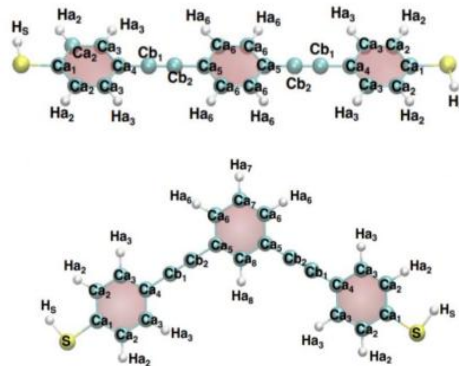


NEMD simulations with QM-derived force fields

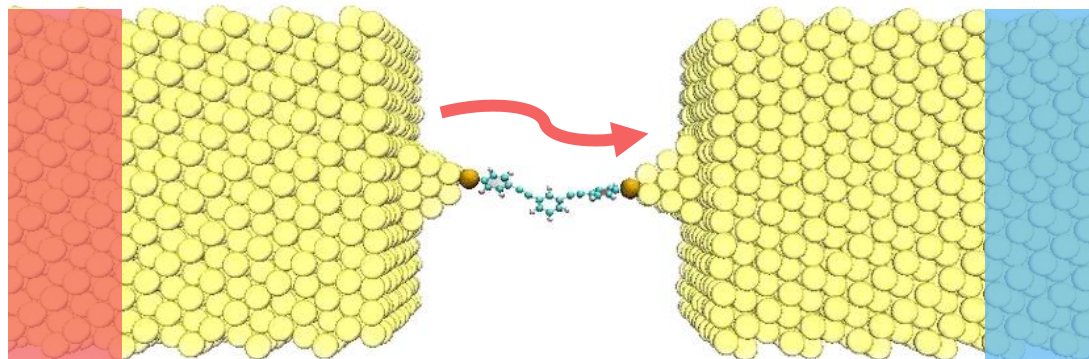
- Intramolecular force field sourced from QM data



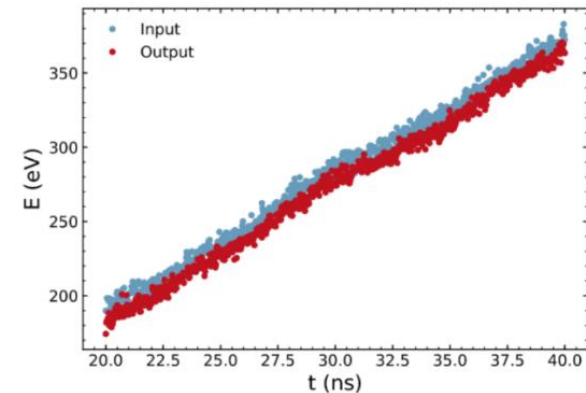
G. Prampolini



- How to measure heat in MD?

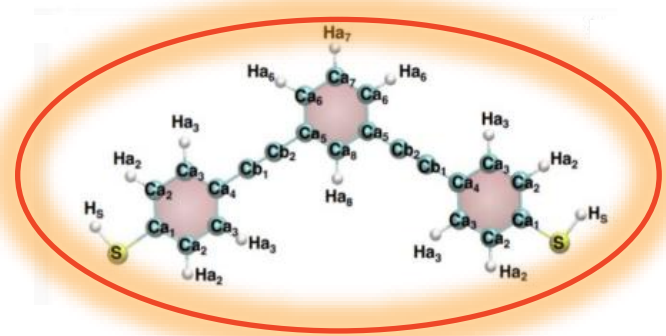
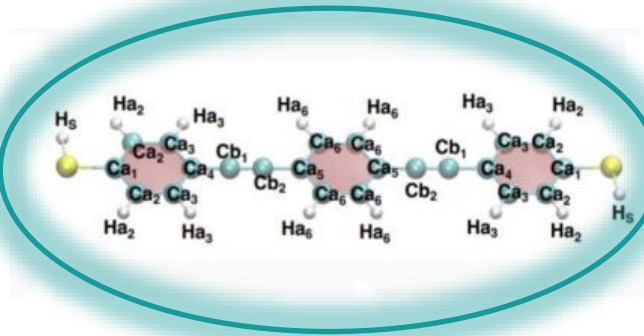


$$G_{th} = \frac{\dot{Q}}{\Delta T}$$



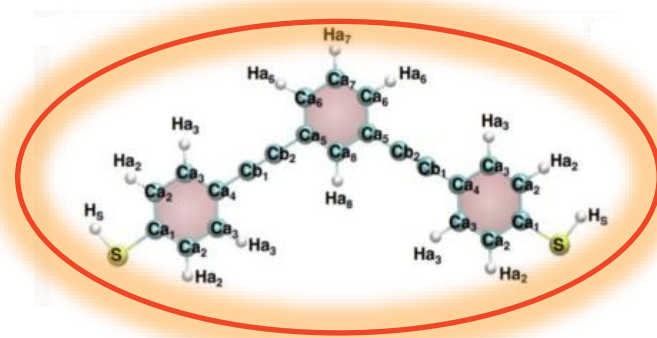
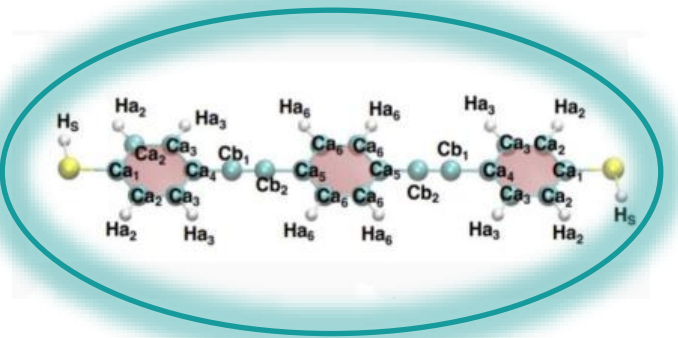
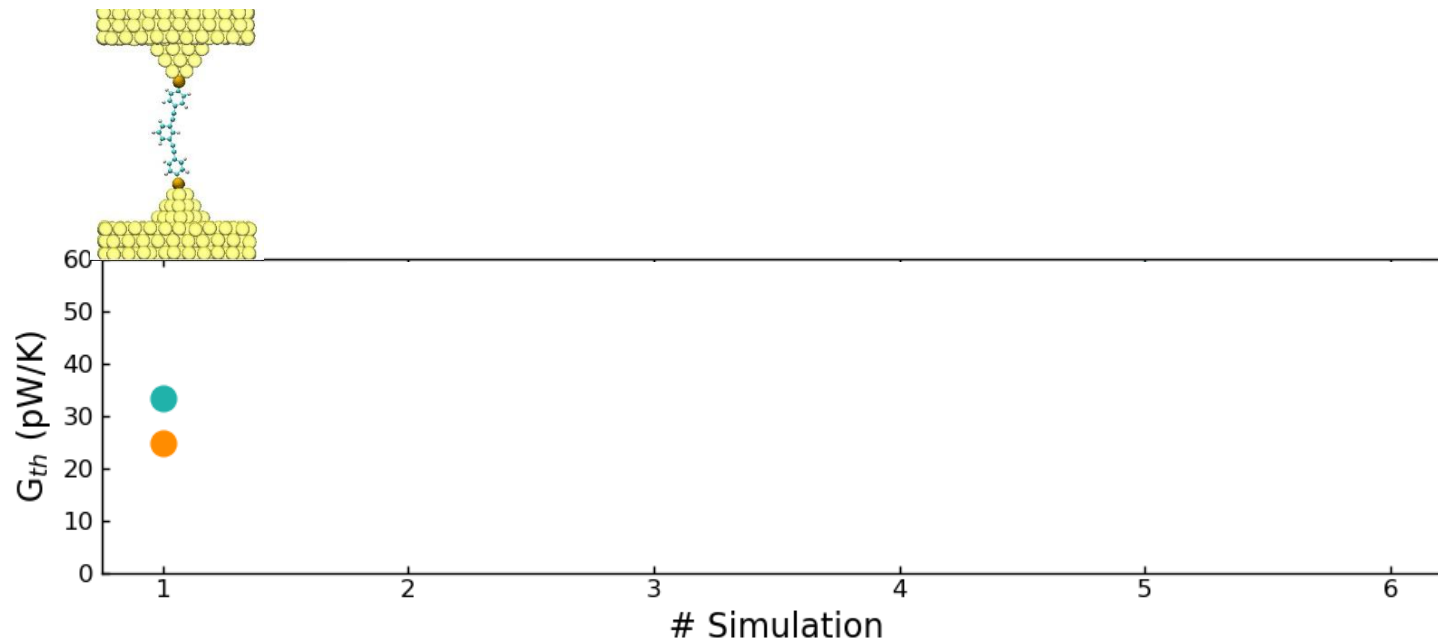
NEMD thermal conductance

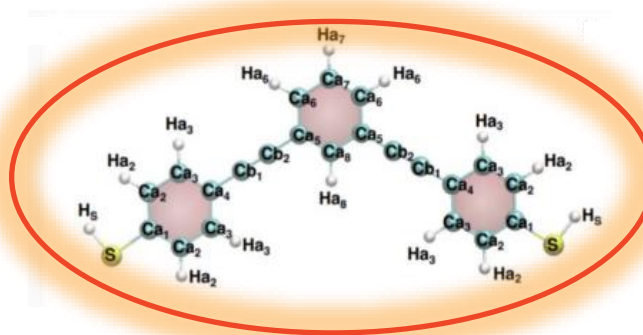
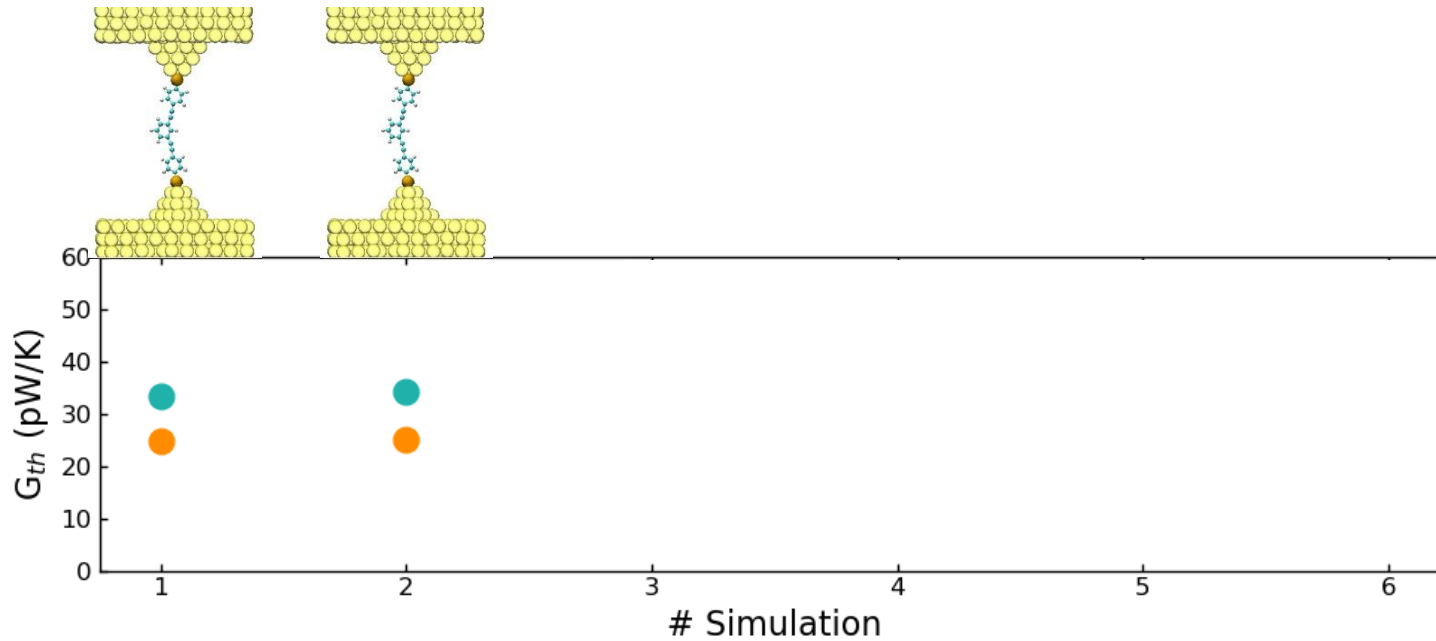
NPT \rightarrow Pulling (0.35 nN) \rightarrow Thermal Bias (40 K) \rightarrow Production (30 ns)



NEMD thermal conductance

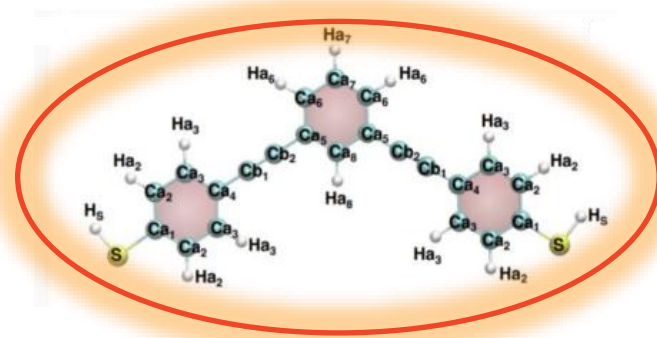
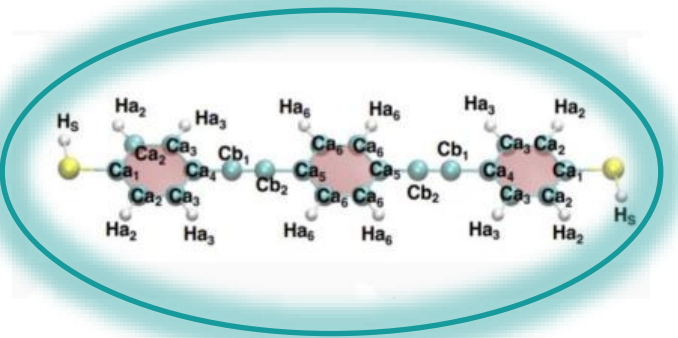
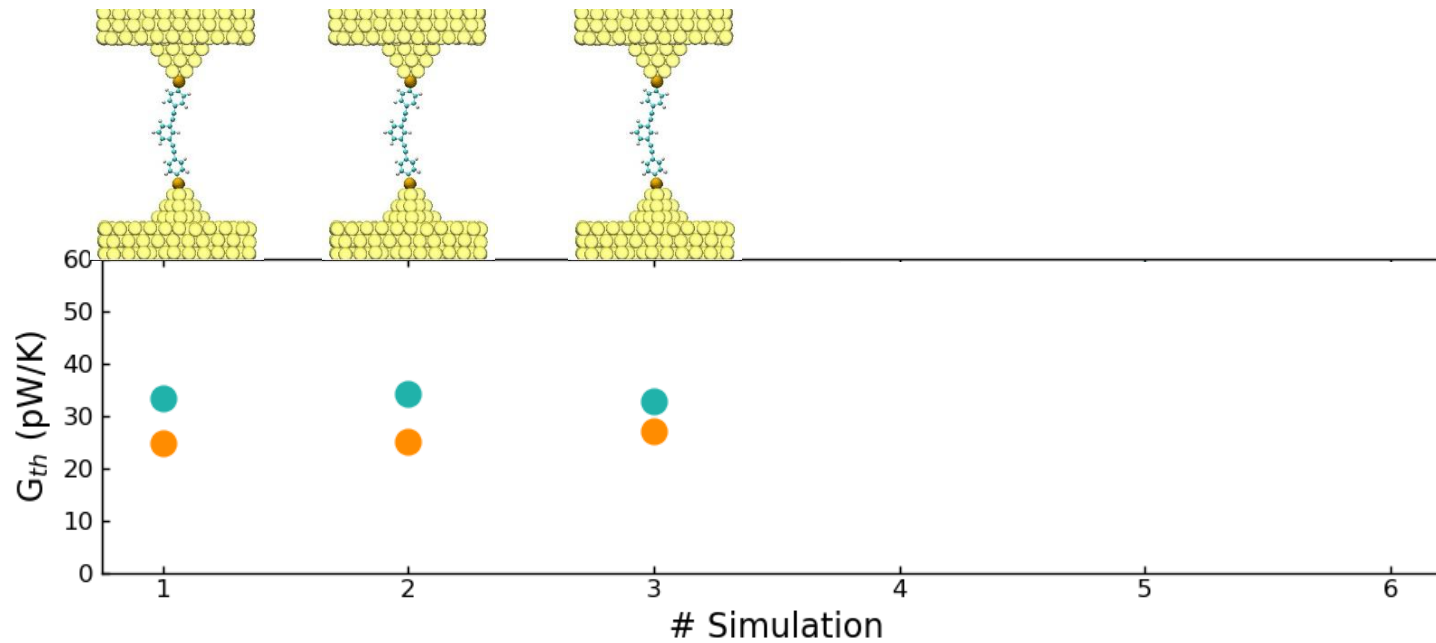
NPT \rightarrow Pulling (0.35 nN) \rightarrow Thermal Bias (40 K) \rightarrow Production (30 ns)





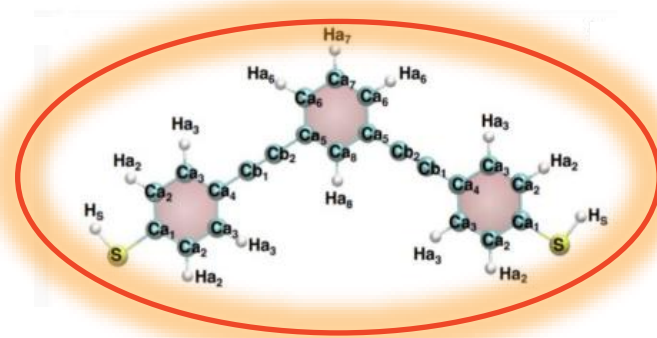
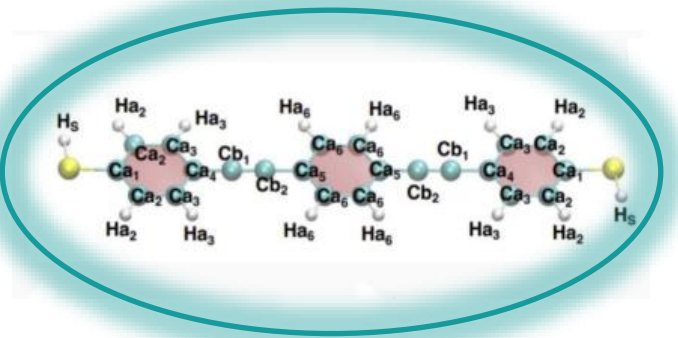
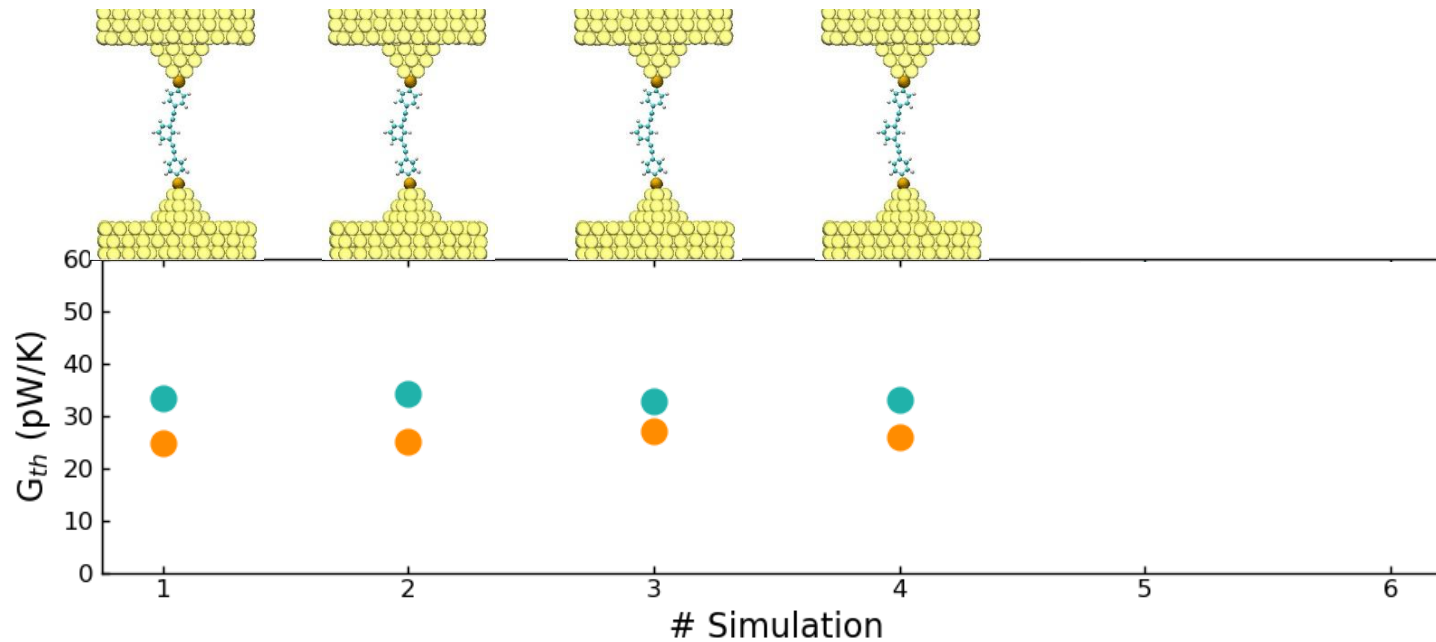
NEMD thermal conductance

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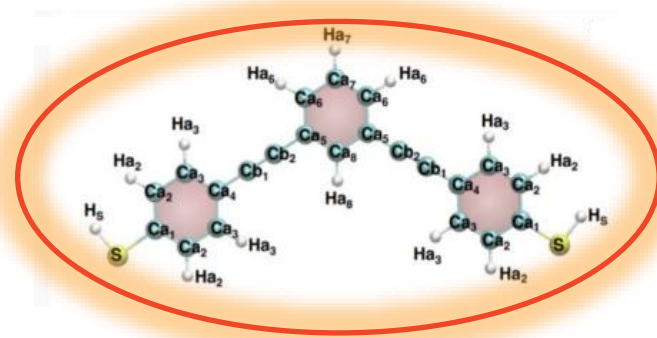
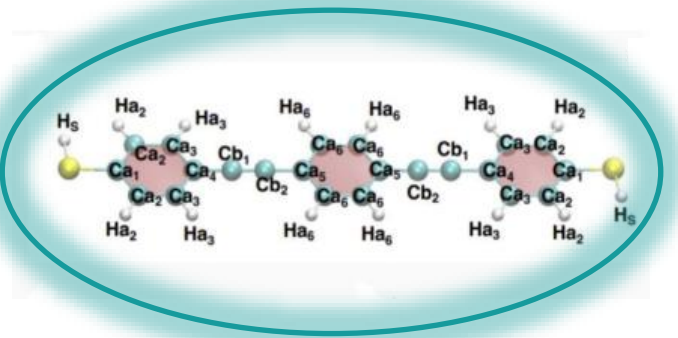
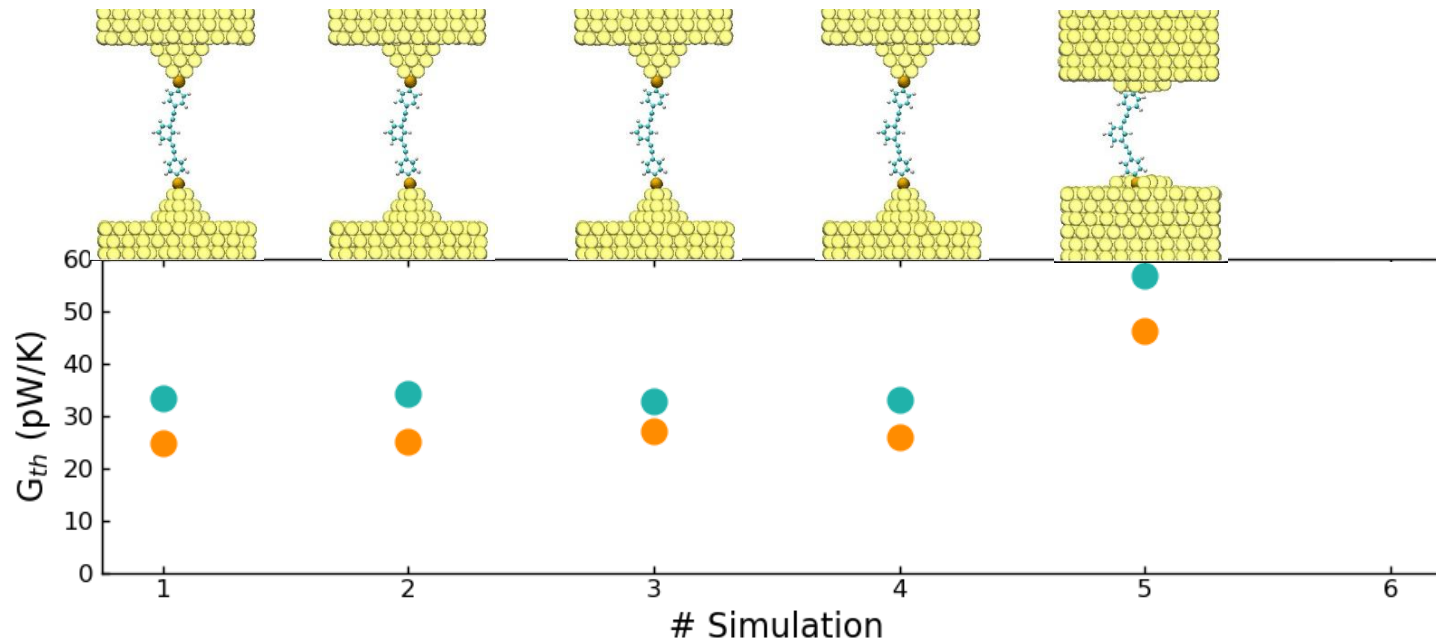
NEMD thermal conductance

NPT → Pulling (0.35 nN) → Thermal Bias (40 K) → Production (30 ns)



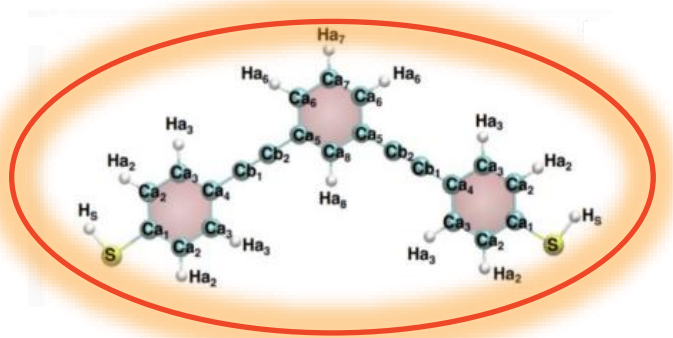
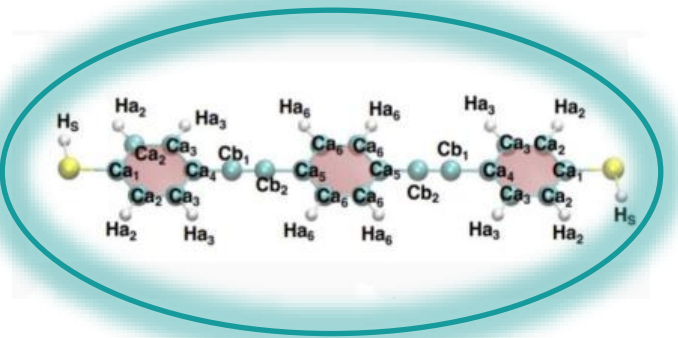
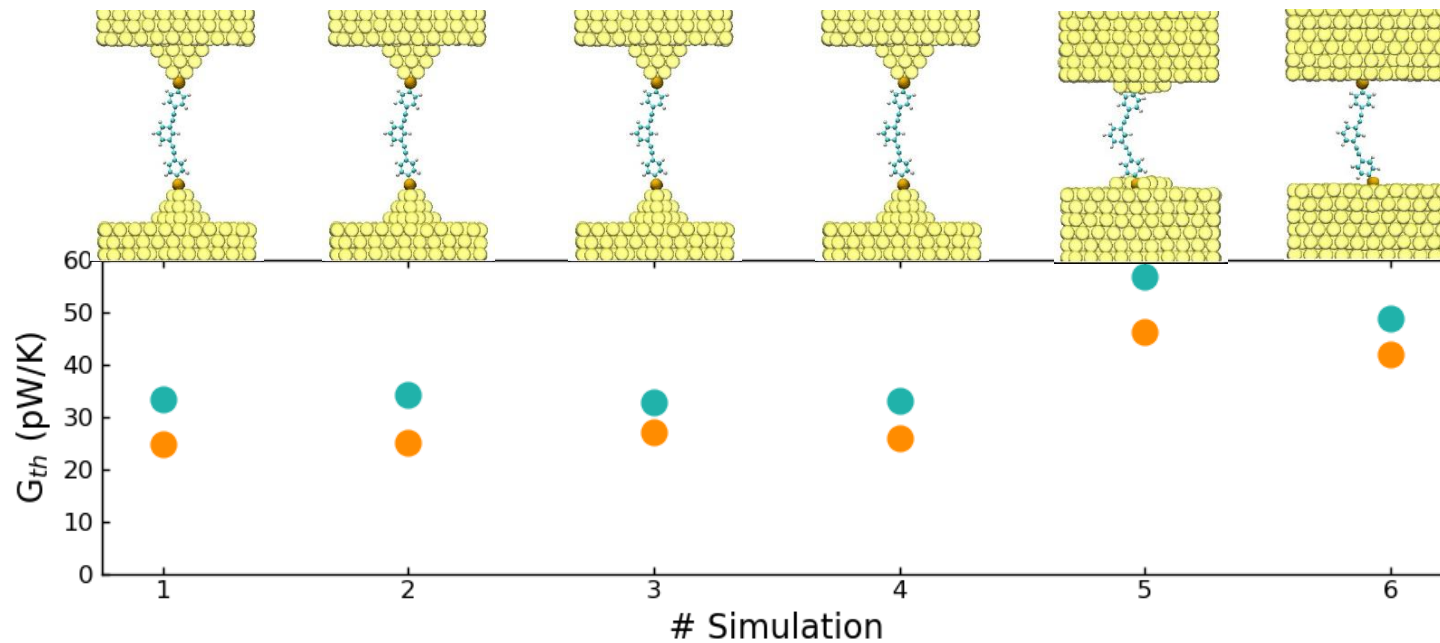
NEMD thermal conductance

NPT → Pulling (0.35 nN) → Thermal Bias (40 K) → Production (30 ns)

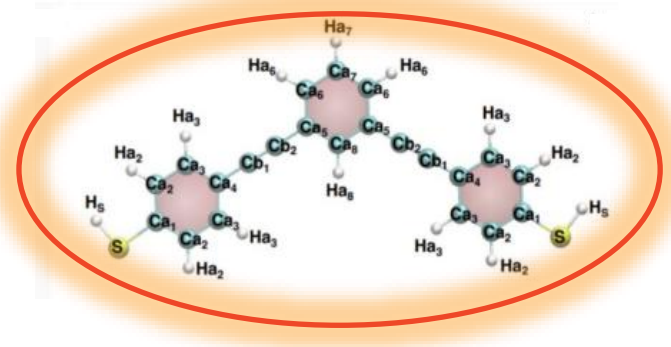
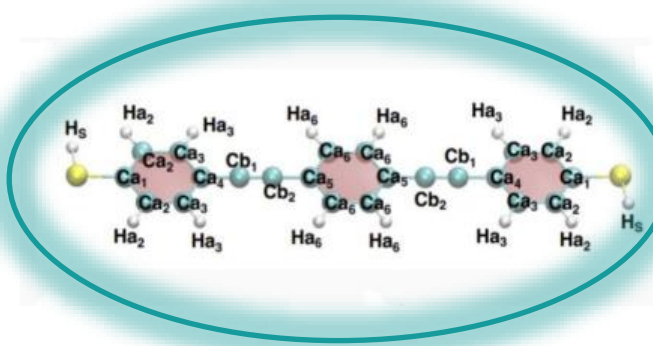


NEMD thermal conductance

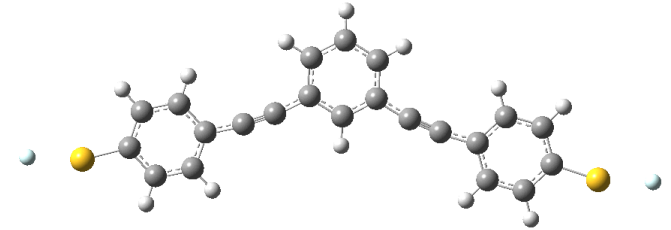
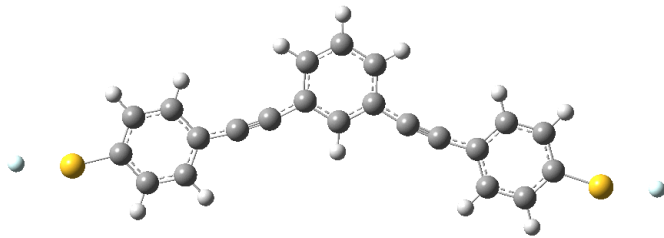
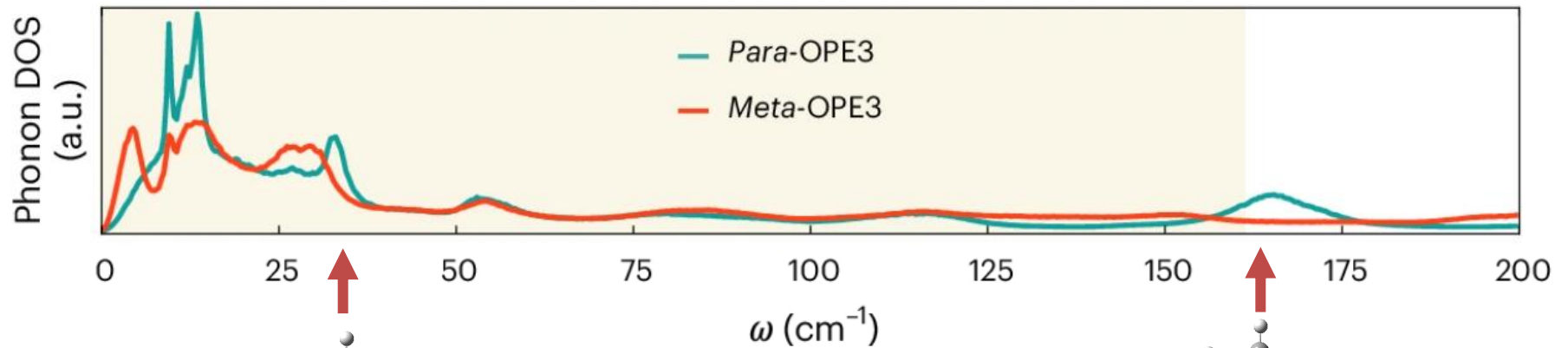
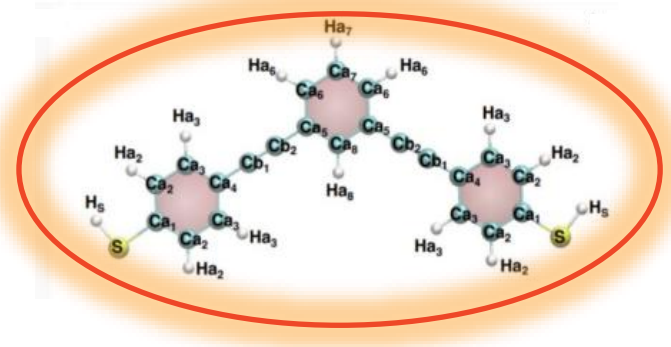
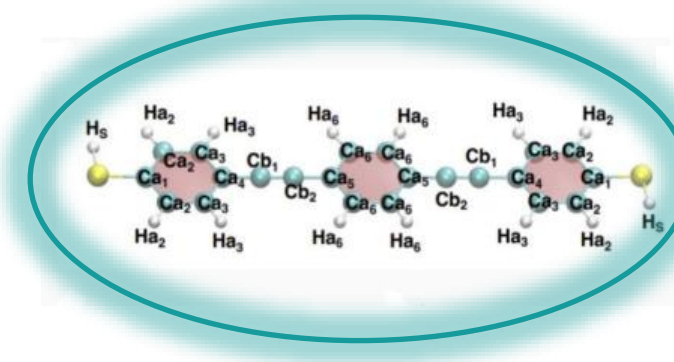
NPT \rightarrow Pulling (0.35 nN) \rightarrow Thermal Bias (40 K) \rightarrow Production (30 ns)



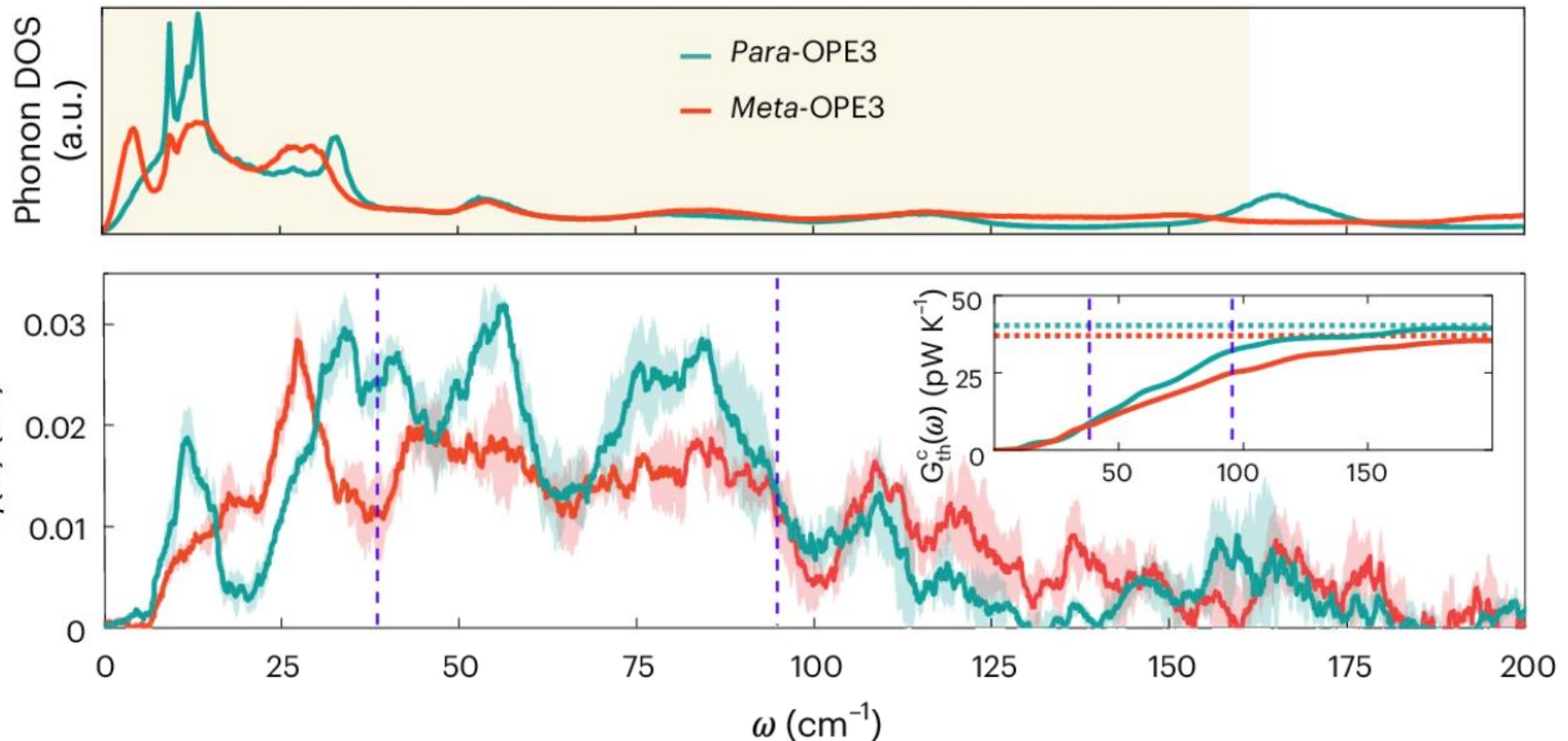
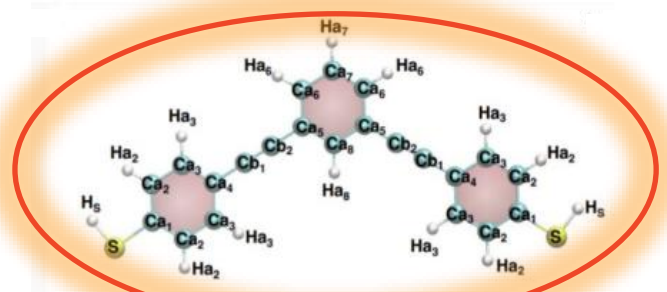
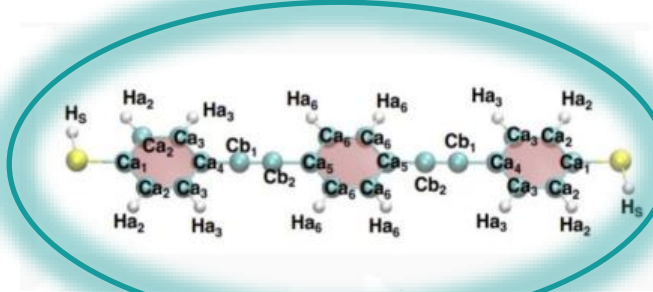
Spectral conductance and vibrational occupation



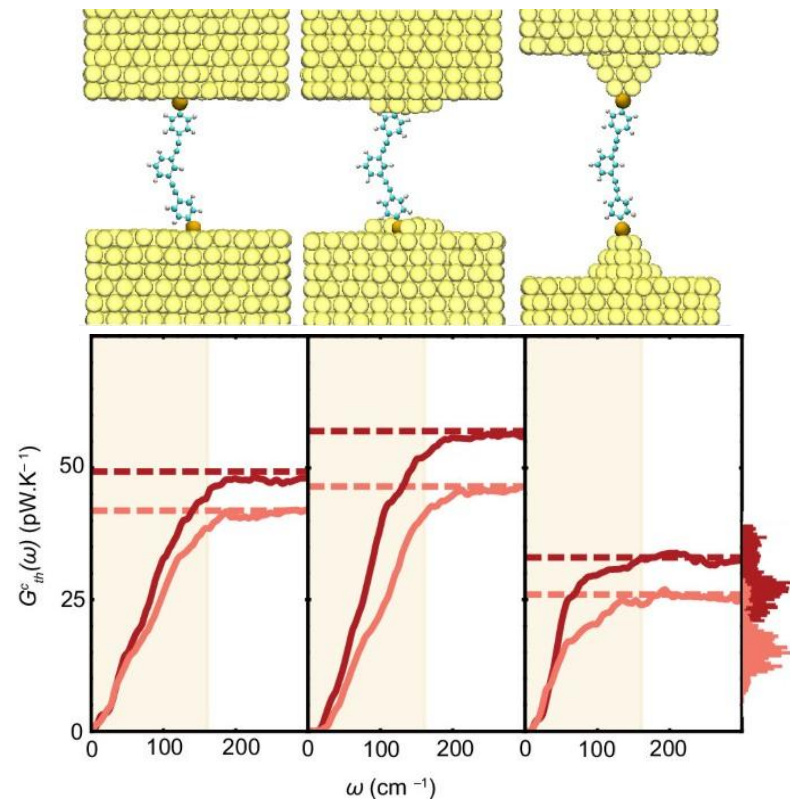
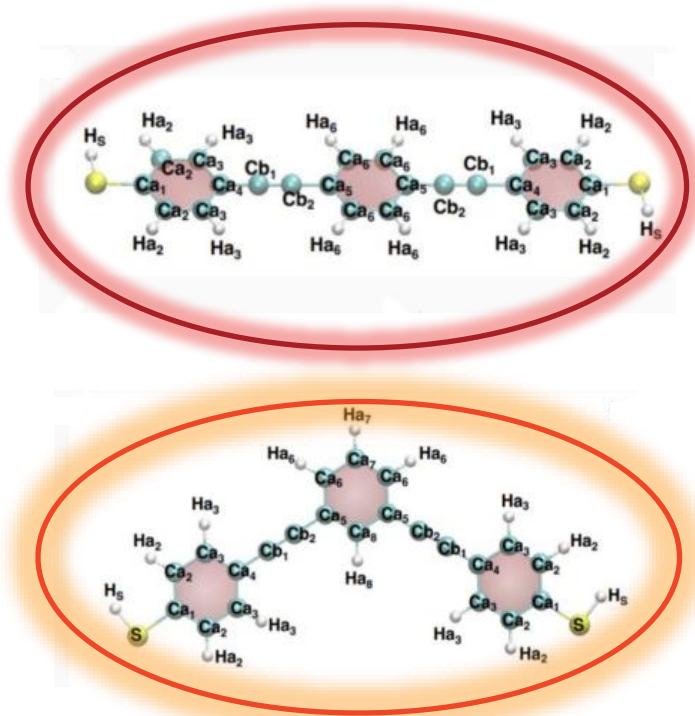
Spectral conductance and vibrational occupation



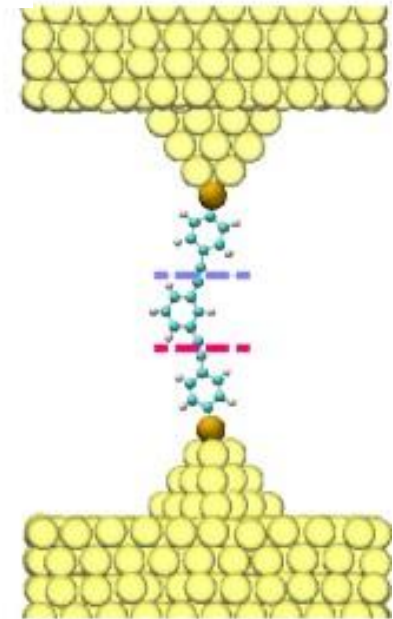
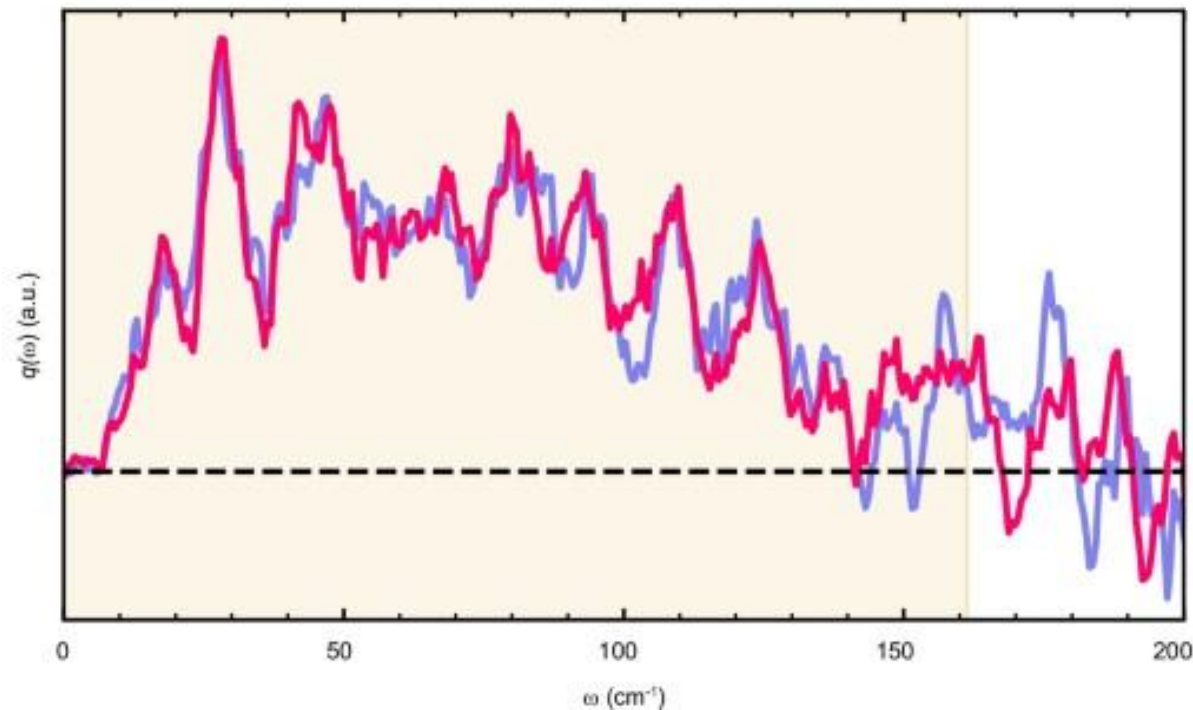
Spectral conductance and vibrational occupation



Spectral conductance and vibrational occupation



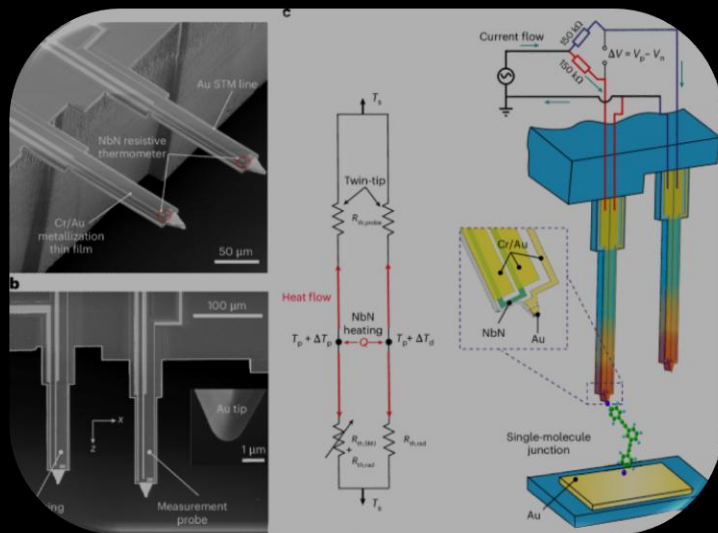
Spectral conductance and vibrational occupation



Coherent heat-transport

Results

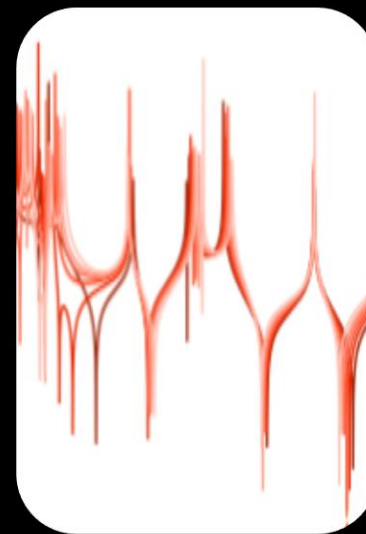
Measurements



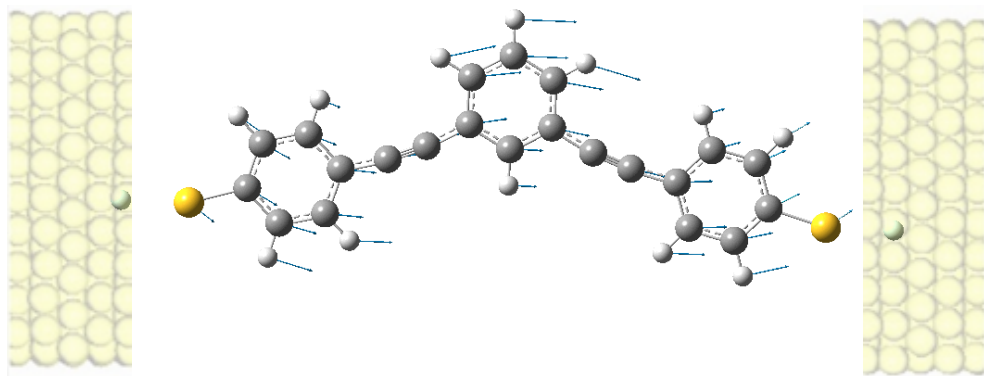
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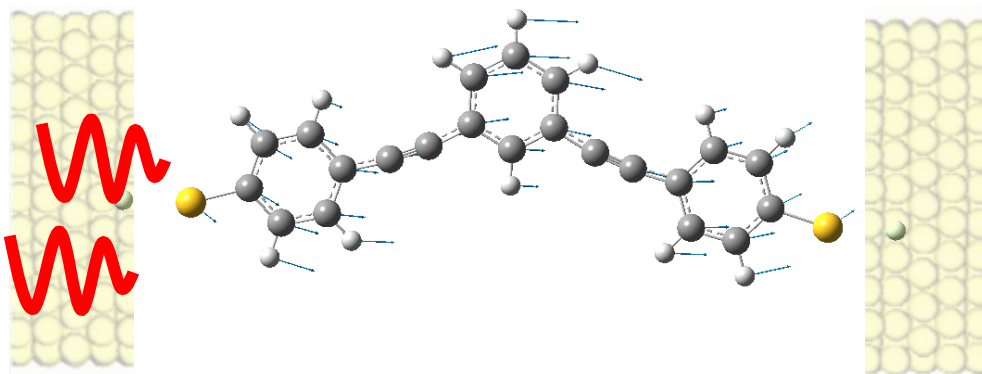
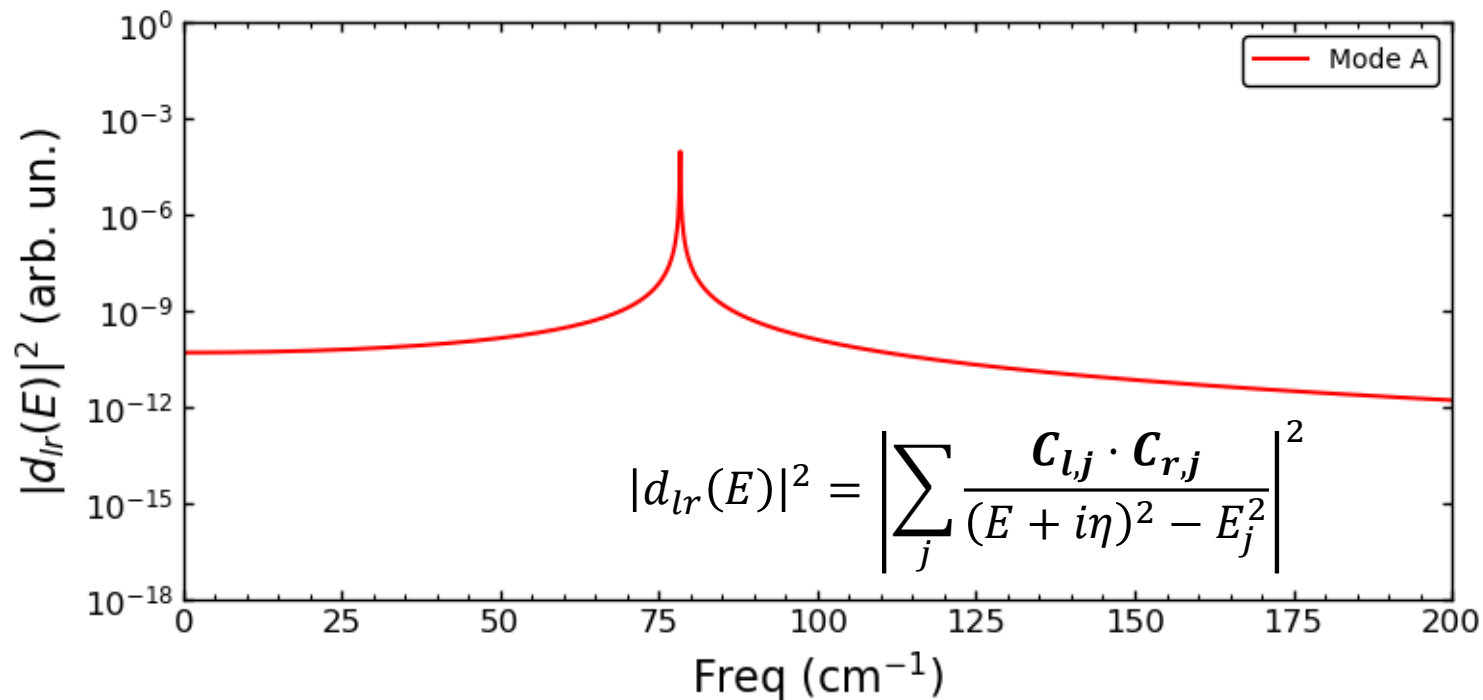
Interference



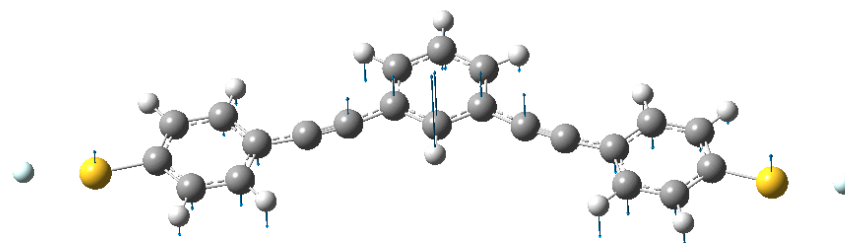
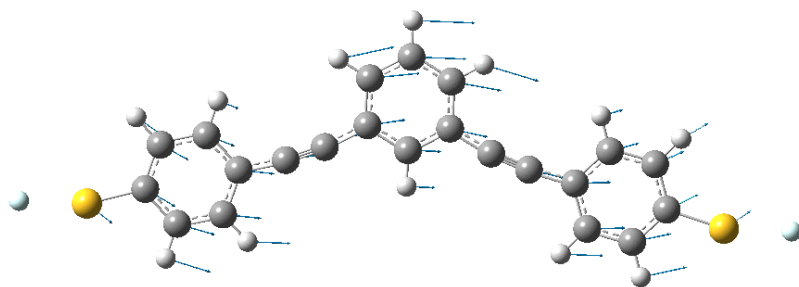
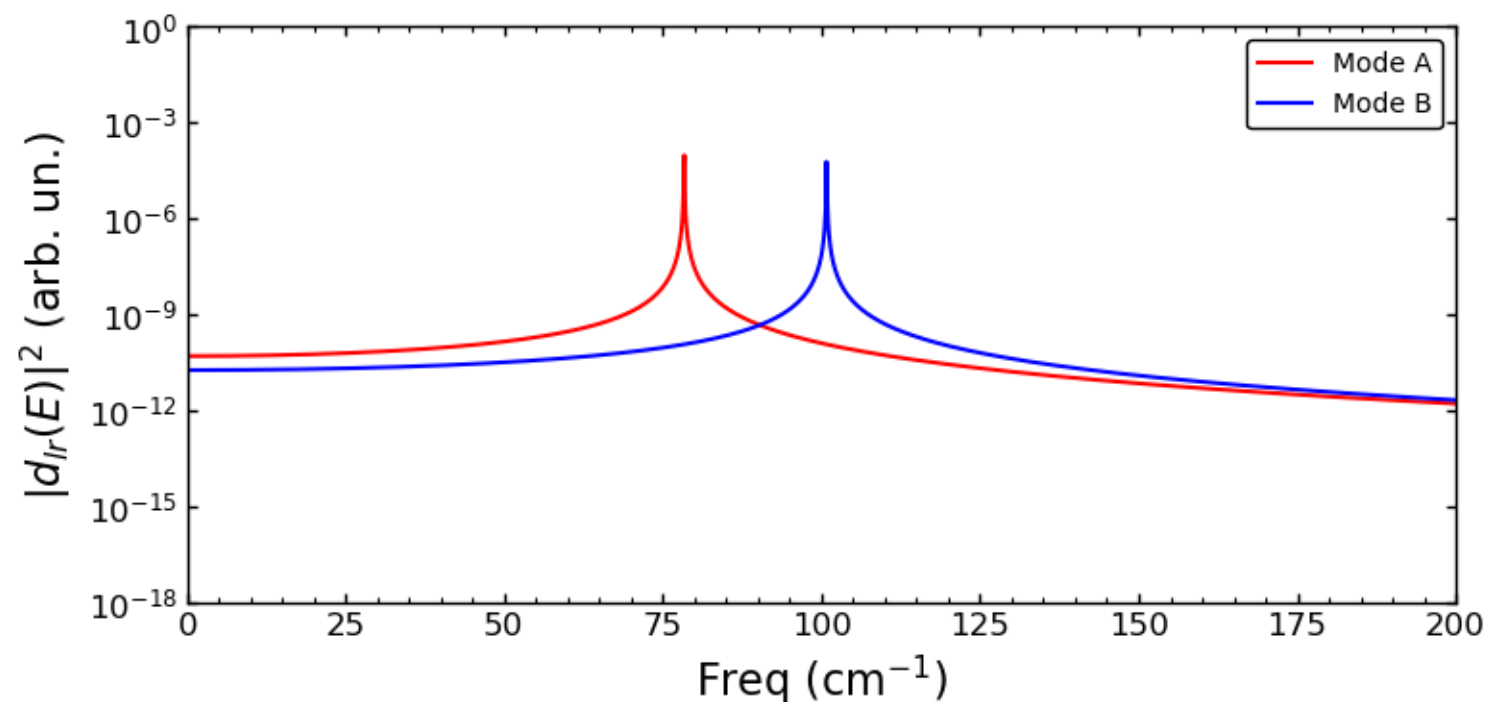
Vibrational interference: two-mode antiresonance



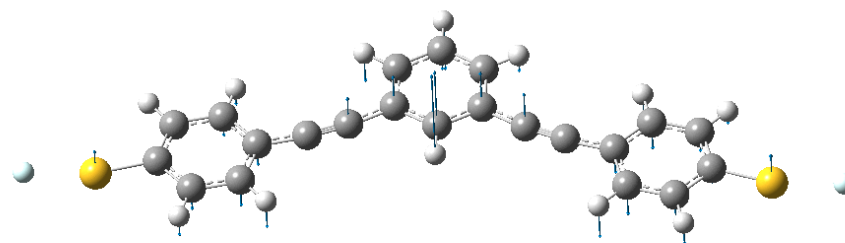
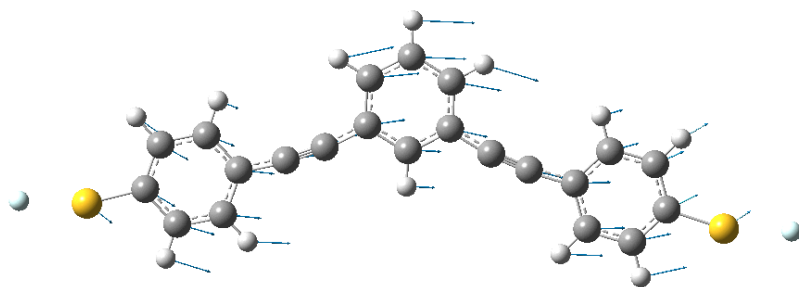
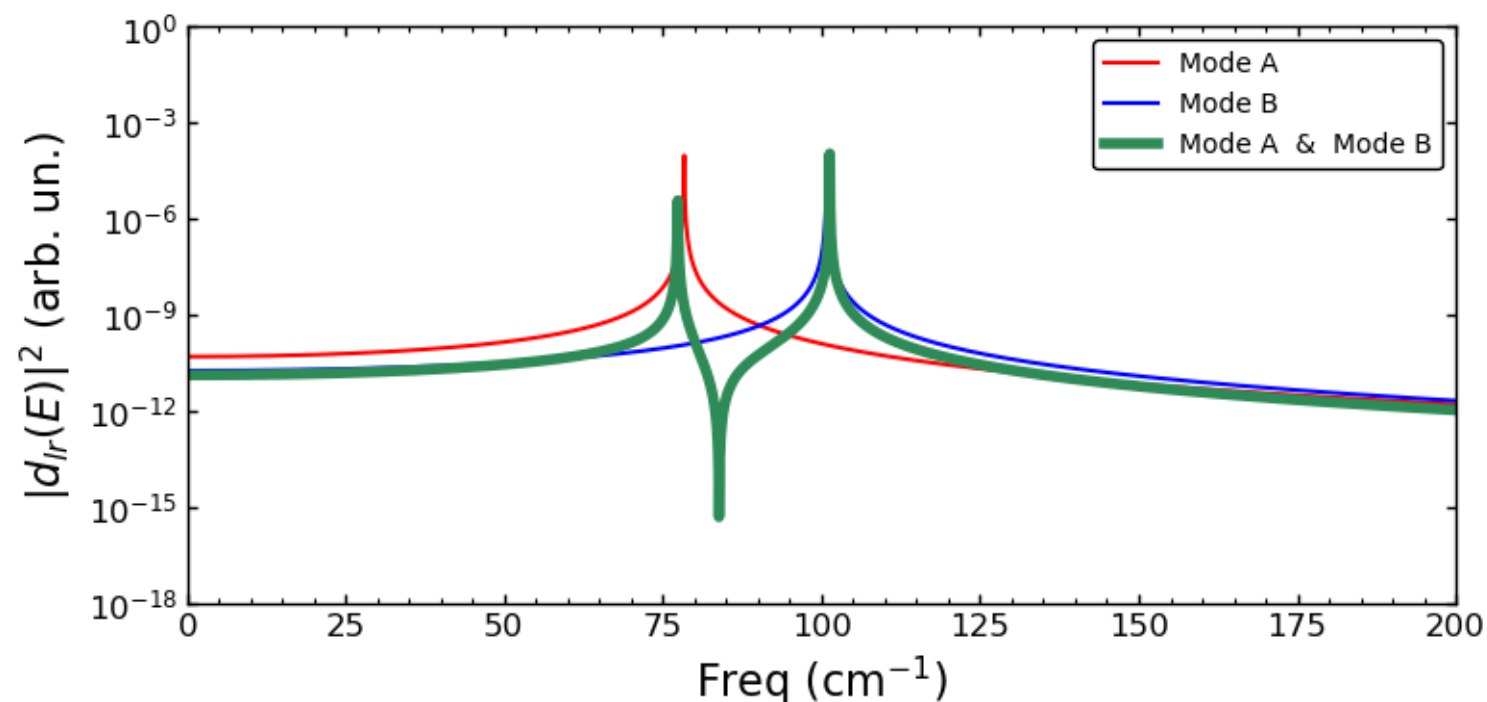
Vibrational interference: two-mode antiresonance



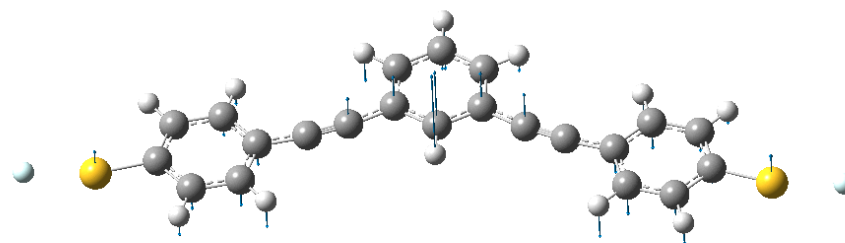
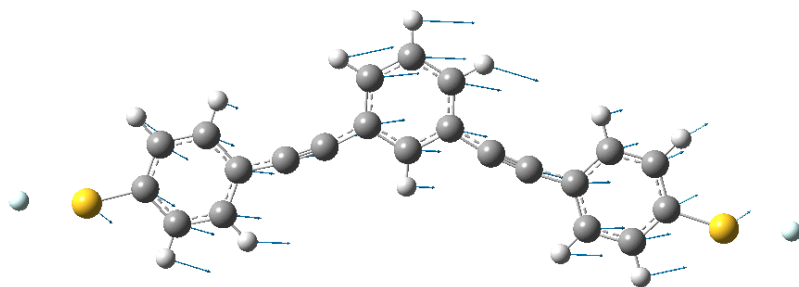
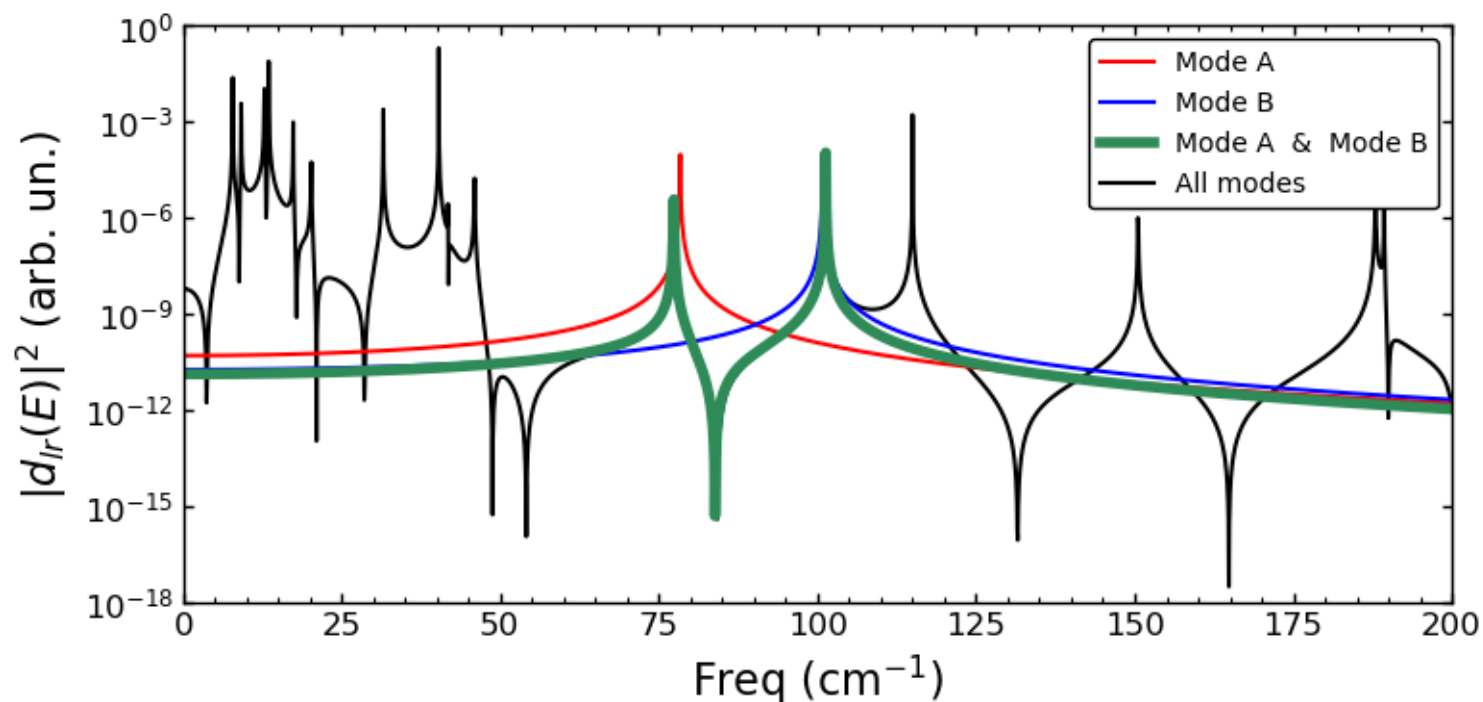
Vibrational interference: two-mode antiresonance



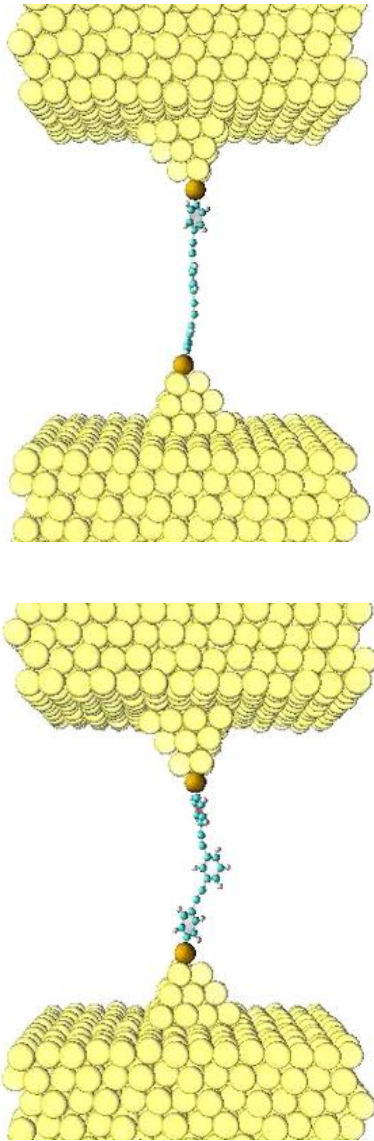
Vibrational interference: two-mode antiresonance



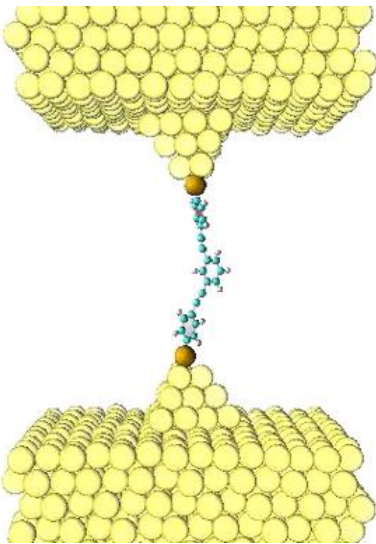
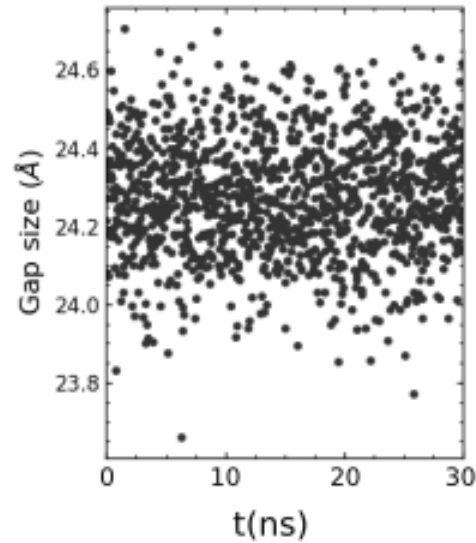
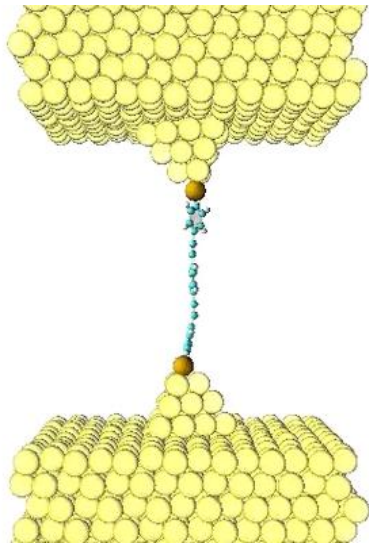
Vibrational interference: two-mode antiresonance



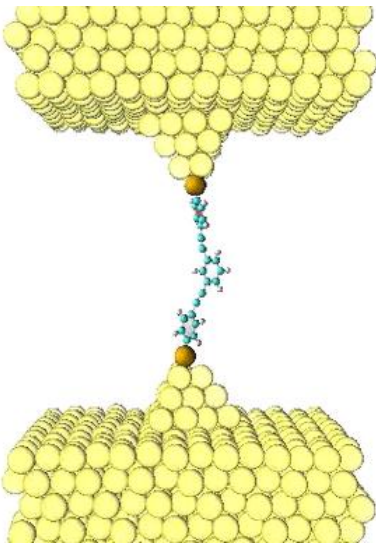
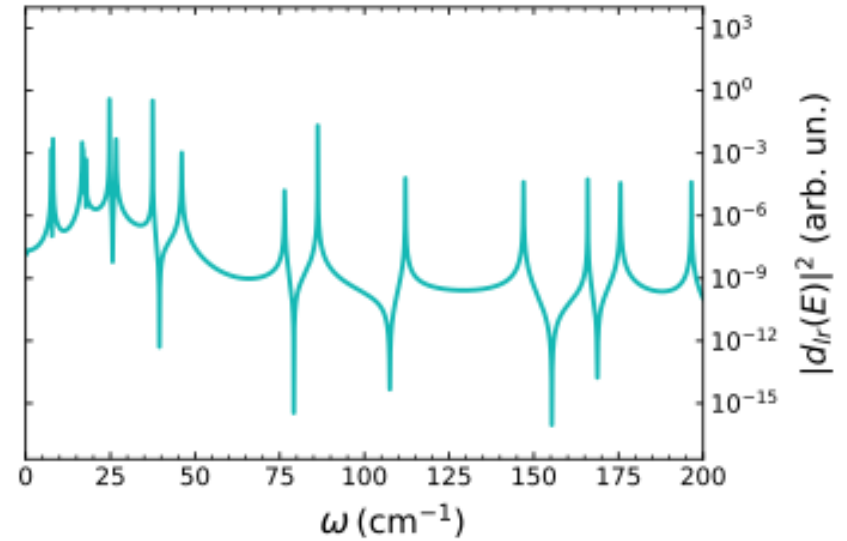
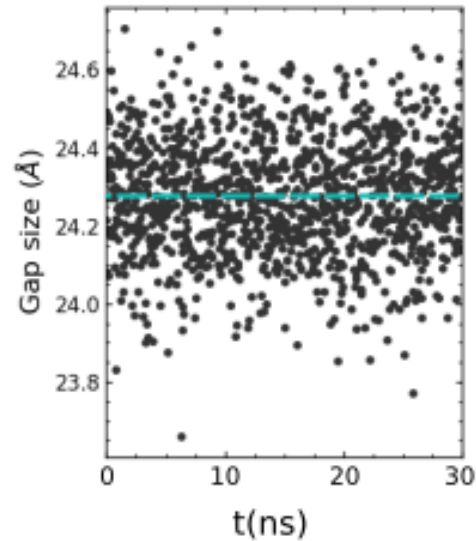
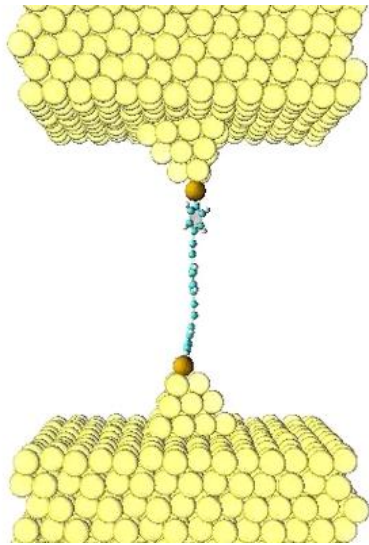
Vibrational interference: accounting for temperature



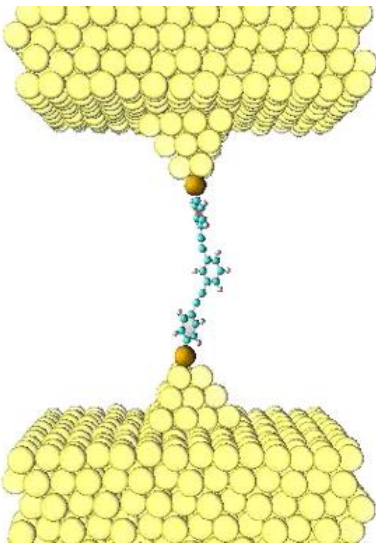
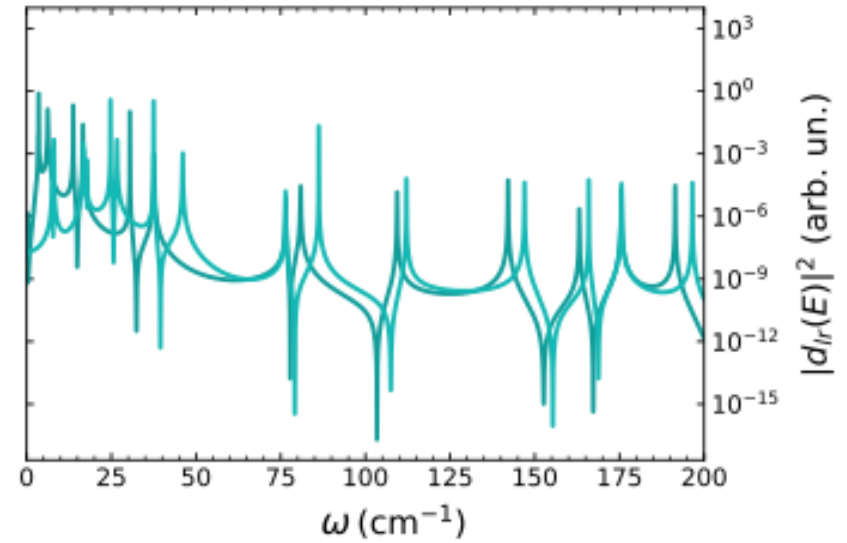
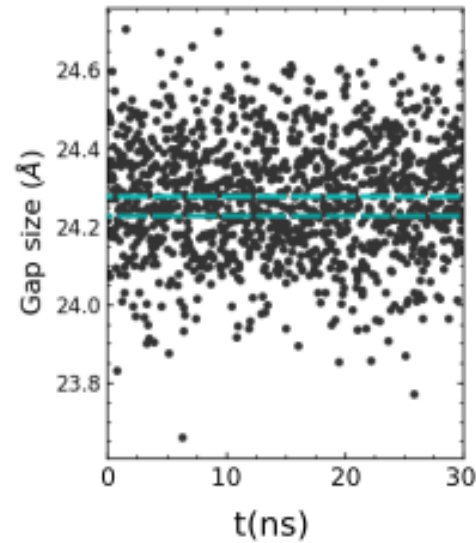
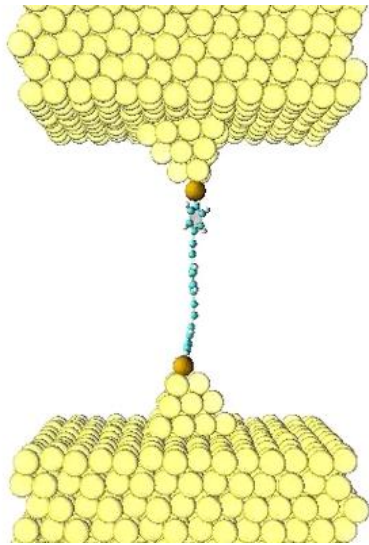
Vibrational interference: accounting for temperature



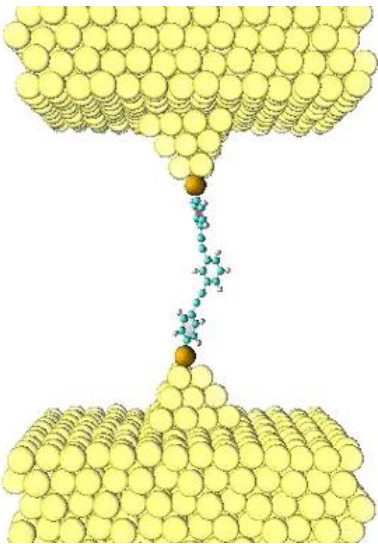
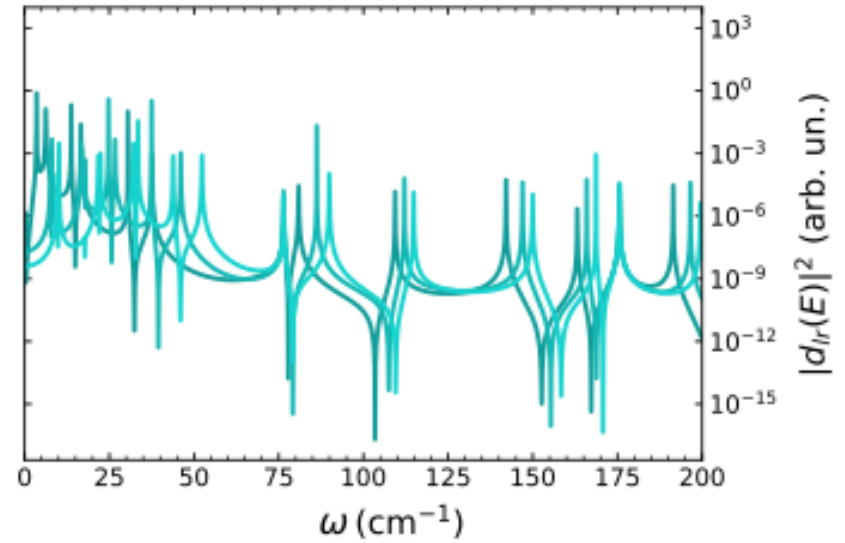
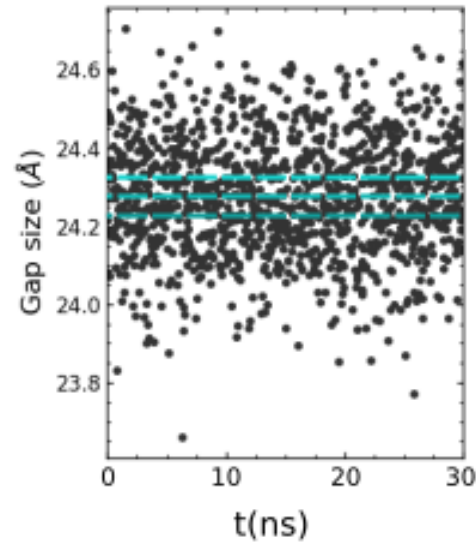
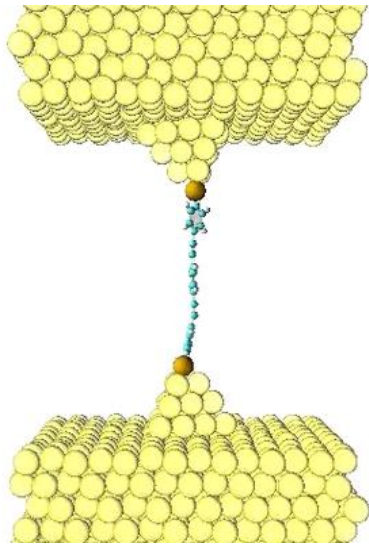
Vibrational interference: accounting for temperature



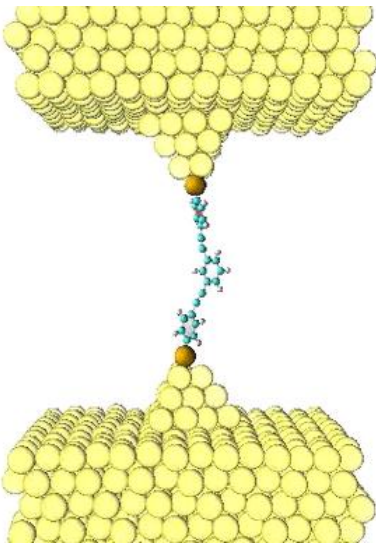
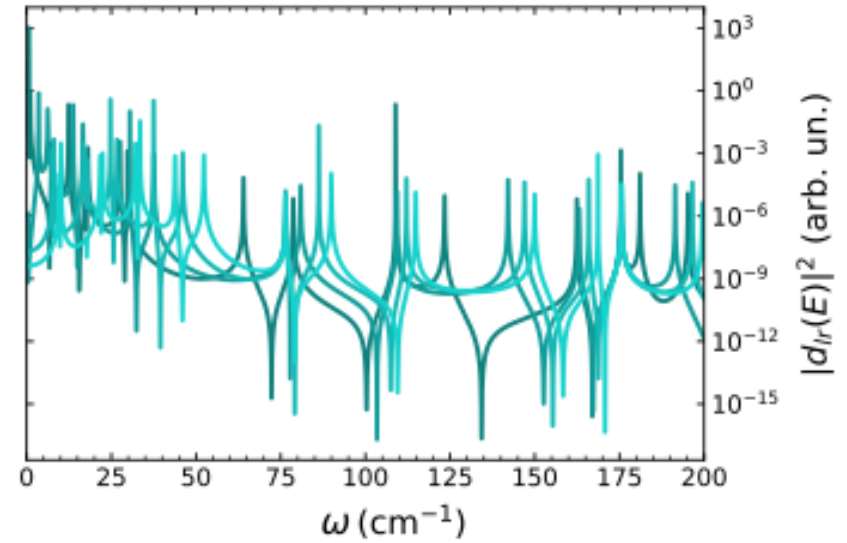
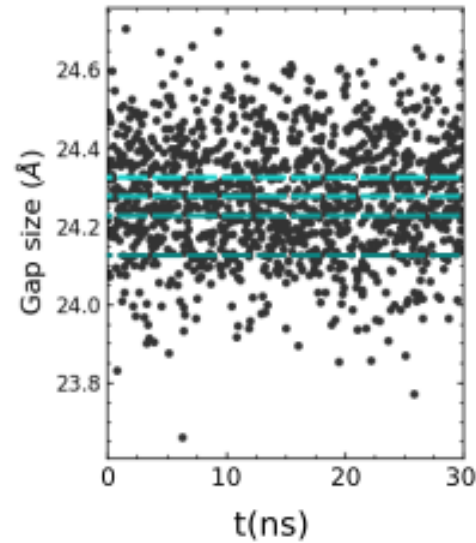
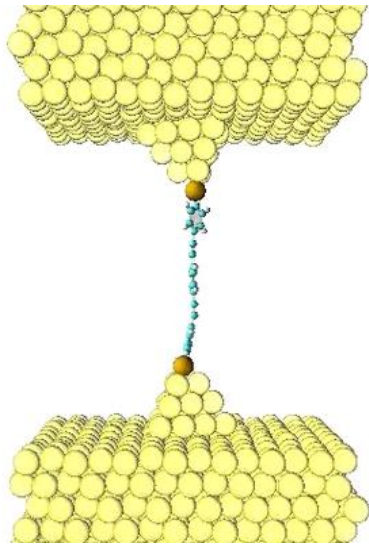
Vibrational interference: accounting for temperature



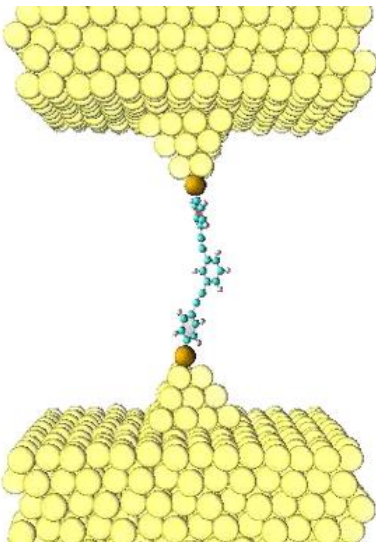
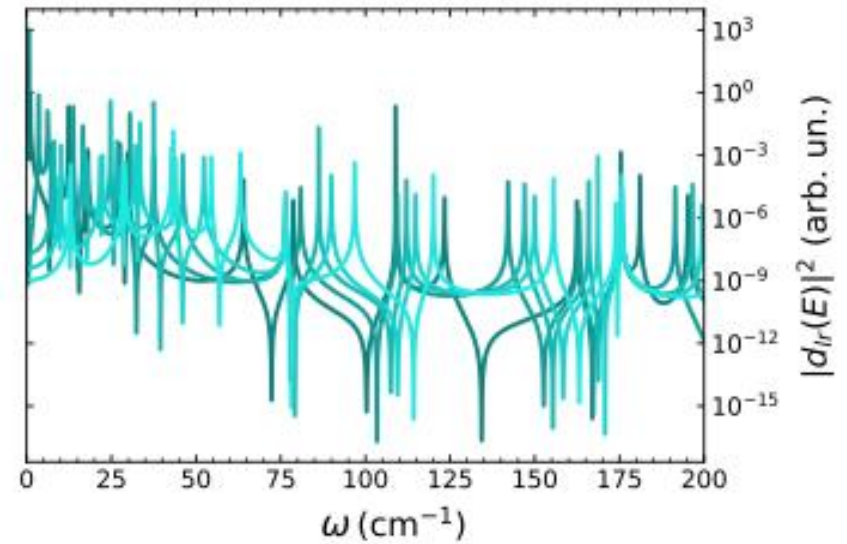
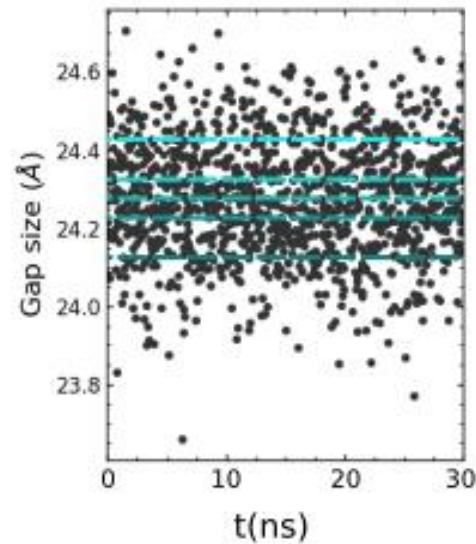
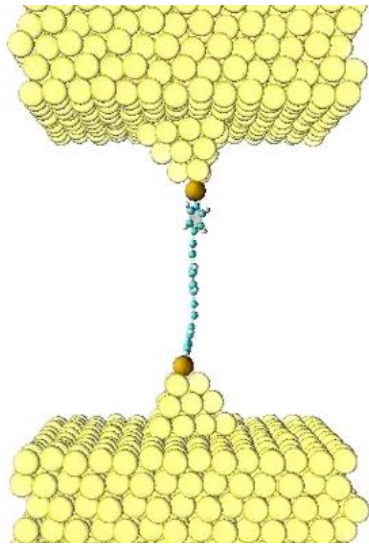
Vibrational interference: accounting for temperature



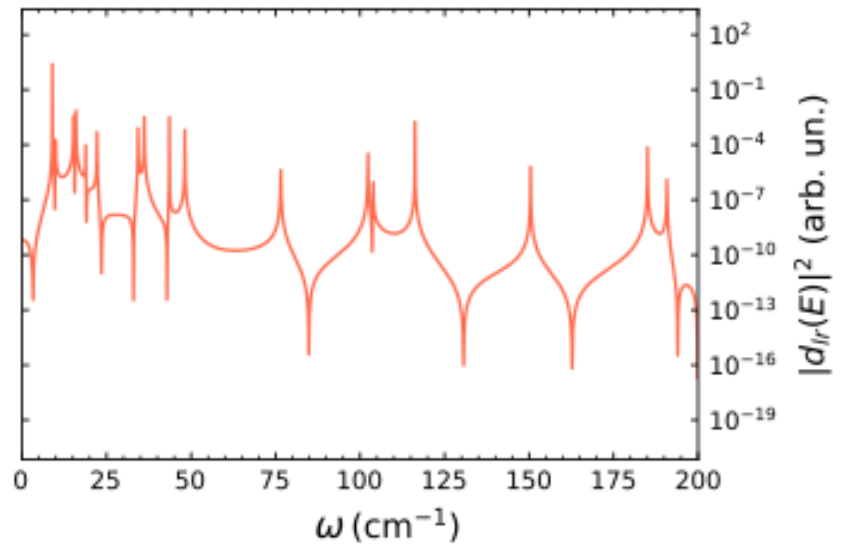
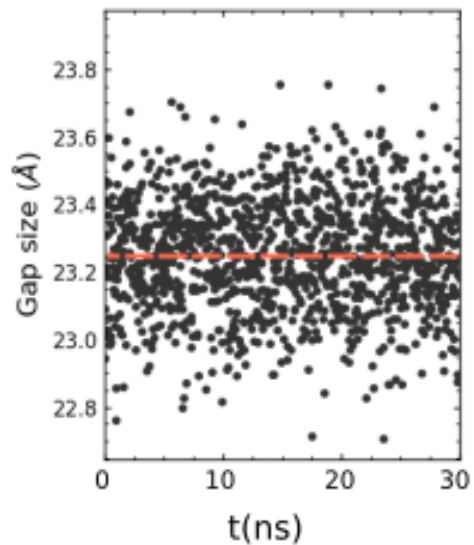
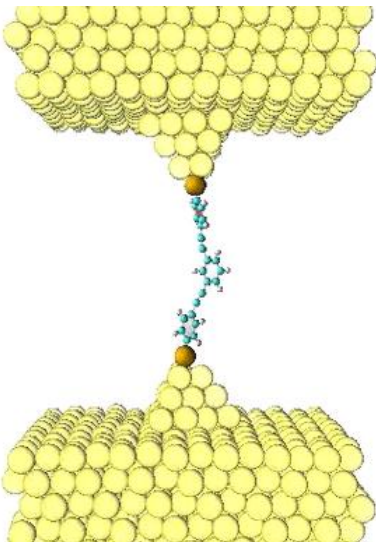
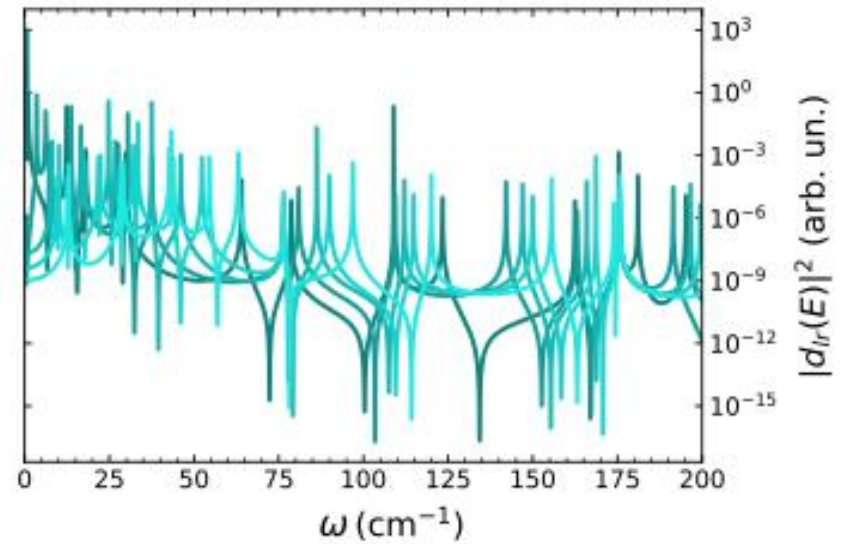
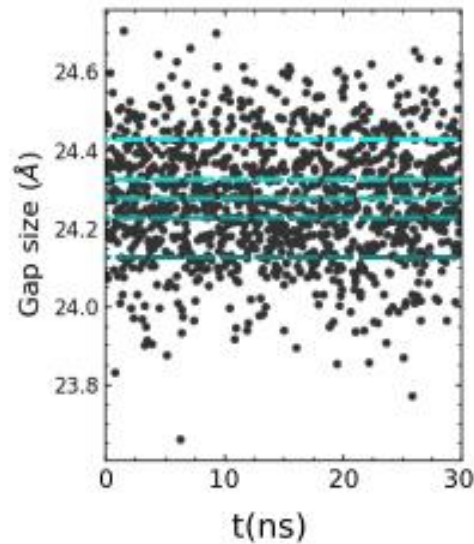
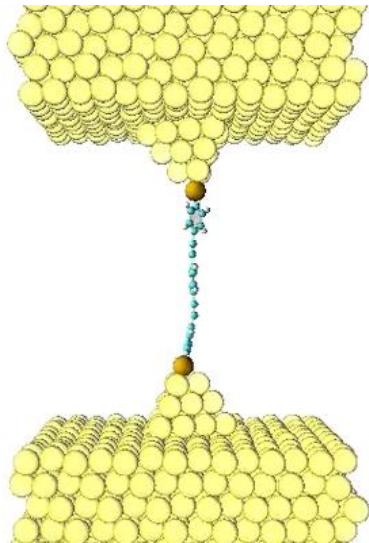
Vibrational interference: accounting for temperature



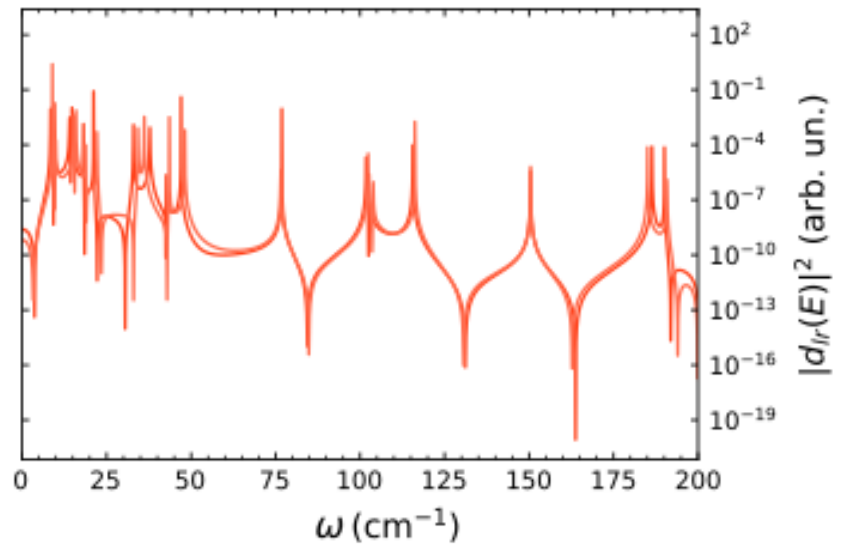
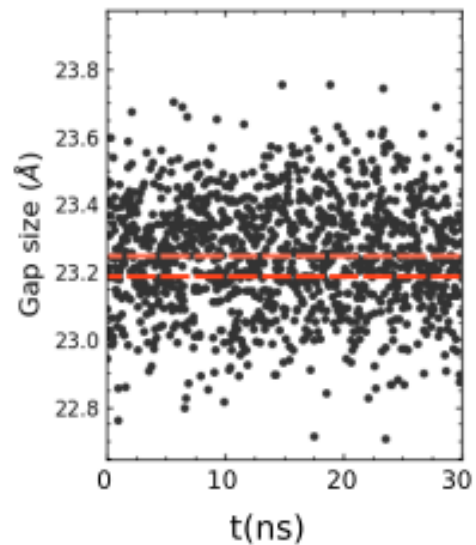
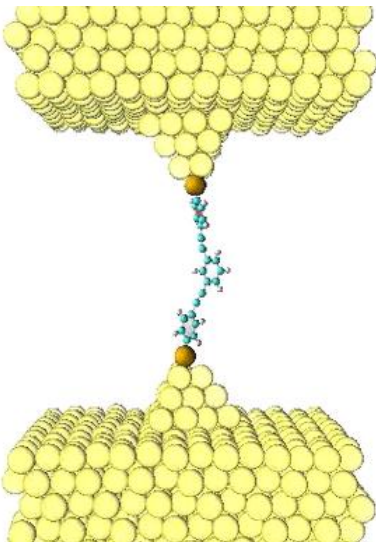
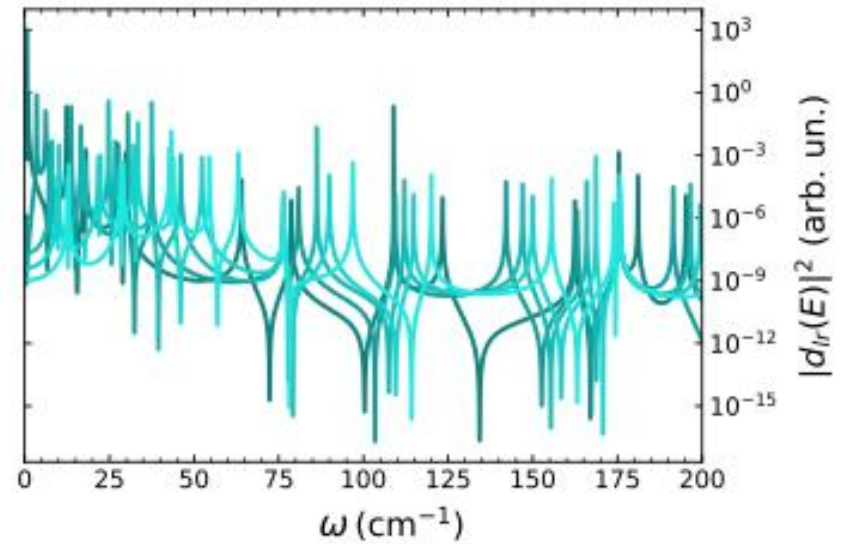
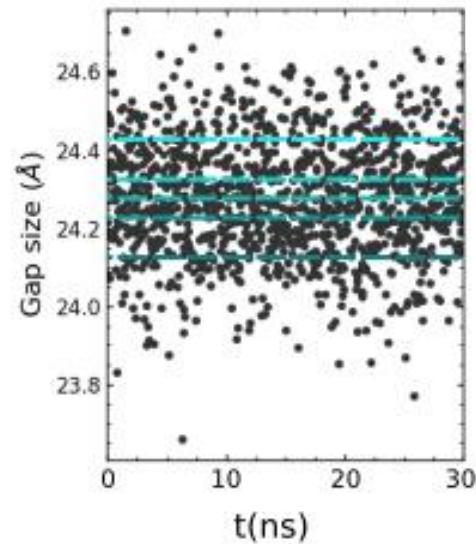
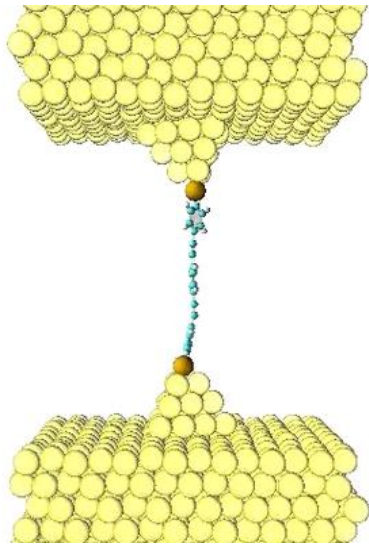
Vibrational interference: accounting for temperature



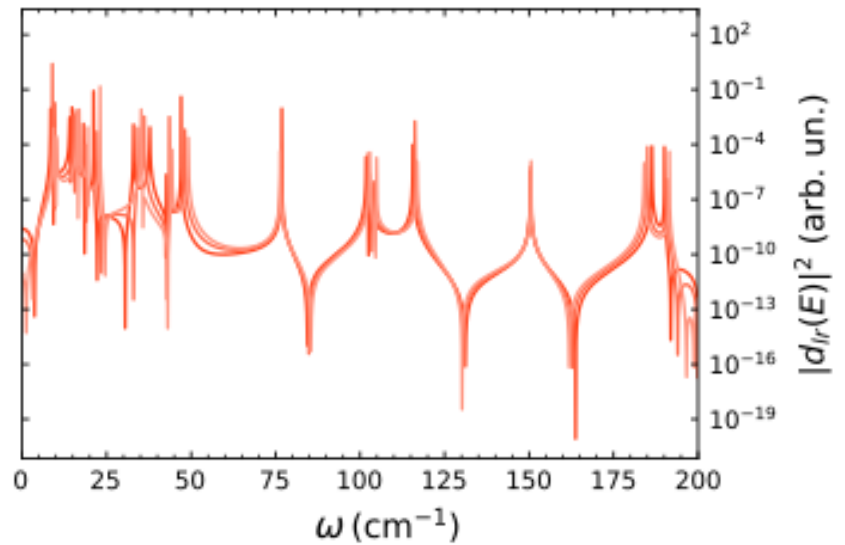
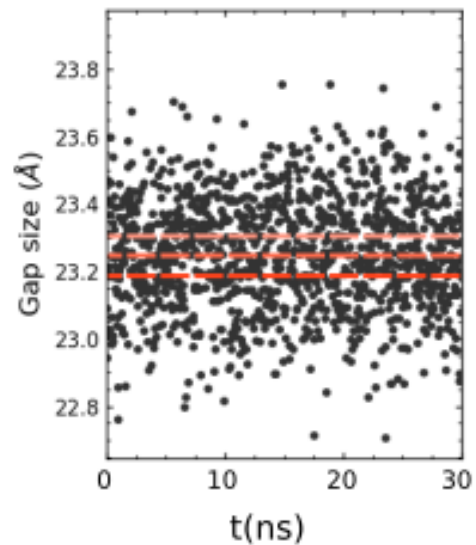
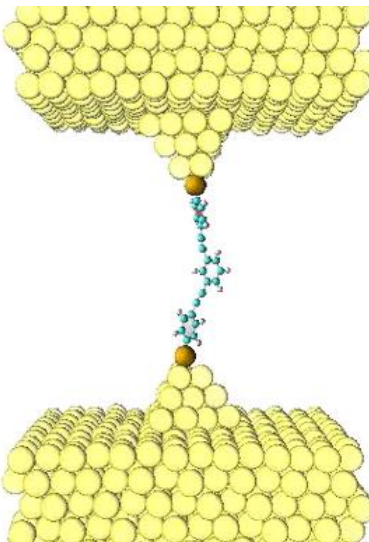
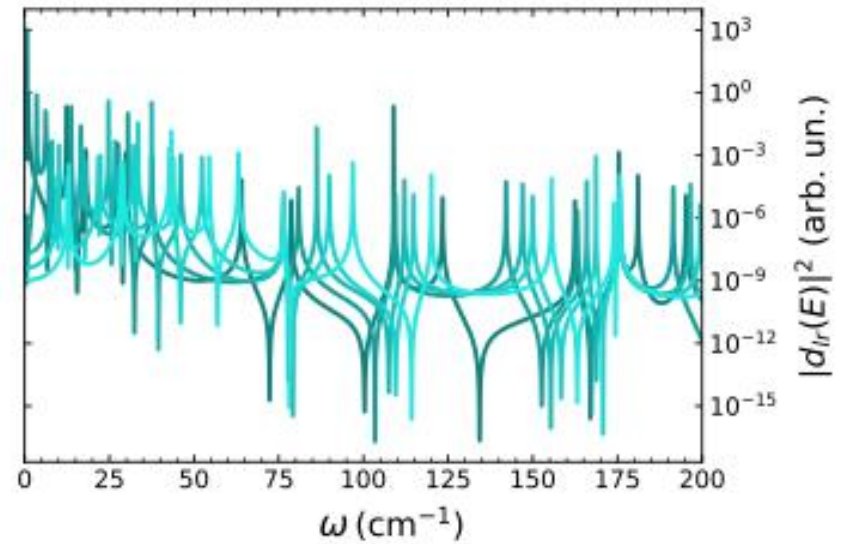
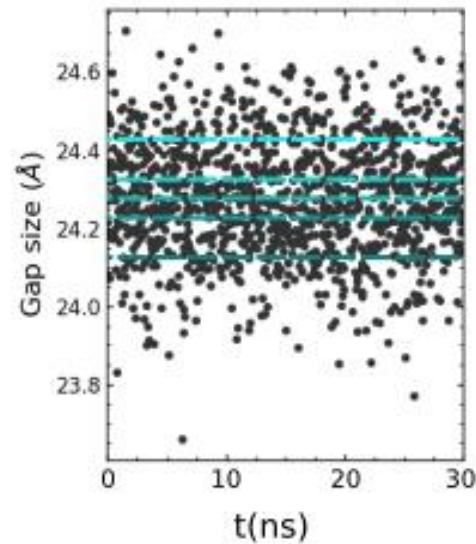
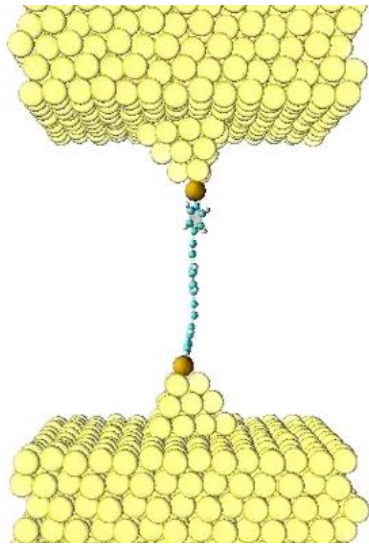
Vibrational interference: accounting for temperature



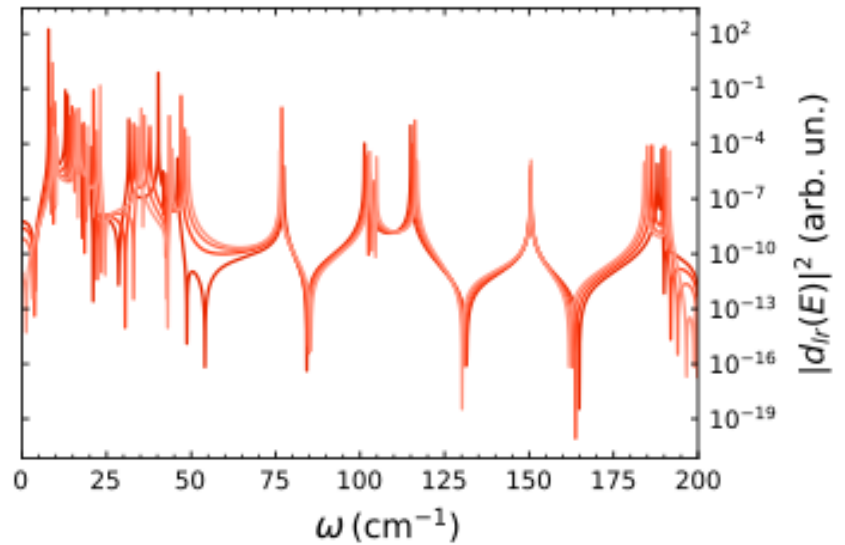
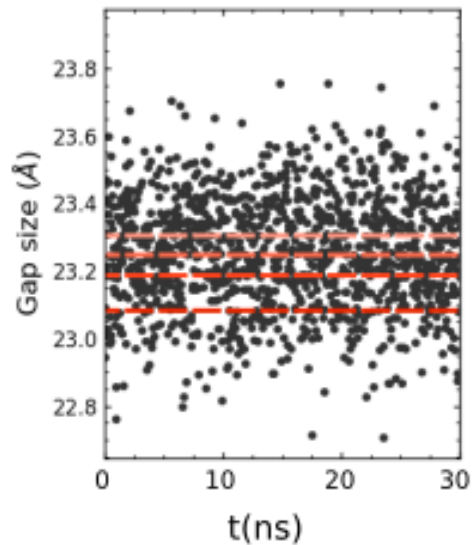
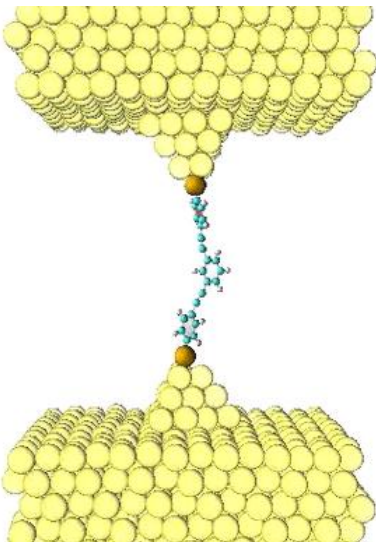
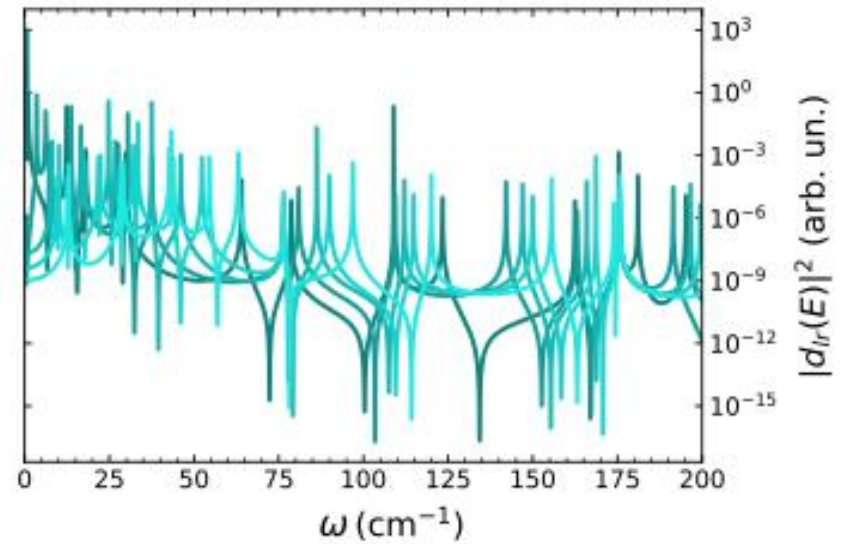
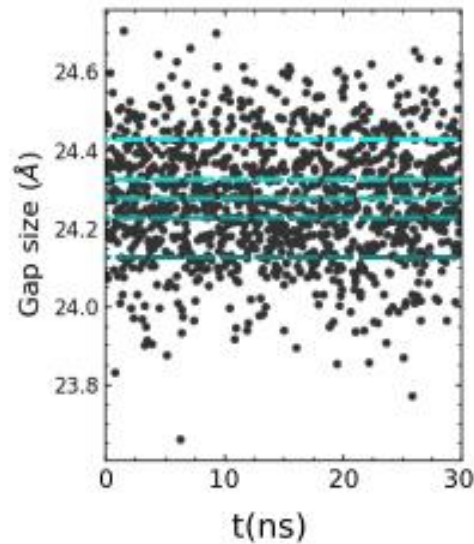
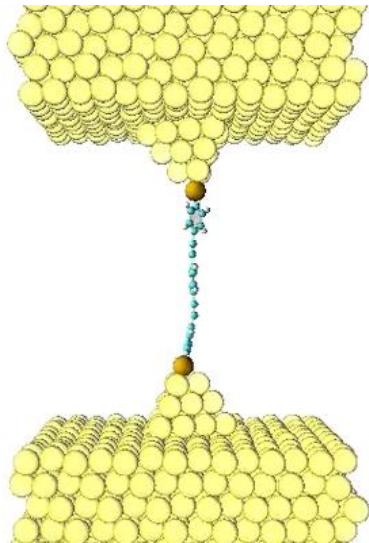
Vibrational interference: accounting for temperature



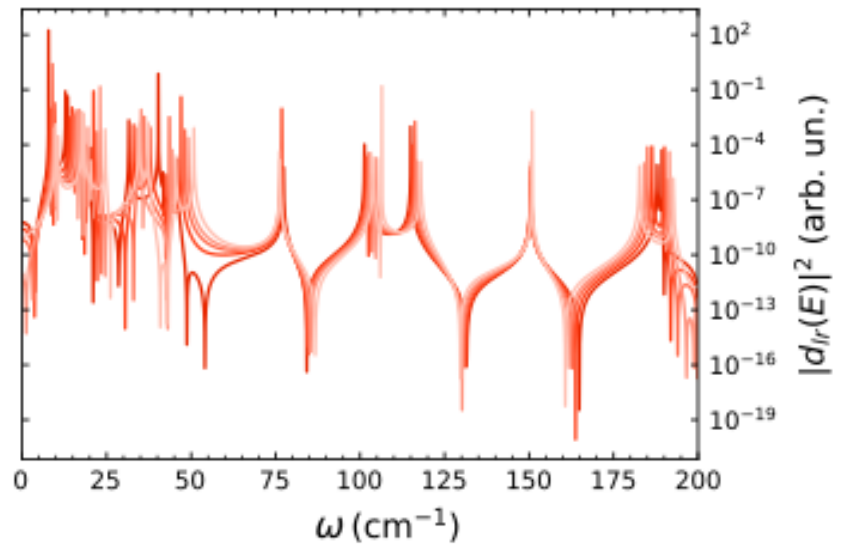
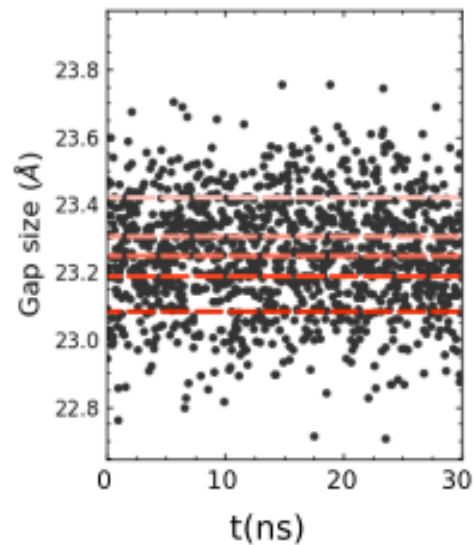
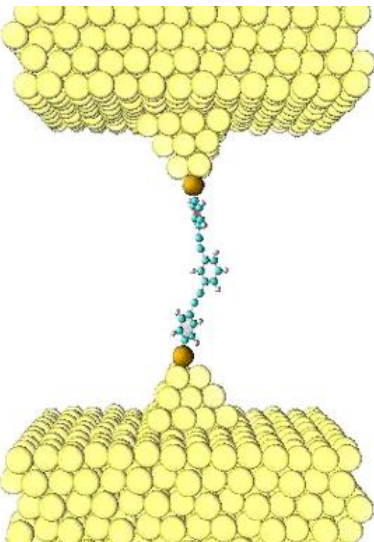
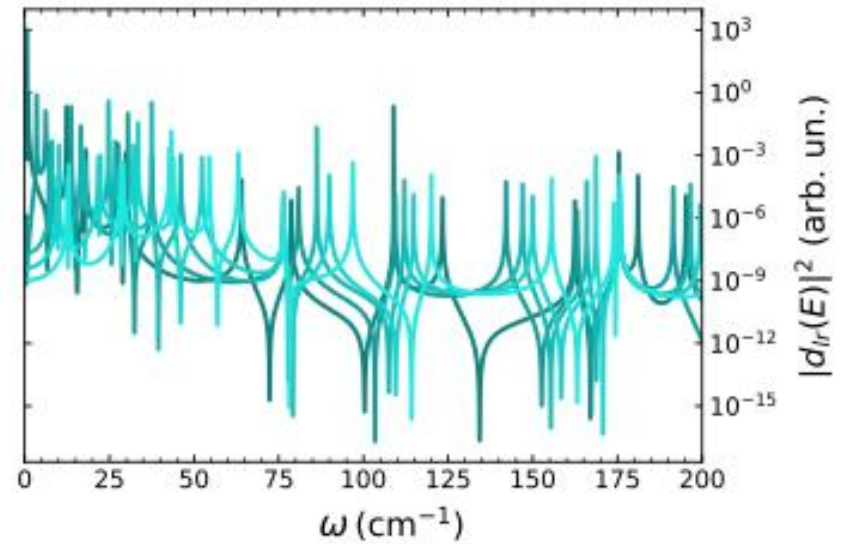
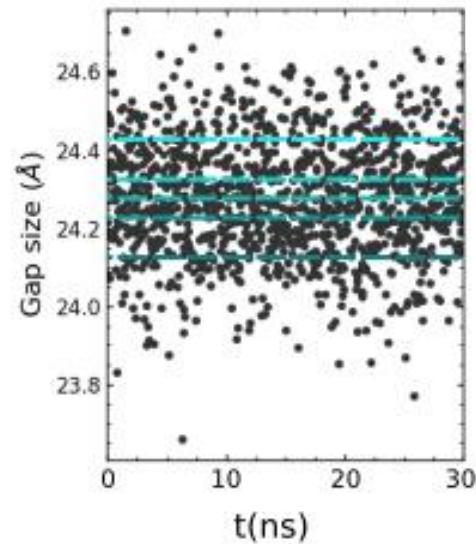
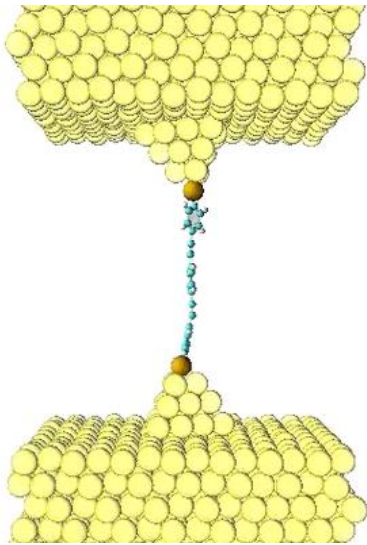
Vibrational interference: accounting for temperature



Vibrational interference: accounting for temperature



Vibrational interference: accounting for temperature

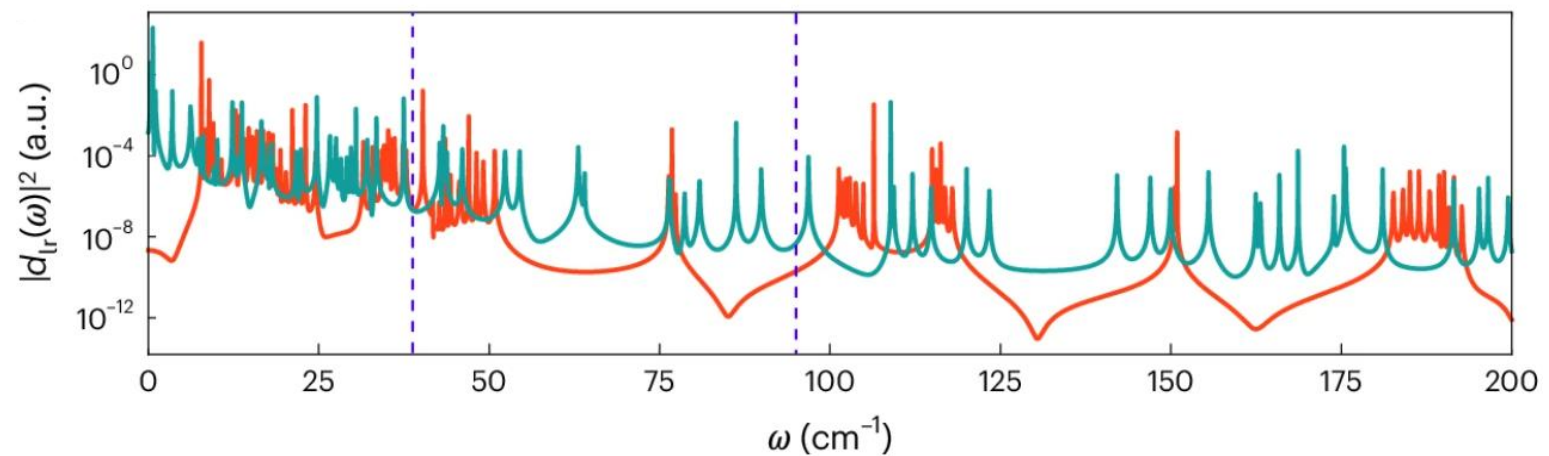
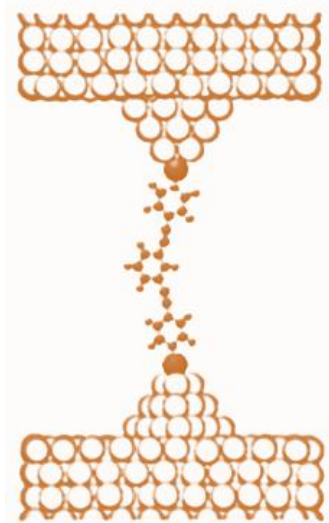


Vibrational interference: accounting for temperature

para-OPE3

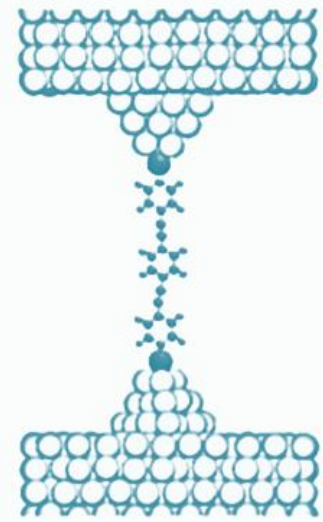


meta-OPE3

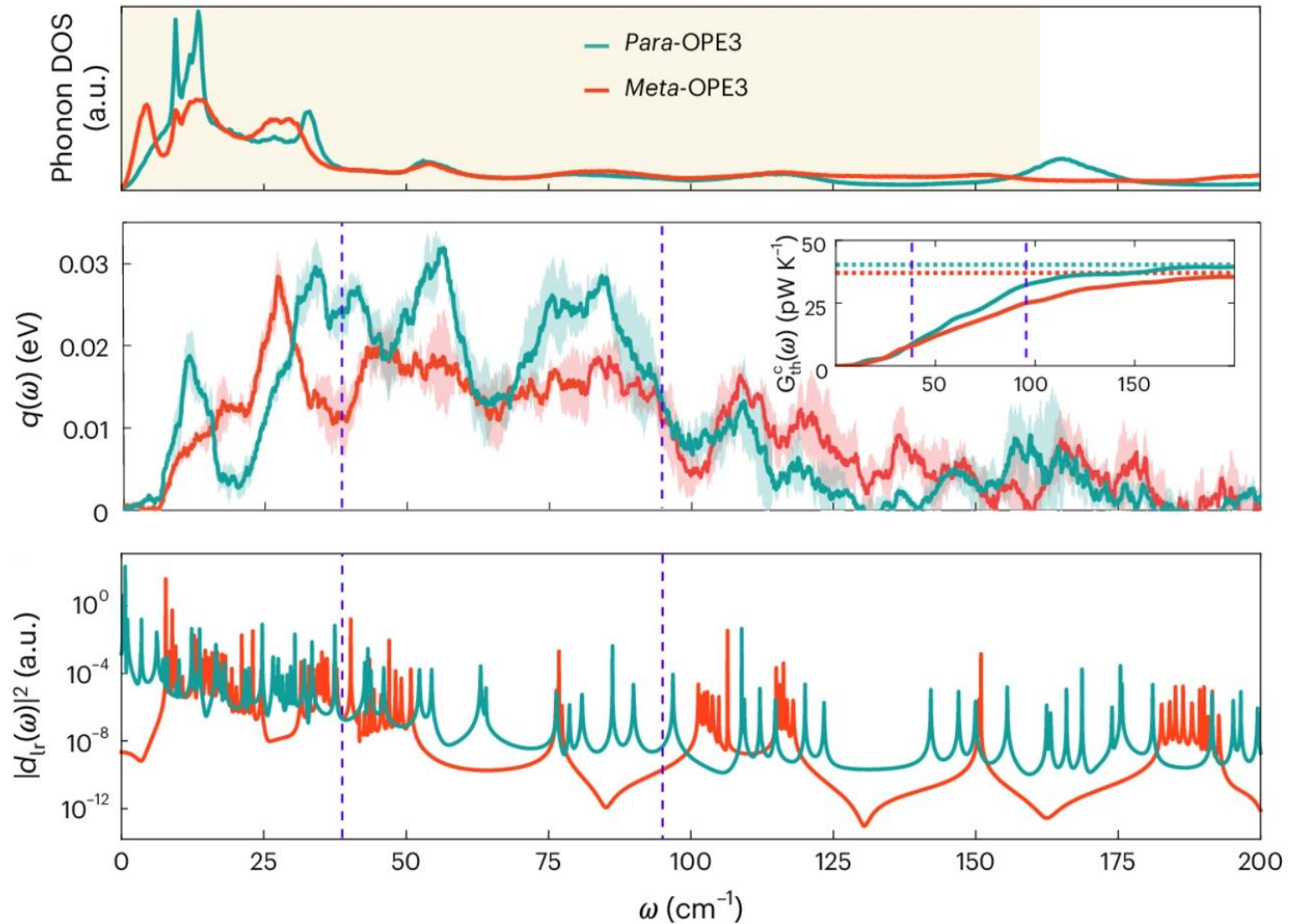


Vibrational interference: accounting for temperature

para-OPE3

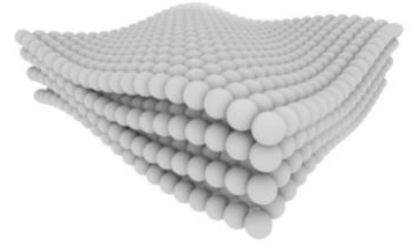


meta-OPE3

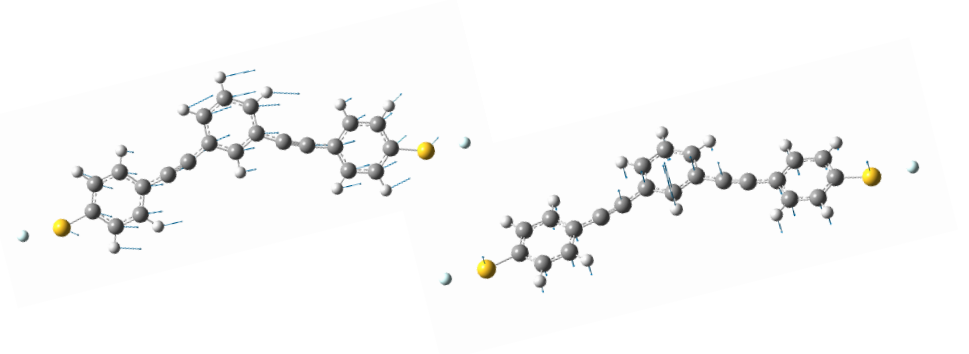


Takeaways

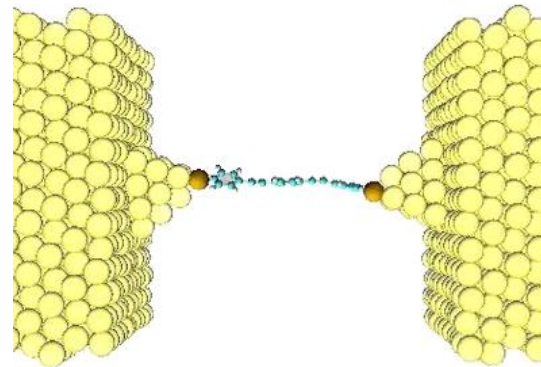
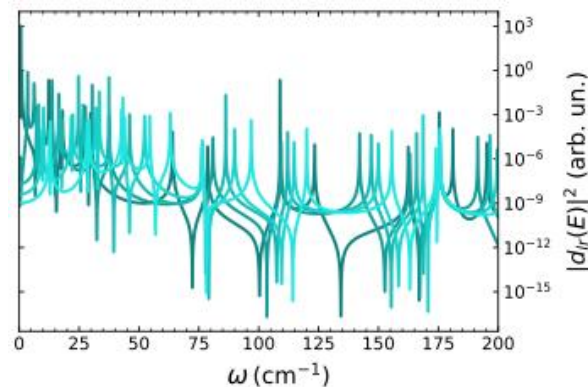
Heat is wave-like at the nanoscale ($L < 100$ nm)



Normal modes can interfere



Finite temperature matters



Acknowledgements



J.G. Vilhena



J.C. Cuevas



G. Prampolini

Thank you for
your attention!

www.nanotrib.com
pab2mrt@gmail.com



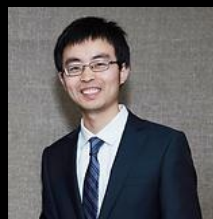
S.C. Yelishala



Y. Zhu



M. Habibi



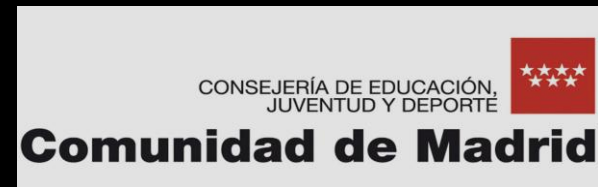
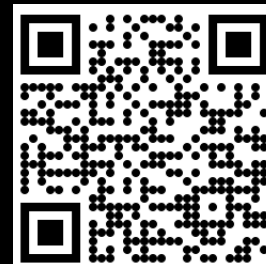
L. Cui



W. Zhang

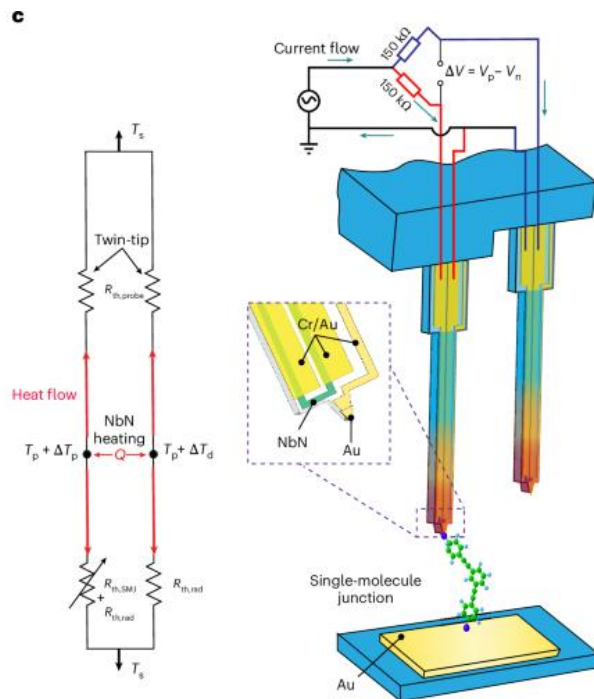
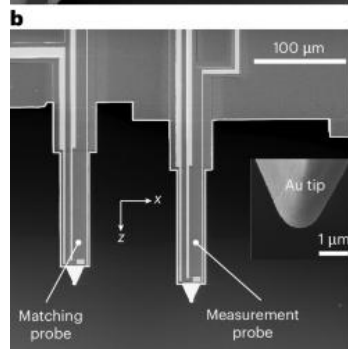
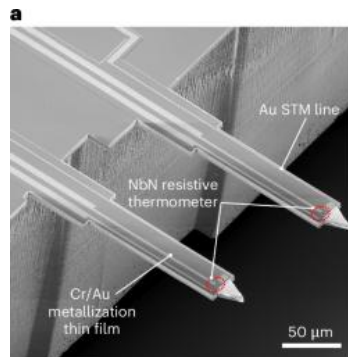
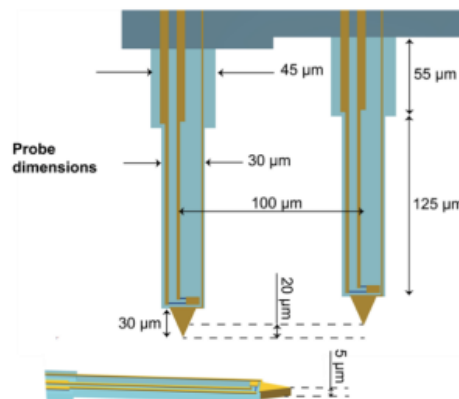
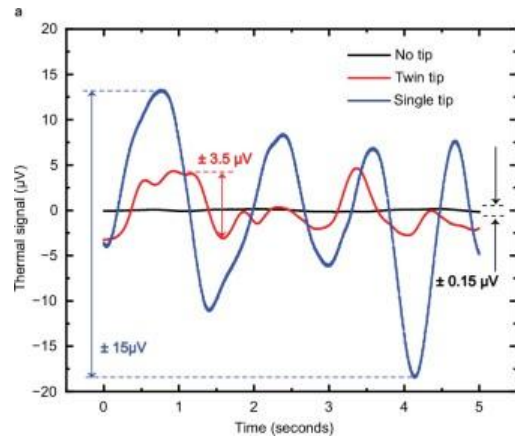


H. Chen

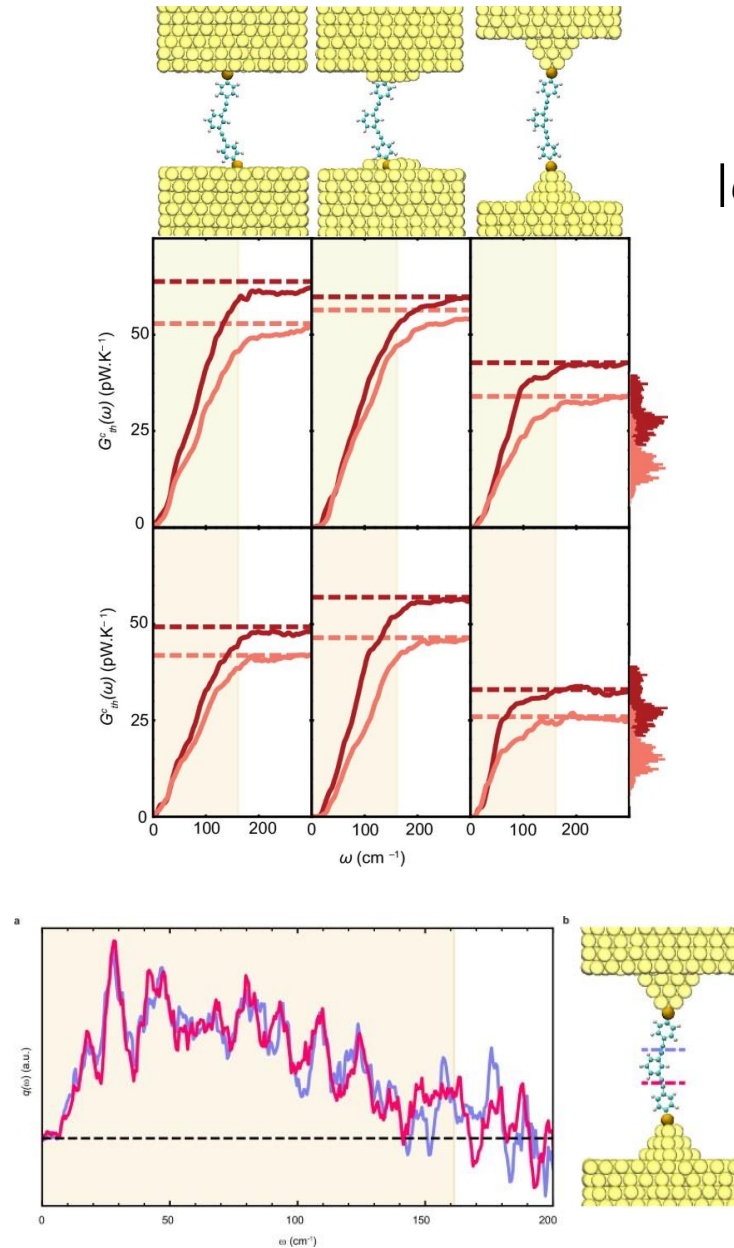
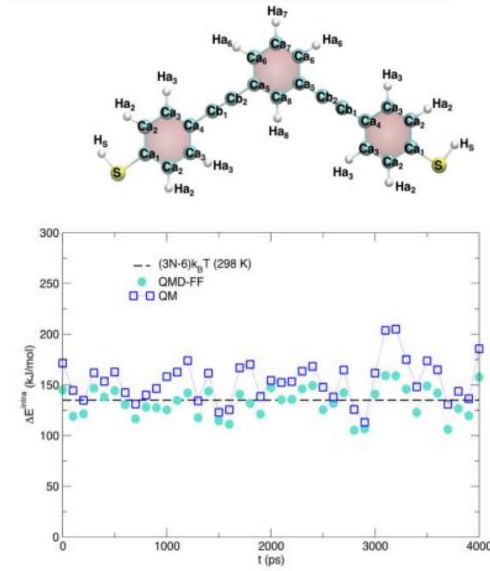
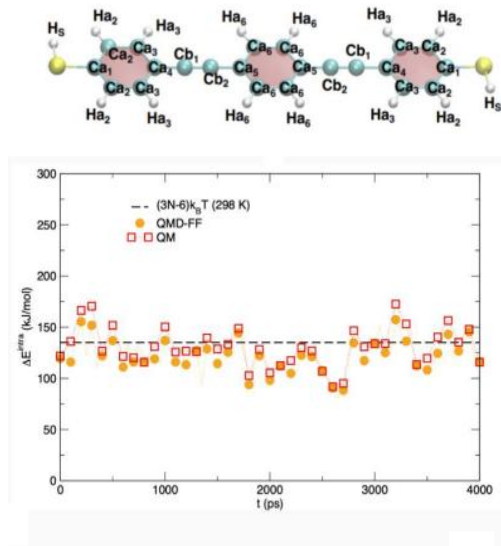


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Extra figures – Experiments



Extra figures – Theory



Kernel of transmission

$$|d_{rl}(E)|^2 = \left| \sum_j \frac{C_{l,j} \cdot C_{r,j}}{(E + i\eta)^2 - E_j^2} \right|^2$$