

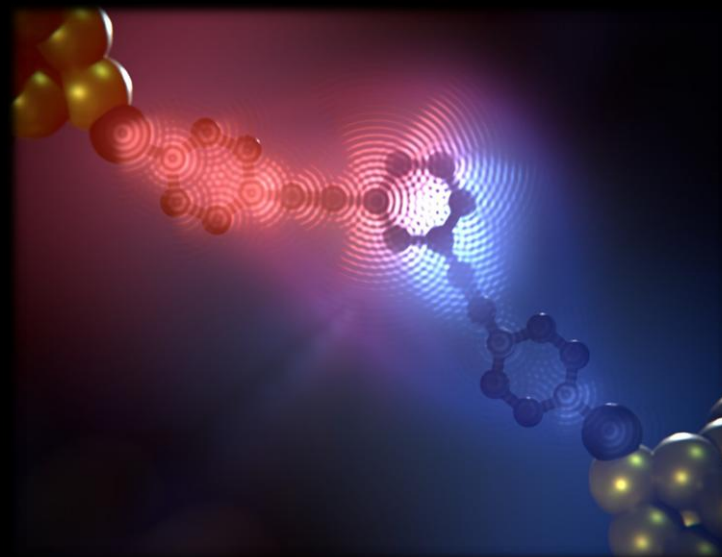
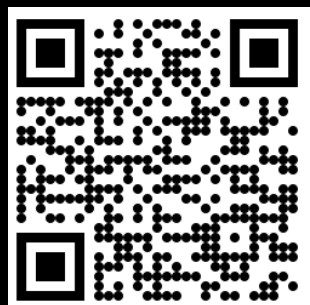
Room-temperature vibrational interference in π -conjugated junctions

P.M. Martinez

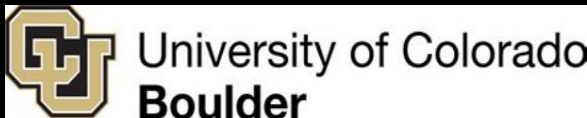


Phonon interference in single-molecule junctions

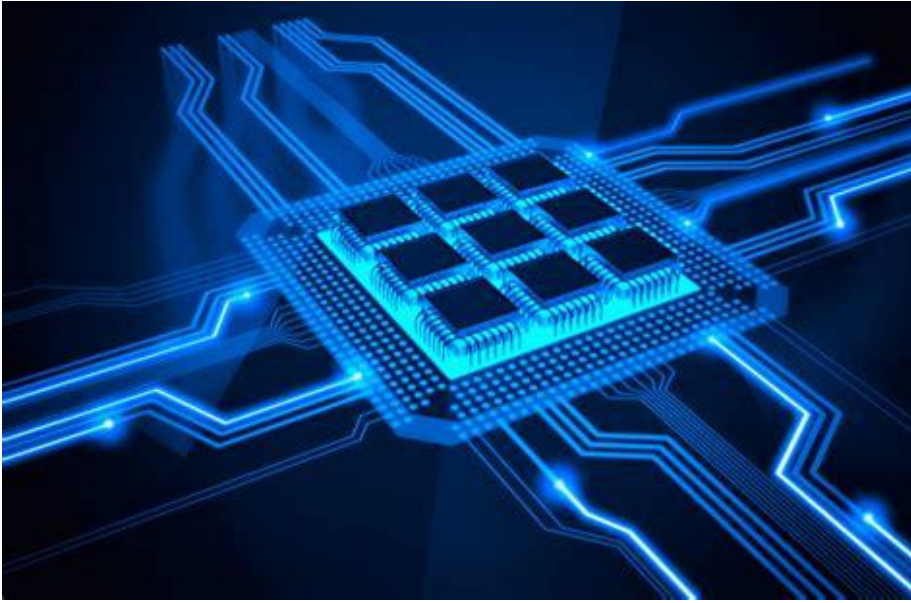
Nat. Mater. **24**, pp. 1258–1264, 2025



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

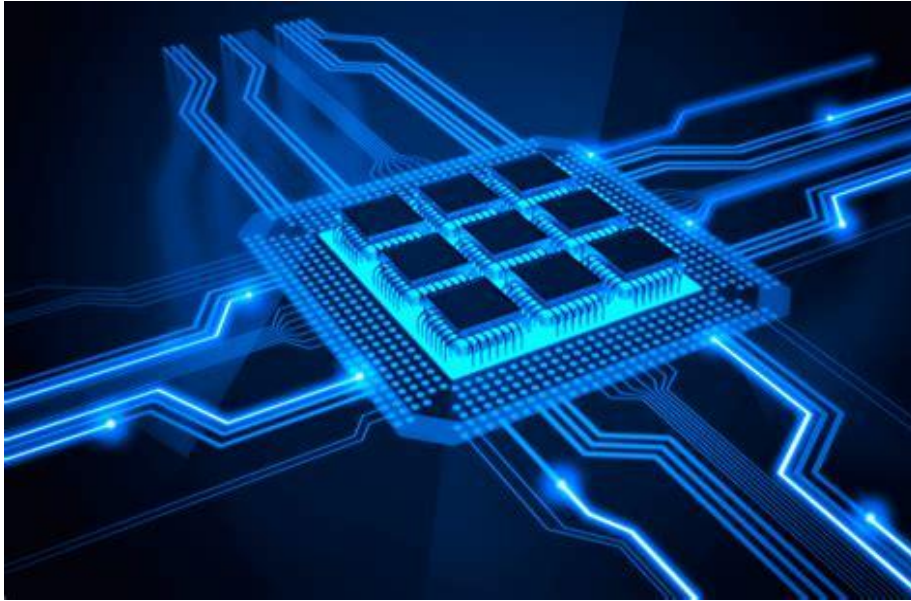


A persistent technological bottleneck



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

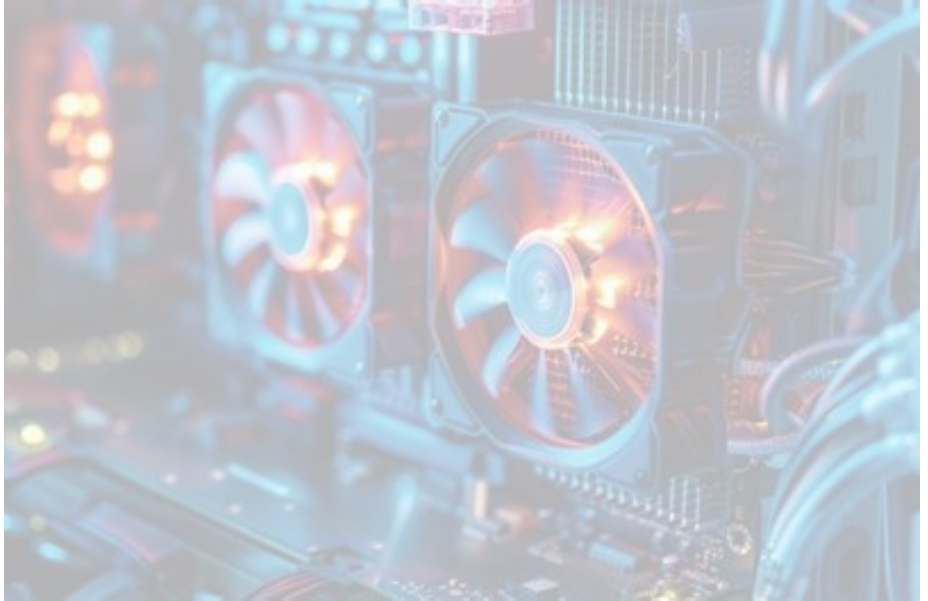
A persistent technological bottleneck



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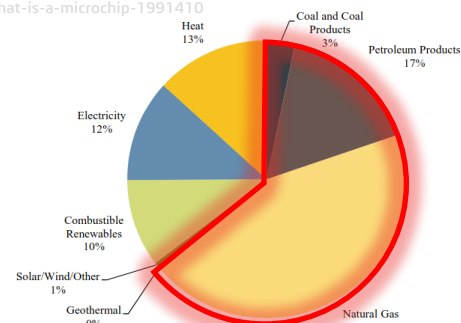
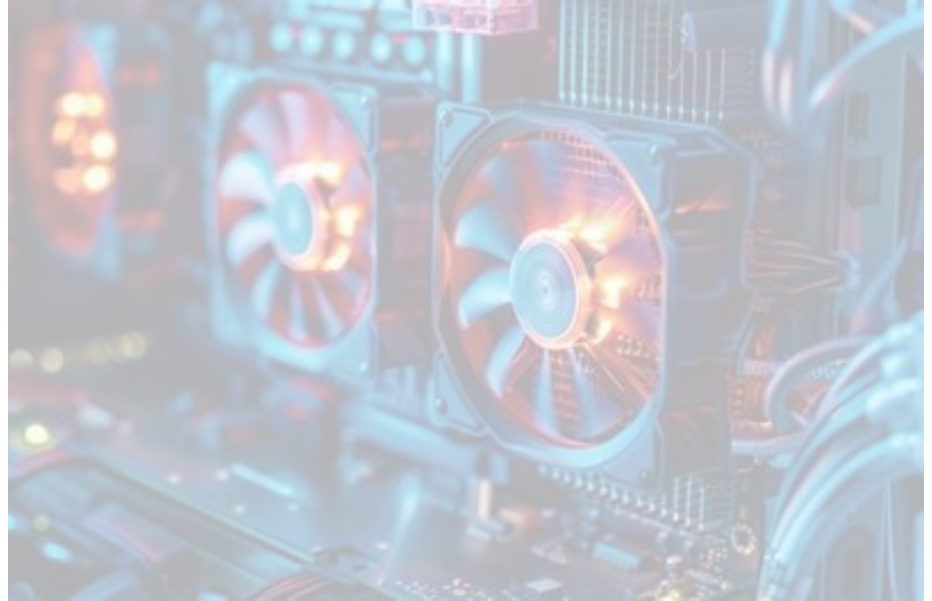


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science institute of Madrid

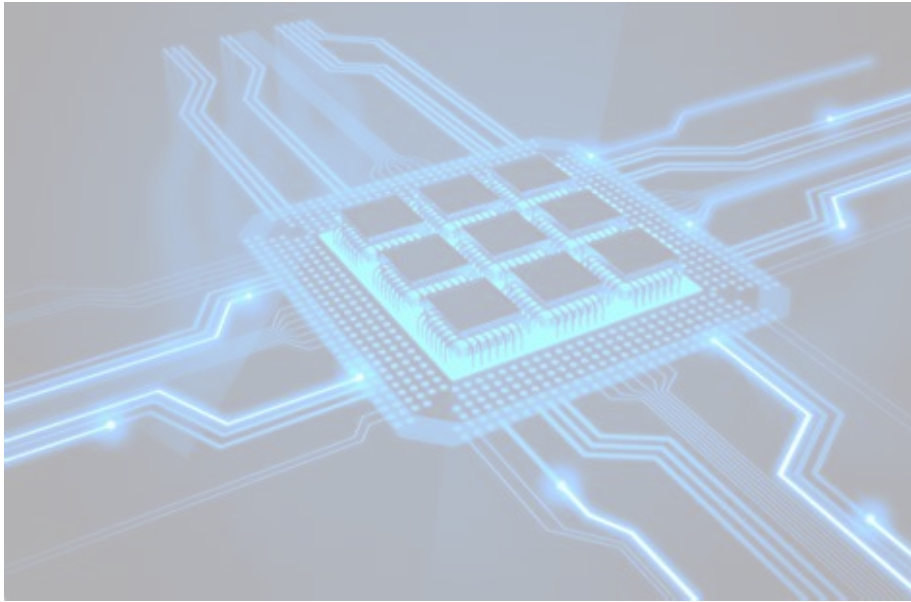
reduce the CO₂ emissions



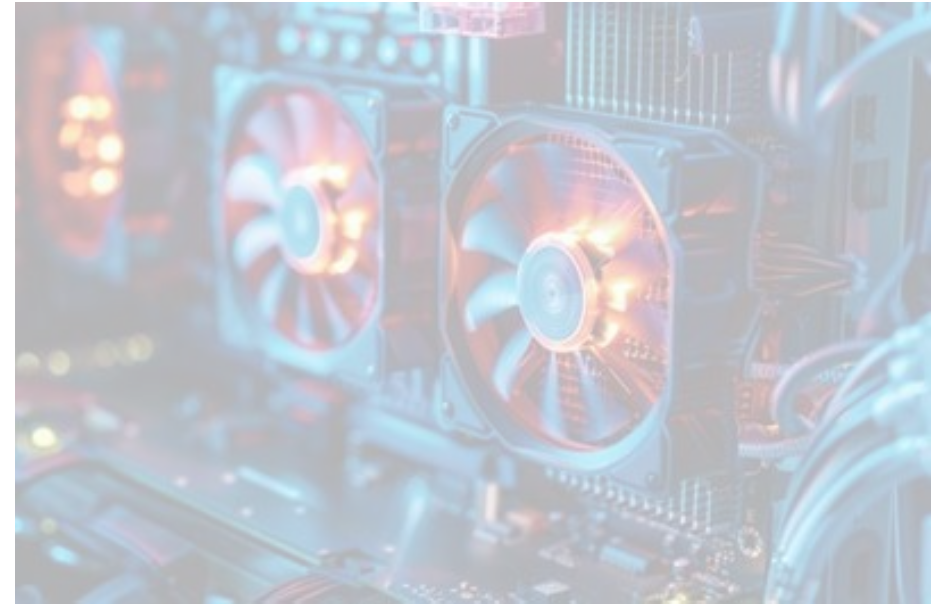
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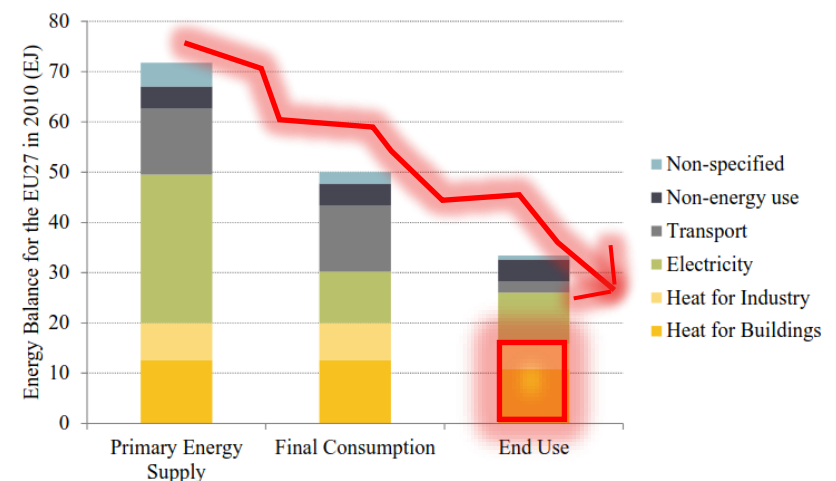
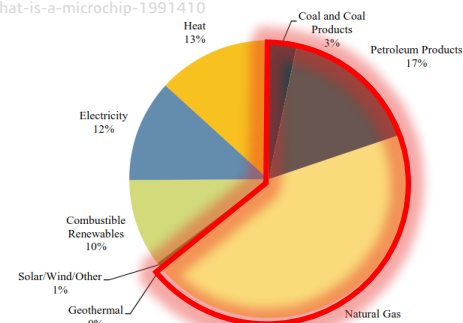
A persistent technological bottleneck



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



Influence of tribology on global energy consumption, costs and emissions
 Research report by the European Commission, 2013. The report assesses the impact of tribology on global energy consumption, costs and emissions. It identifies key areas for improvement and provides recommendations for reducing energy losses and CO₂ emissions. The report is available at: <https://ec.europa.eu/research/tribology/>

~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

Connolly, D., Mathiesen, B. V., Østergaard, P. A., Möller, B., Nielsen, S., Lund, H., Persson, U., Werner, S., Grözinger, J., Boermans, T., Bosquet, M., & Trier, D. (2013). Heat Roadmap Europe 2: Second Pre-Study for the EU27. Department of Development and Planning, Aalborg University

Classical Theory of Heat Transport

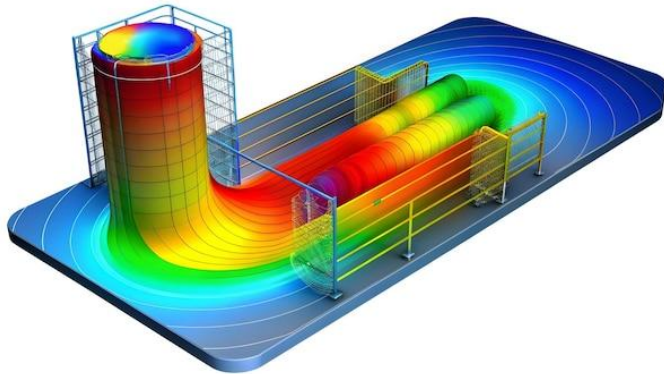
Nearly 200 years ago in France...

Classical Theory of Heat Transport

Nearly 200 years ago in France...

Fourier formulates his renowned Law...

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



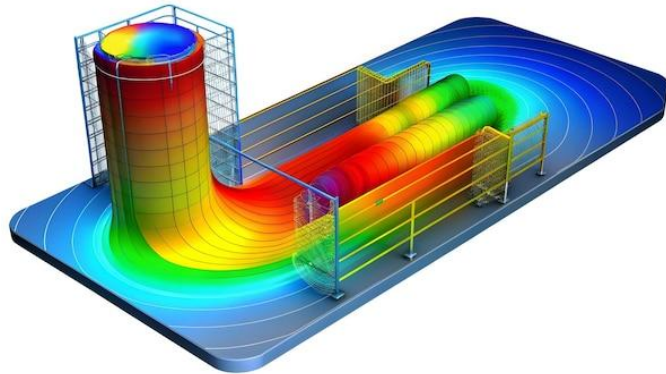
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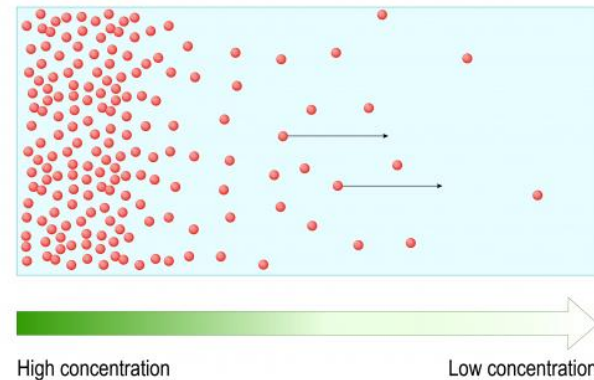
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$$\dot{N} = -D \frac{\partial \phi}{\partial x}$$



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

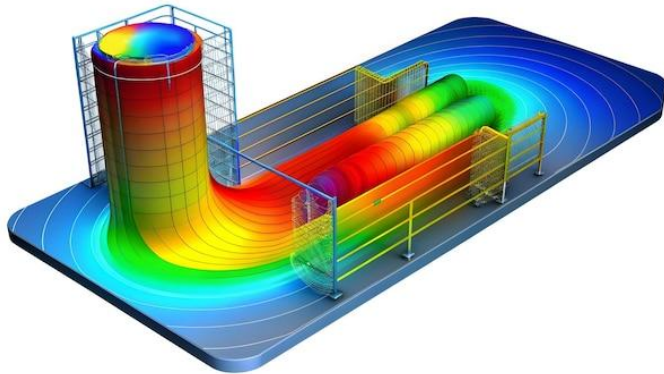
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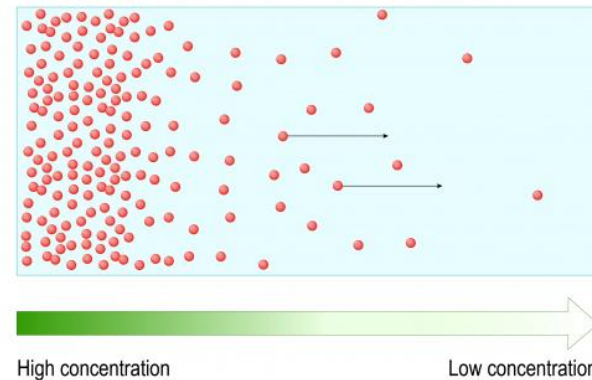
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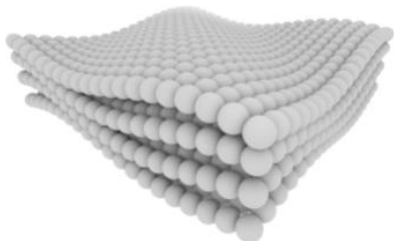


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<https://fity.club/lists/suggestions/diffusion/>

At the submicron scale this picture fails...



[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)

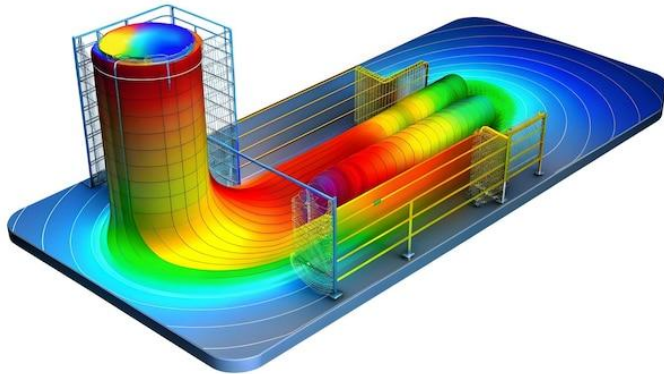
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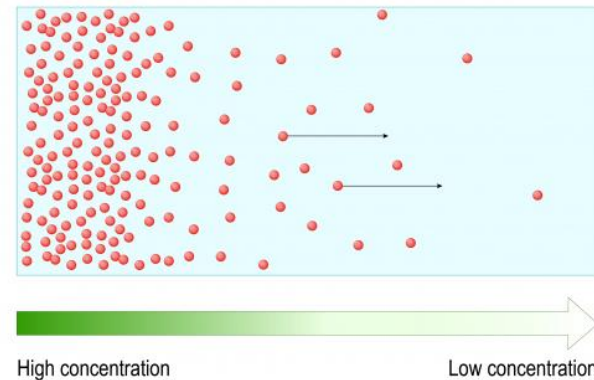
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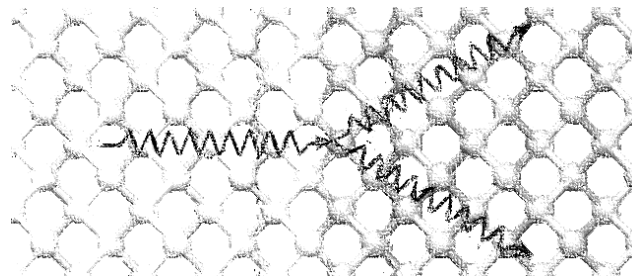
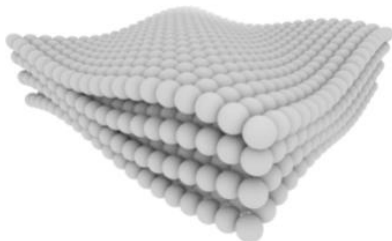


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<https://doi.org/10.1103/PhysRevB.103.174306>

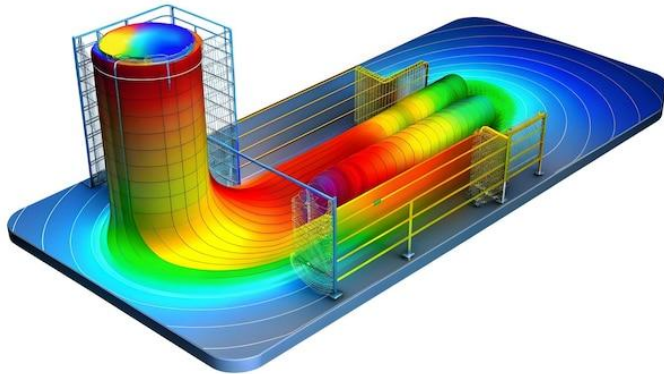
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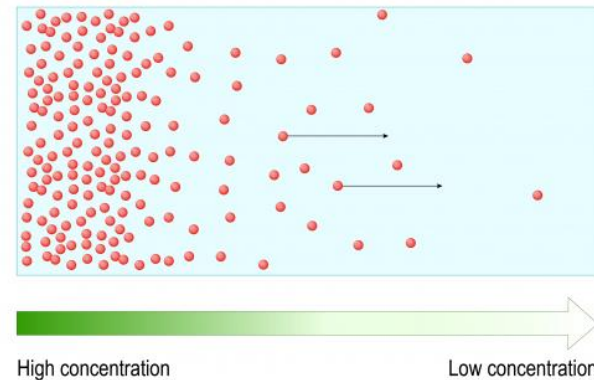
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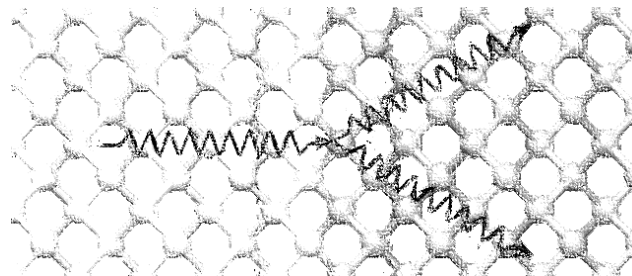
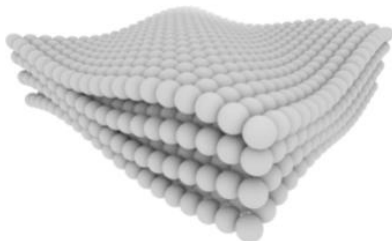


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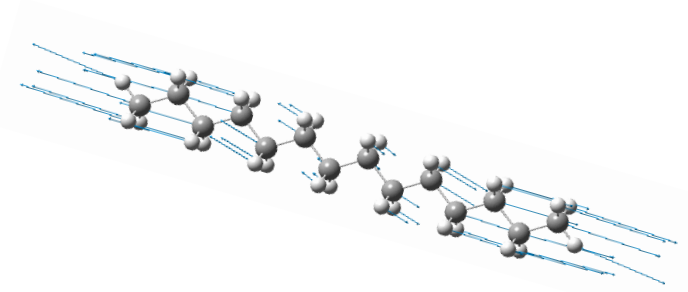
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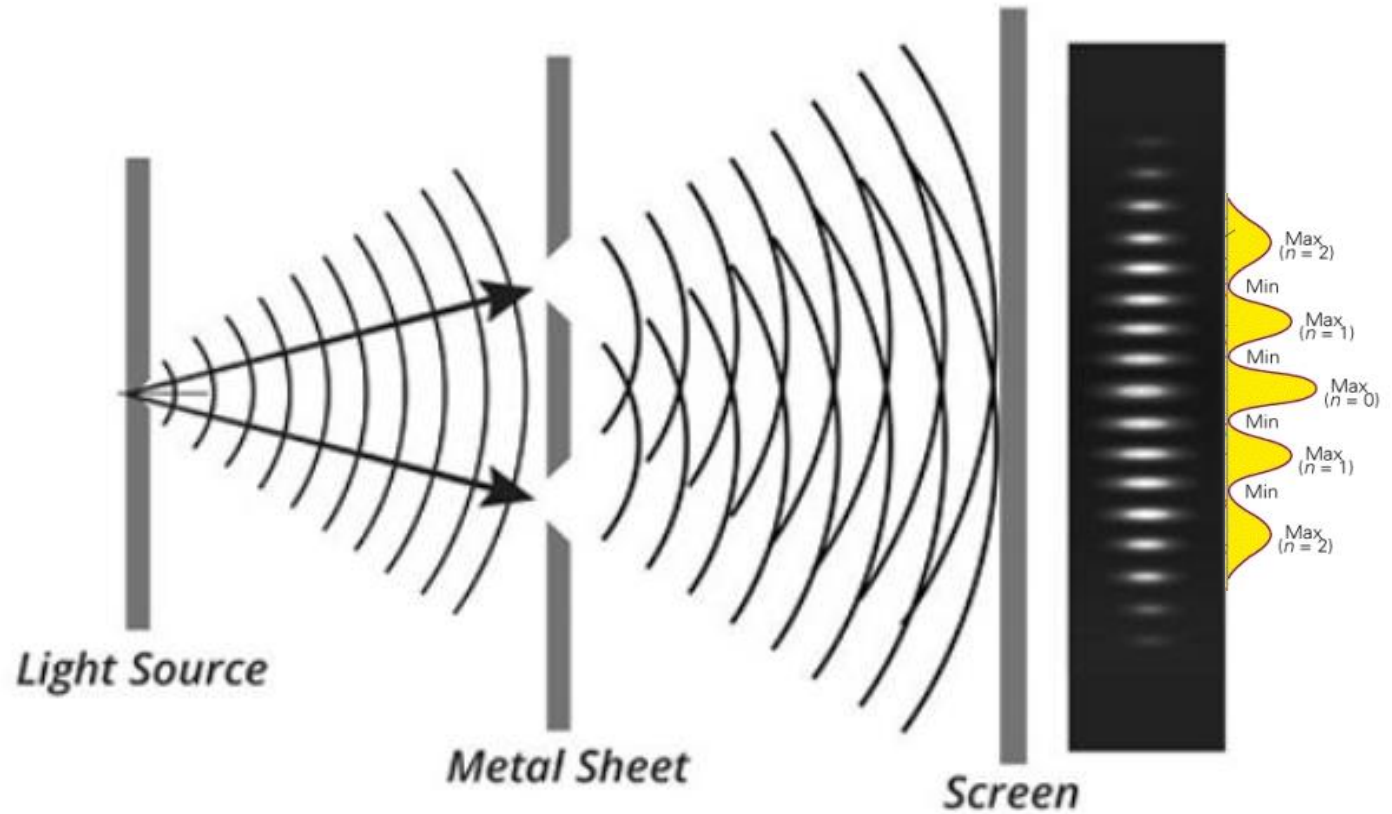


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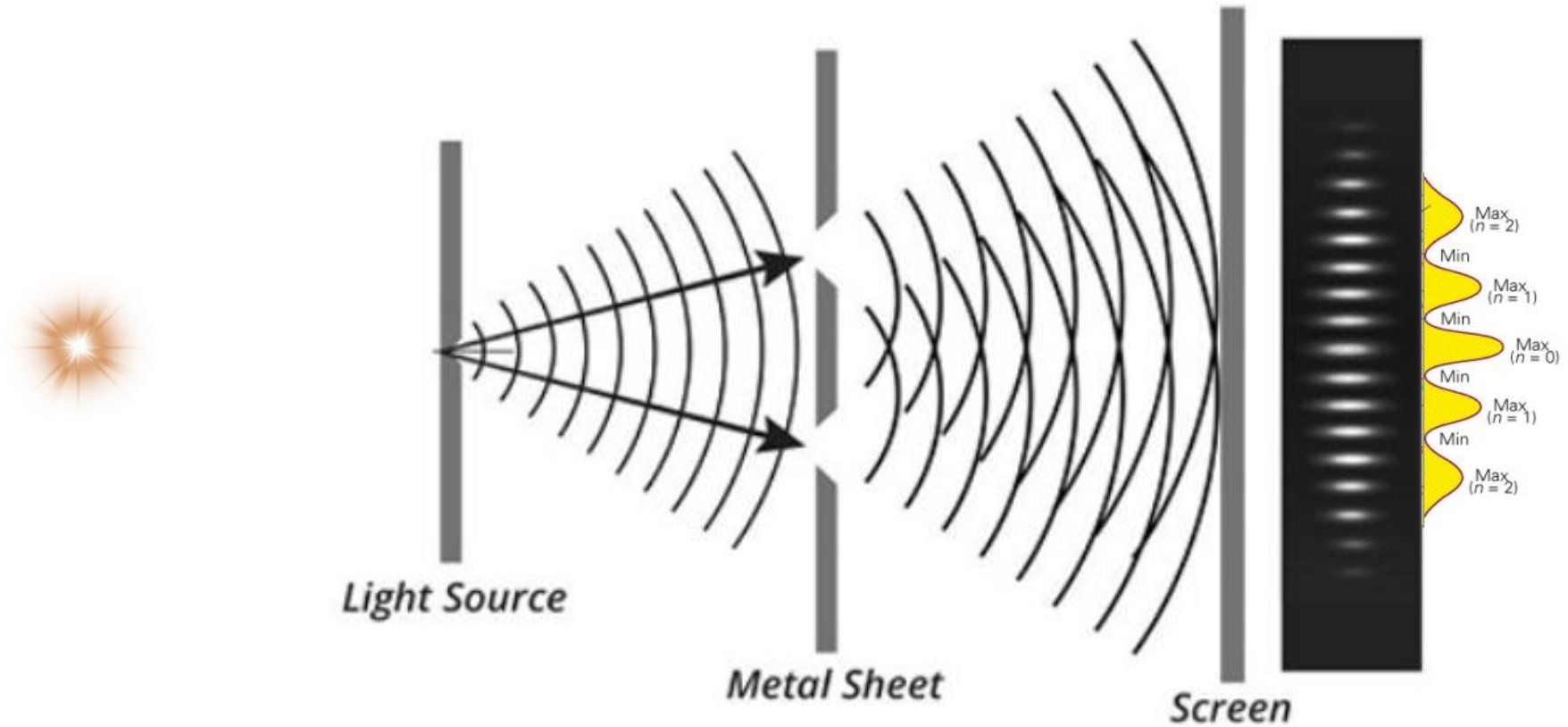
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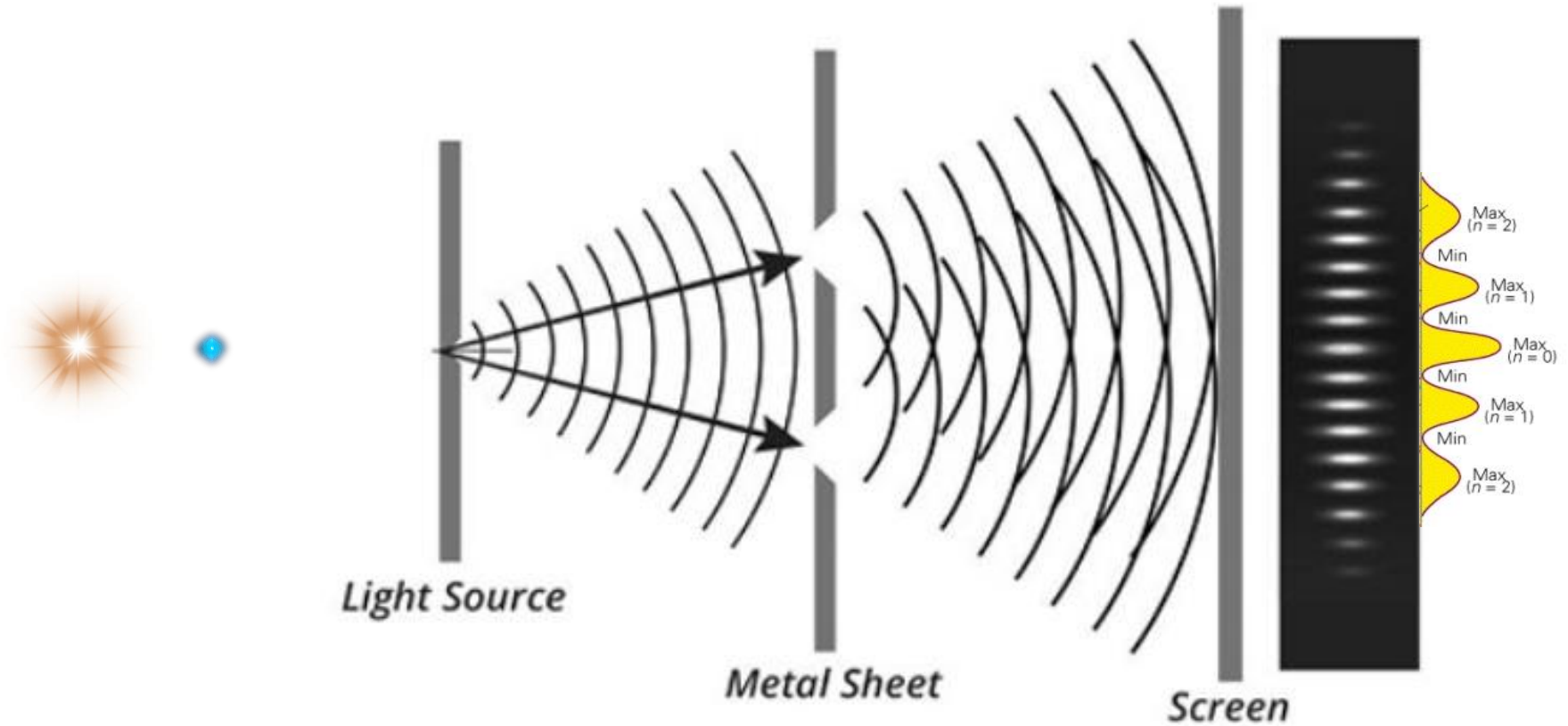
Violations of diffusive transport disclose novel mechanism



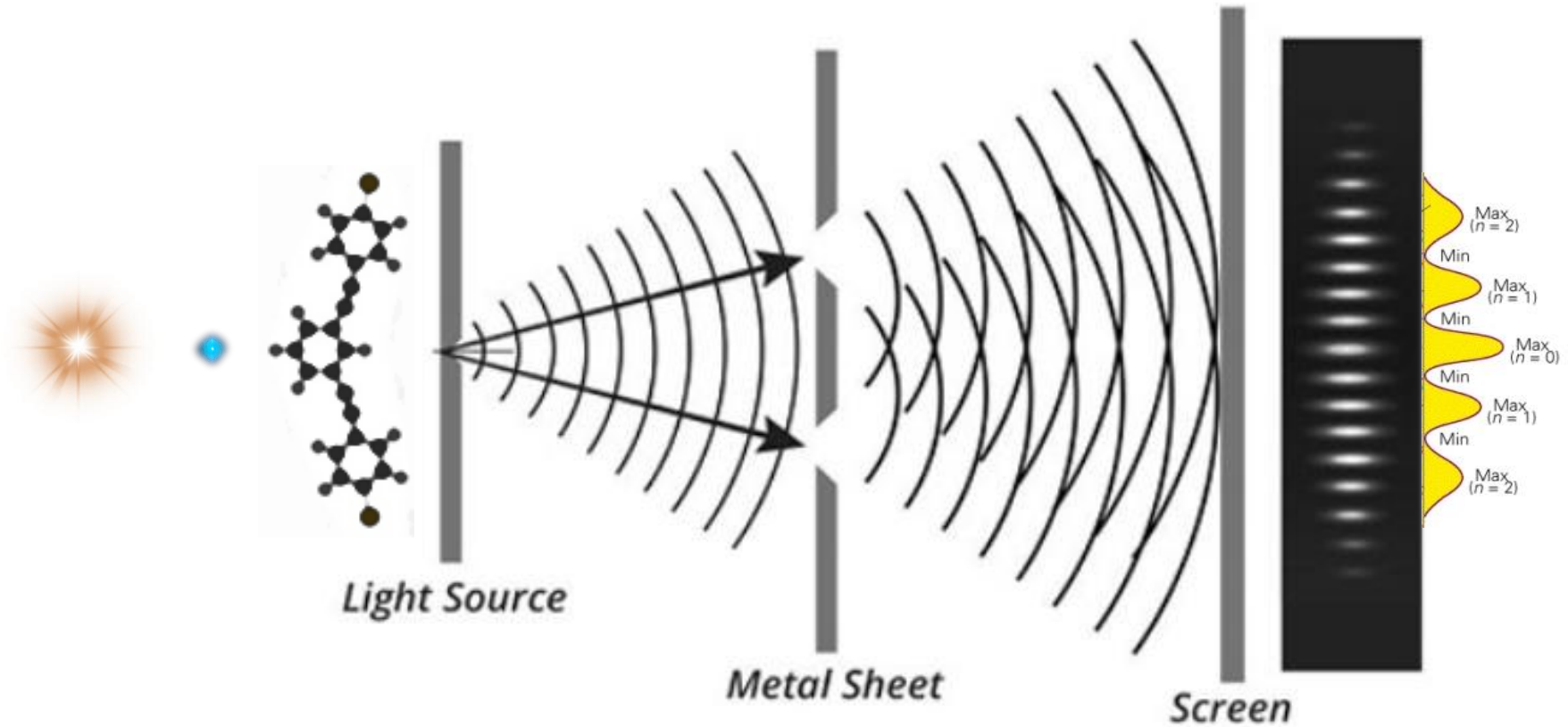
Violations of diffusive transport disclose novel mechanism



Violations of diffusive transport disclose novel mechanism



Violations of diffusive transport disclose novel mechanism



Methods

Methods: Simulations & Experiments (SThM)

➤ All-atom molecular dynamics simulations



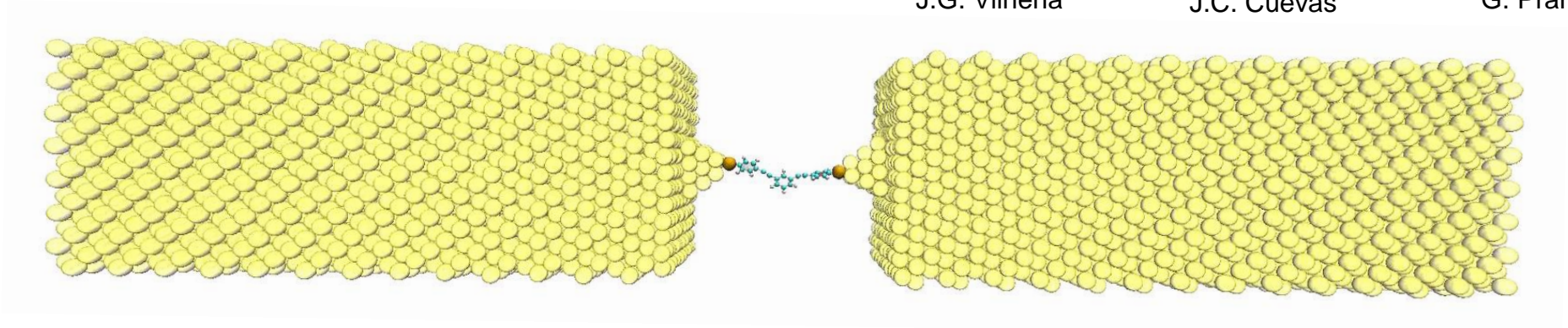
J.G. Vilhena



J.C. Cuevas

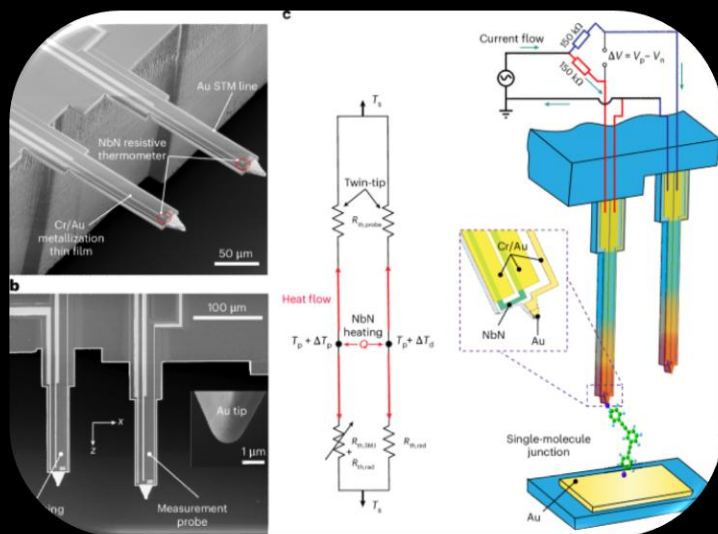


G. Prampolini



Results

Measurements



MD simulation

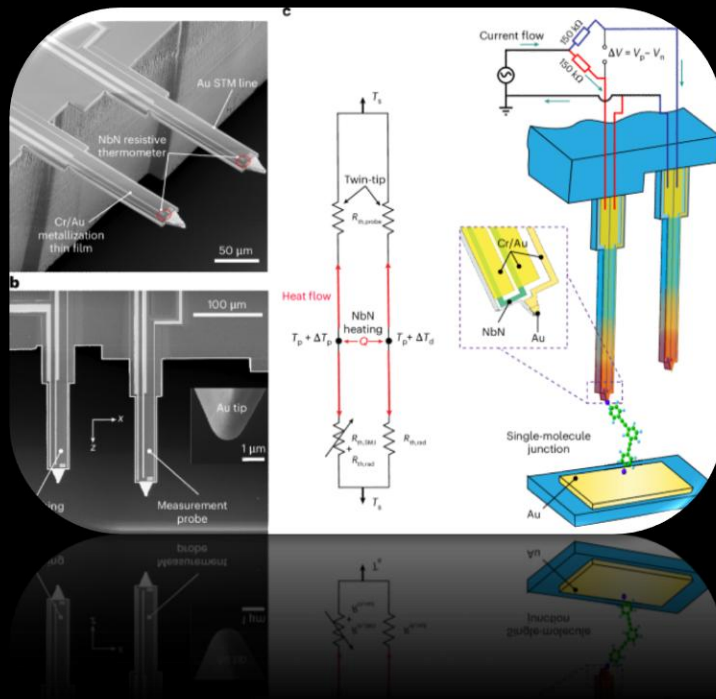


Interference



Results

Measurements

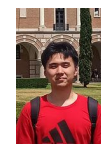


Nat. Mater. 24, pp. 1258–1264, 2025

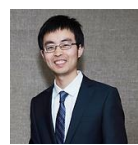
Measurement protocol: single-junction resolution



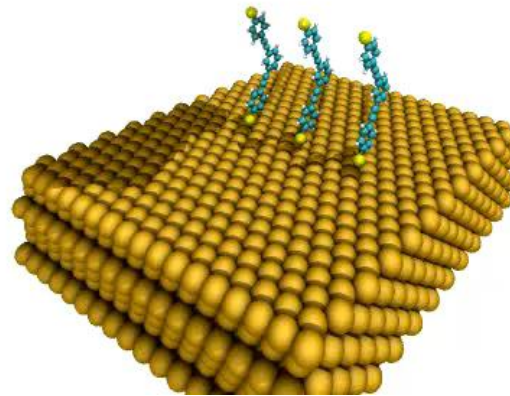
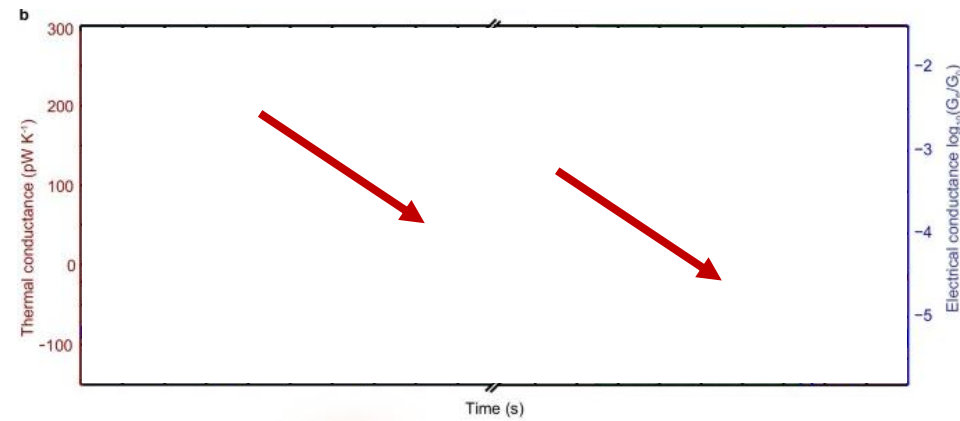
S.C. Yelishala



X. Zhu



L. Cui



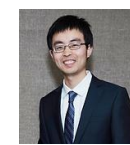
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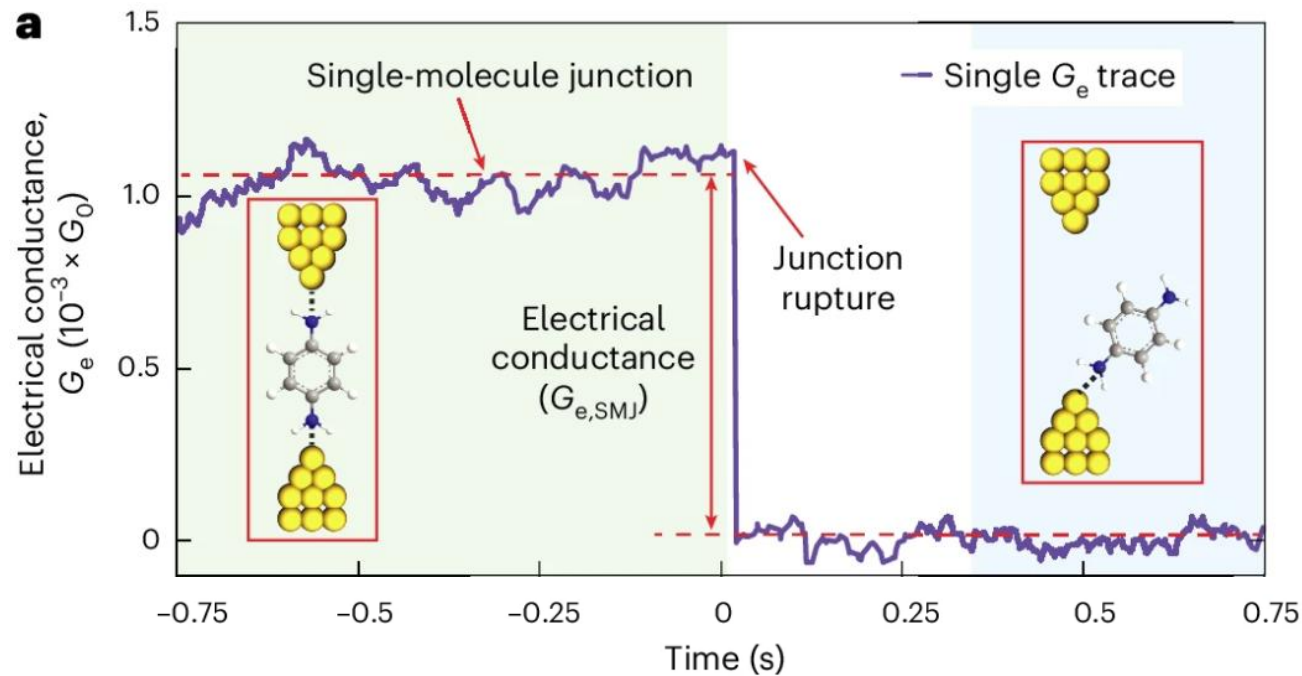
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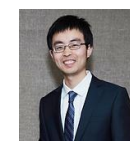
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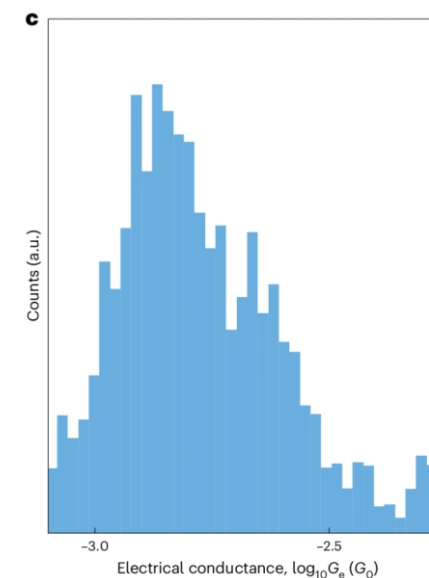
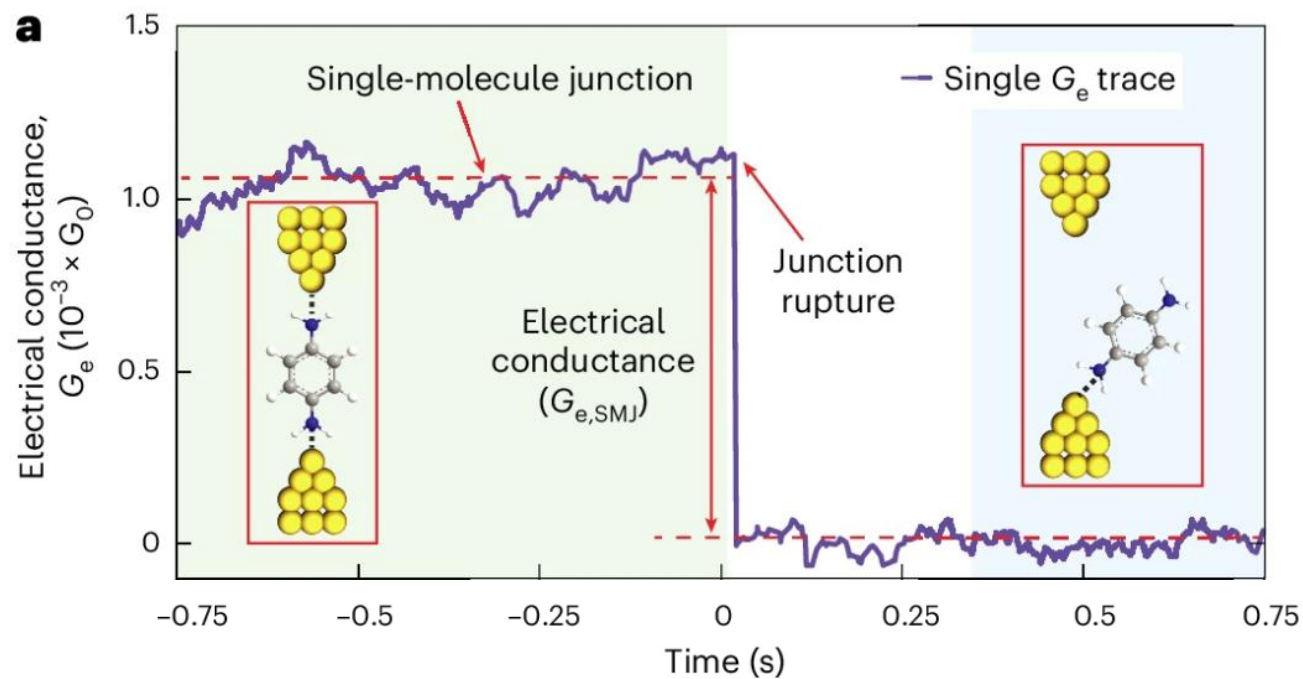
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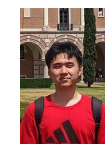
L. Cui



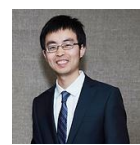
Measurement protocol: single-junction resolution



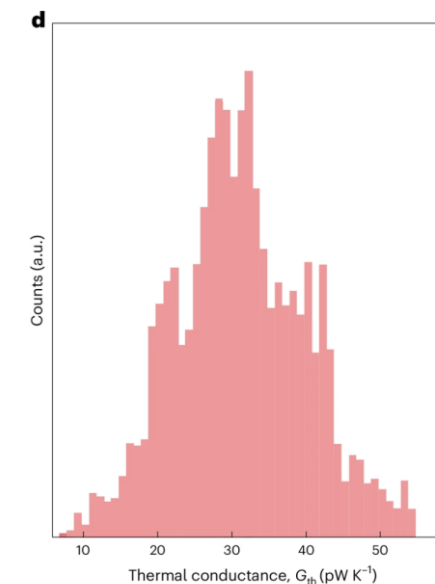
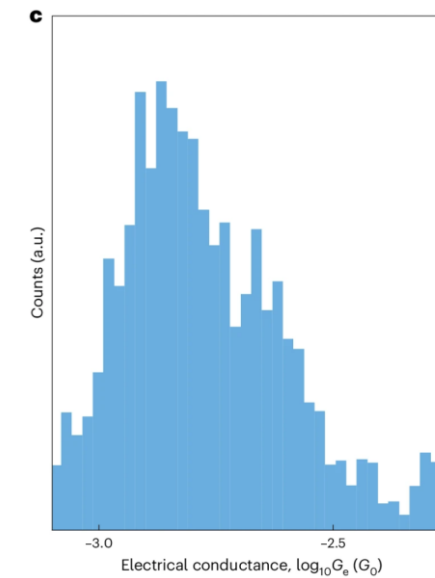
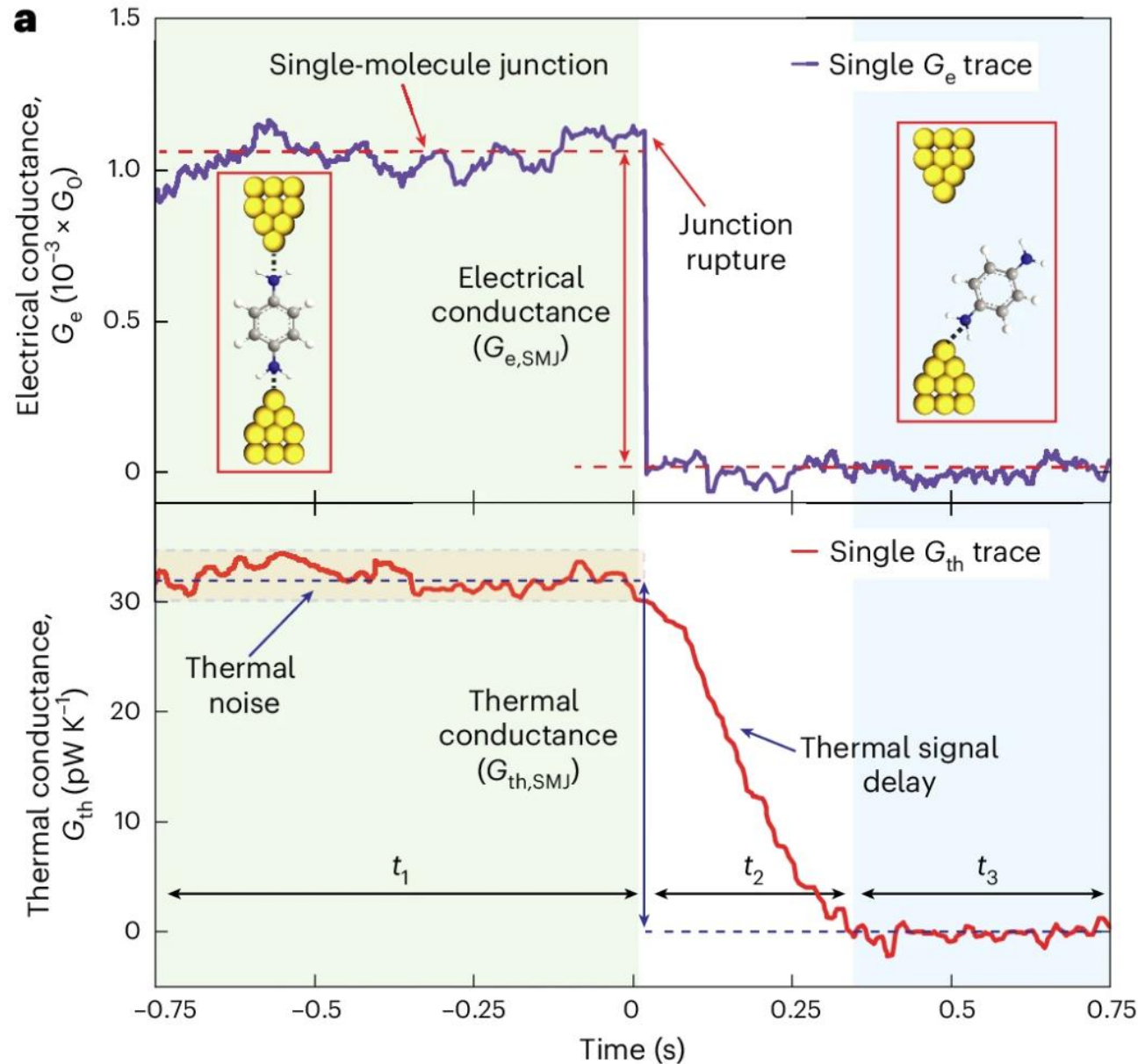
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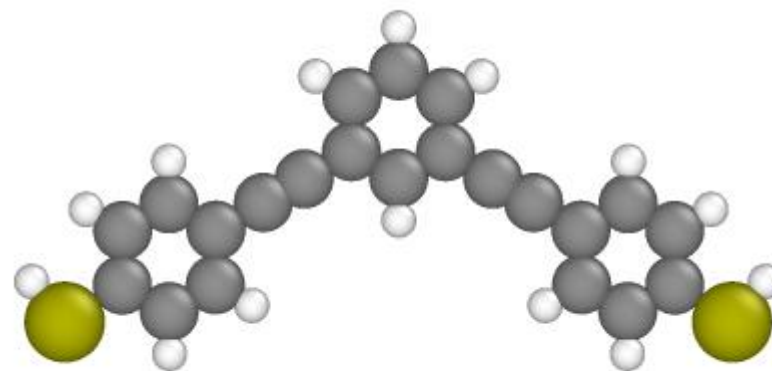
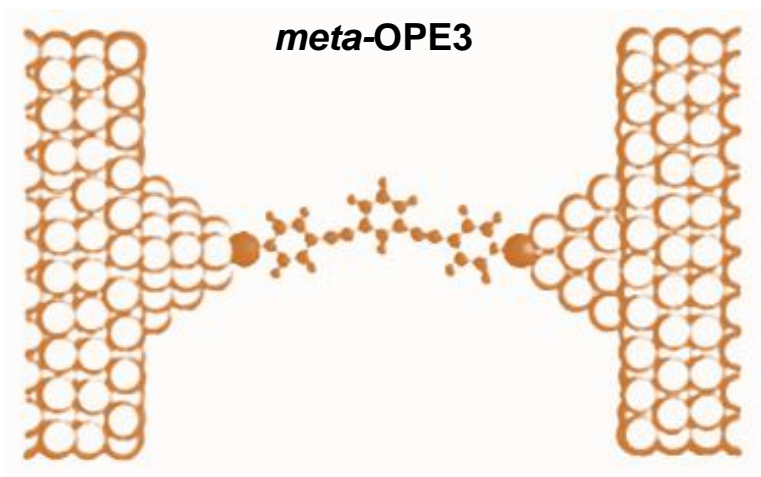
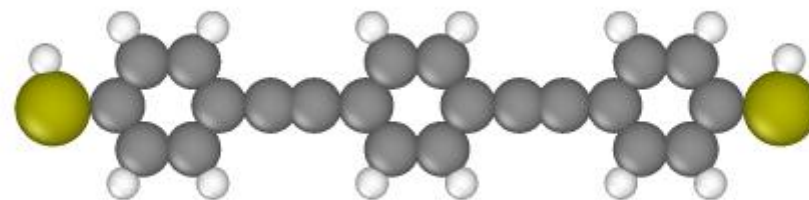
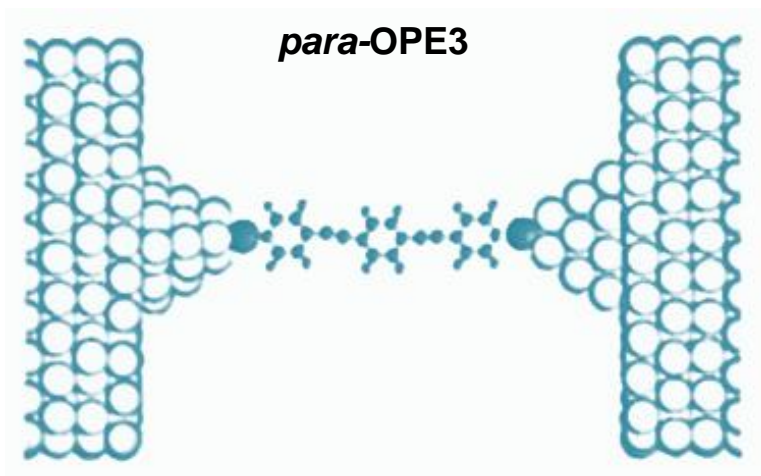
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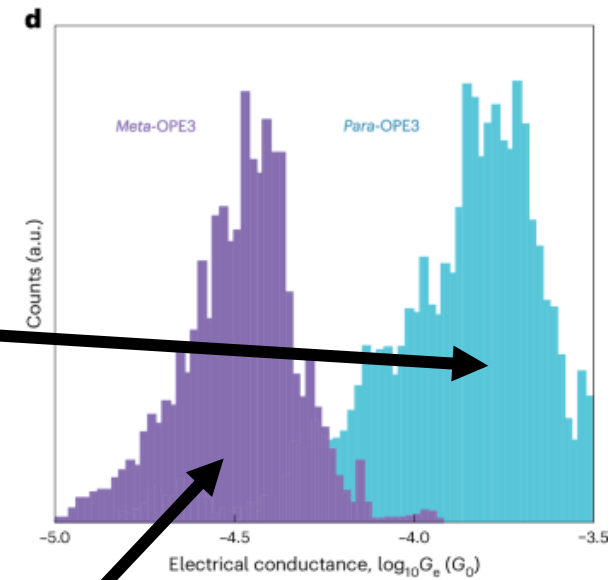
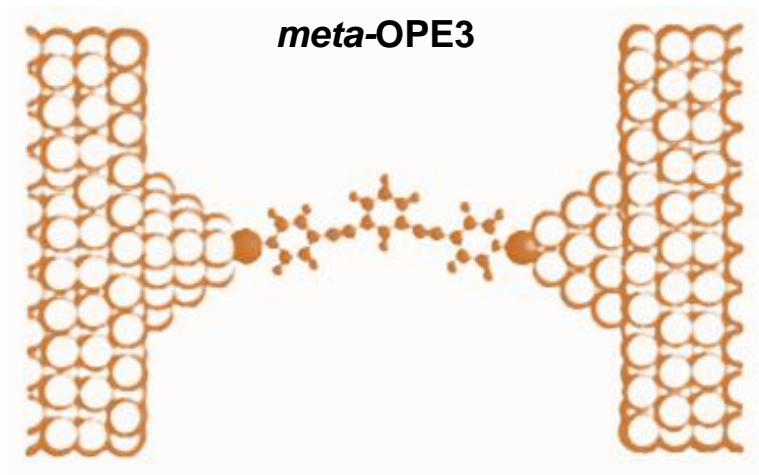
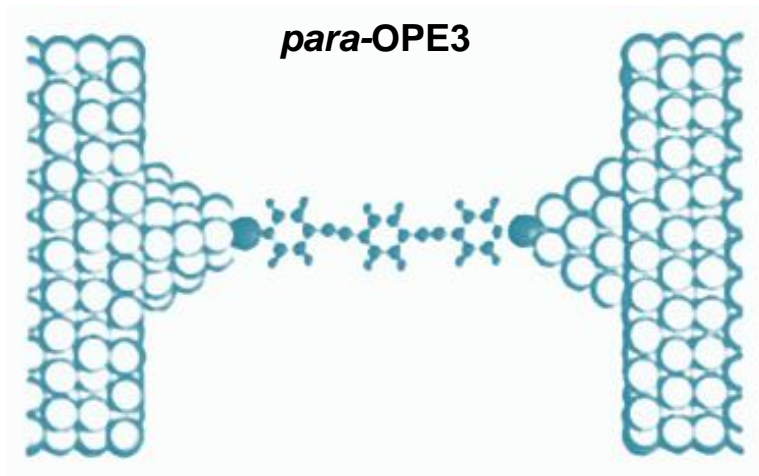
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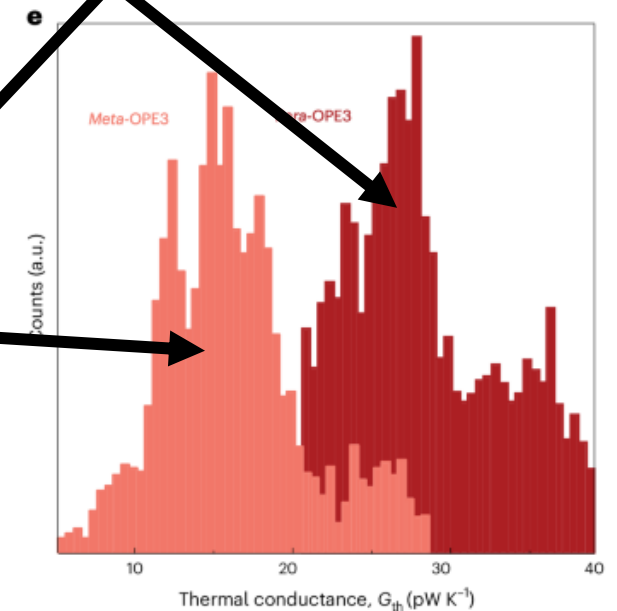
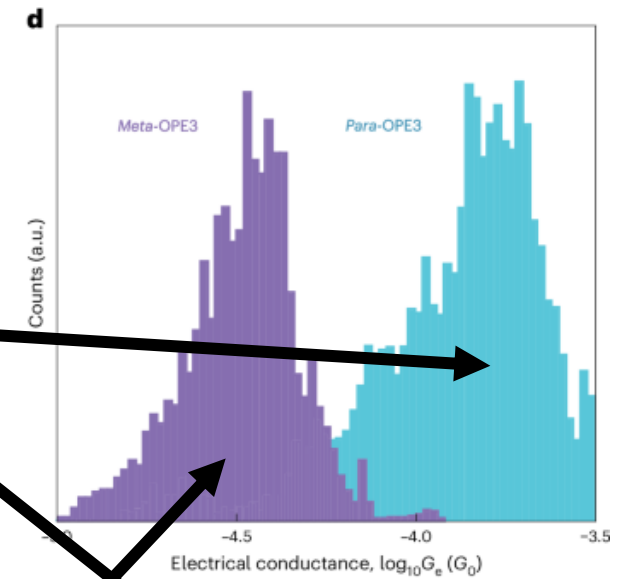
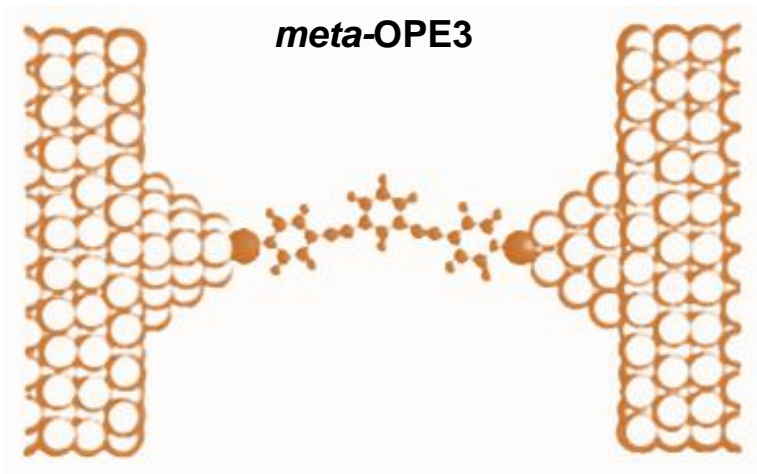
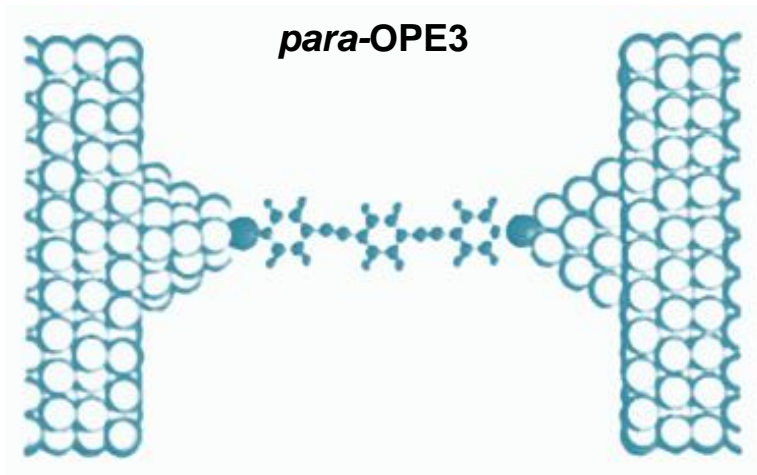
Thermal conductance of *meta*- and *para*-OPE3



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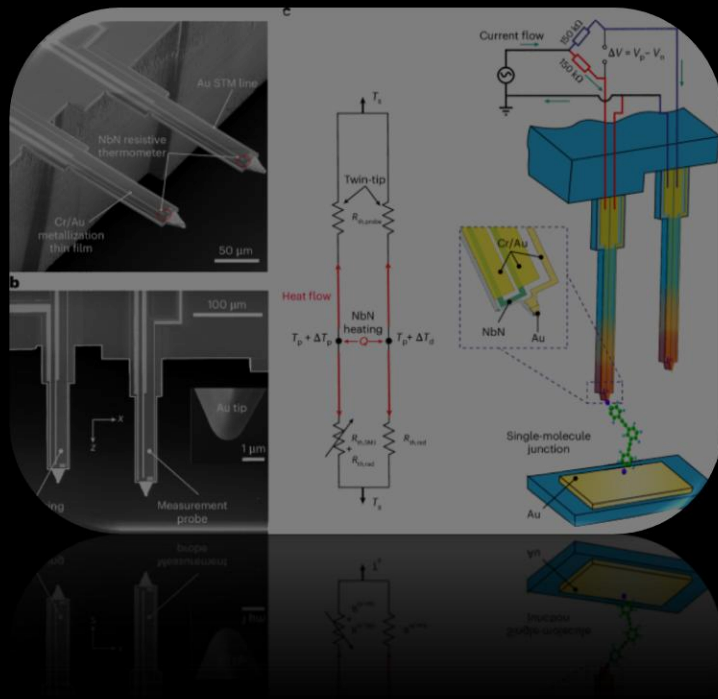


Thermal conductance of *meta*- and *para*-OPE3

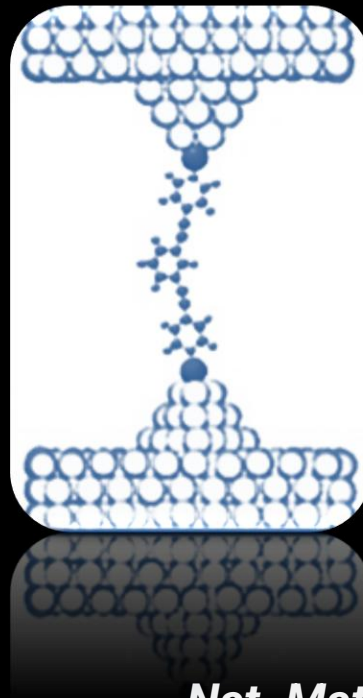


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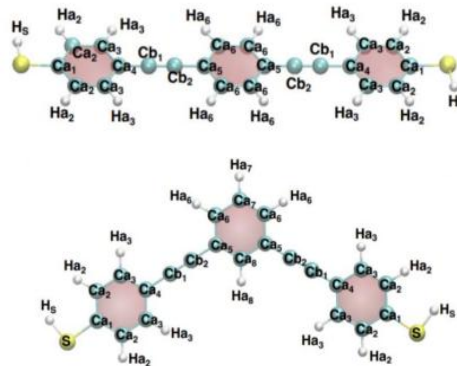
Nat. Mater. 24, pp. 1258–1264, 2025

NEMD simulations with QM-derived force fields

- Intramolecular force field sourced from QM data



G. Prampolini



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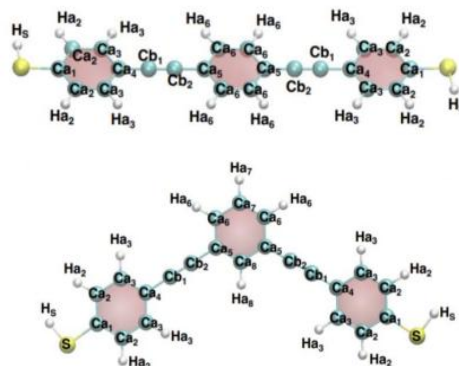
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G. Prampolini



J. Chem. Theory Comput.
21, 3156–3175 (2025)



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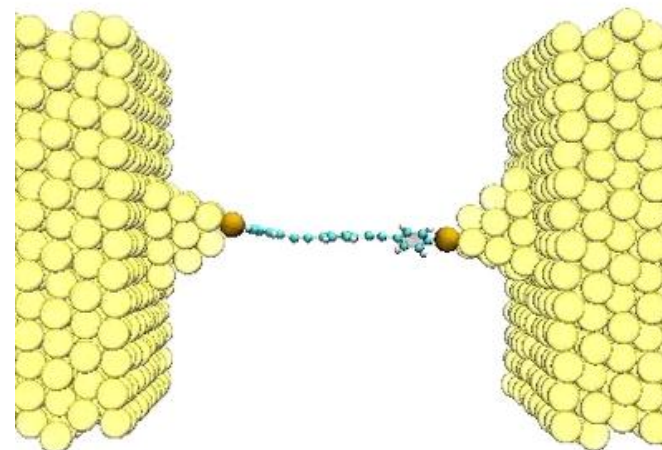
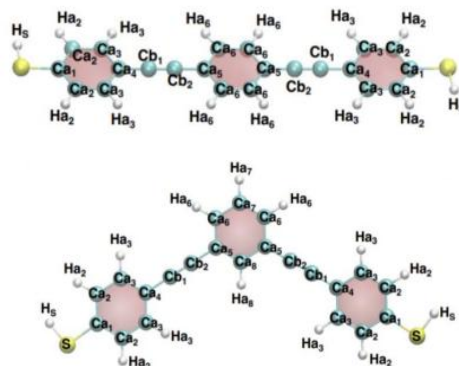
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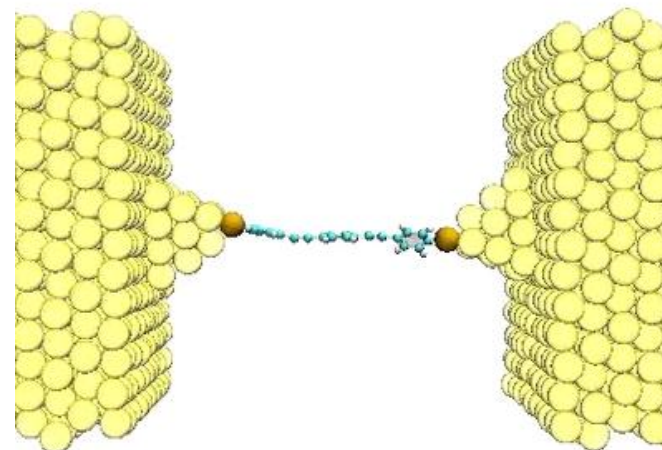
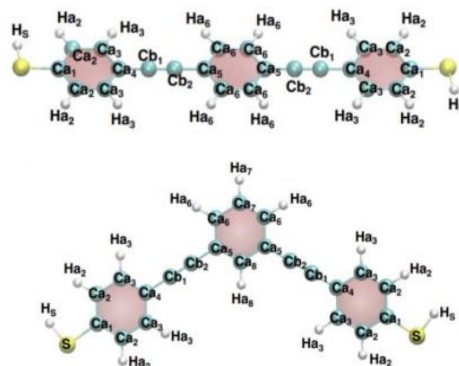
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- How to measure heat in MD?

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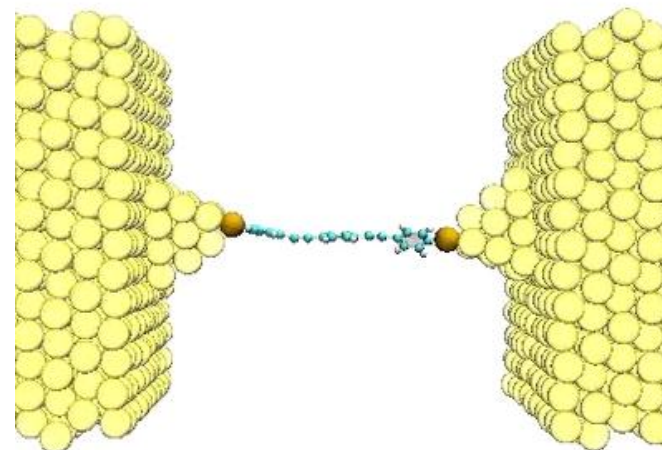
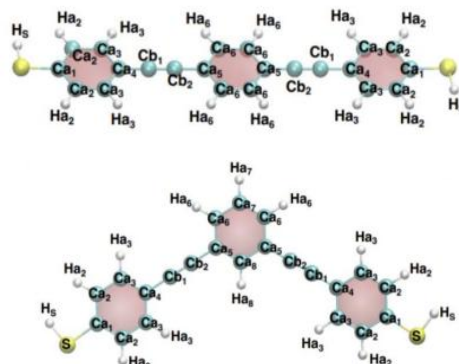
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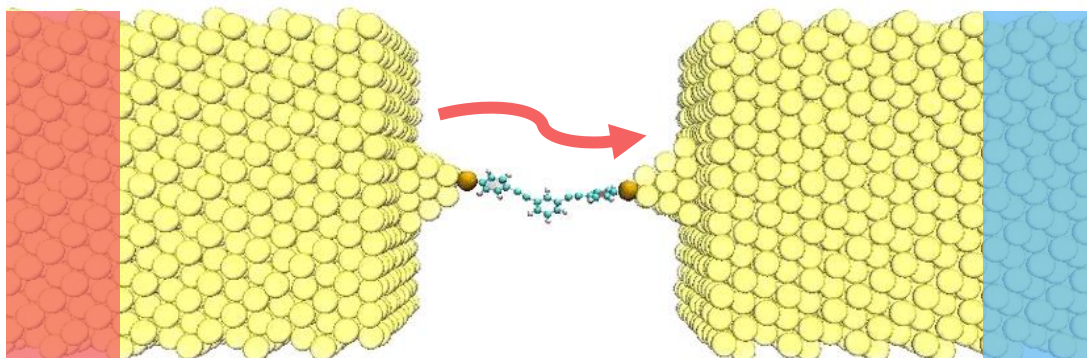
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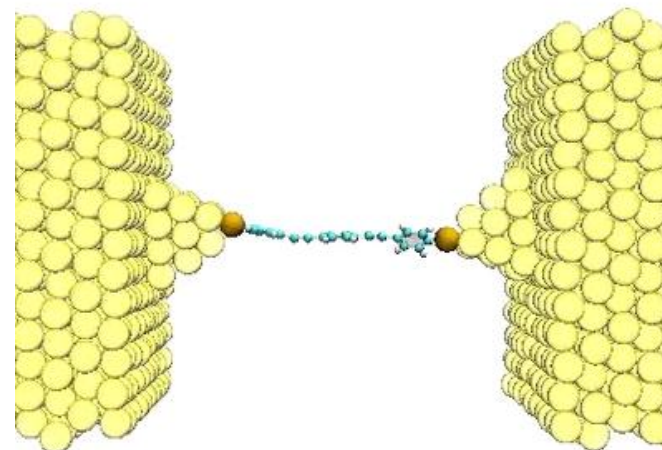
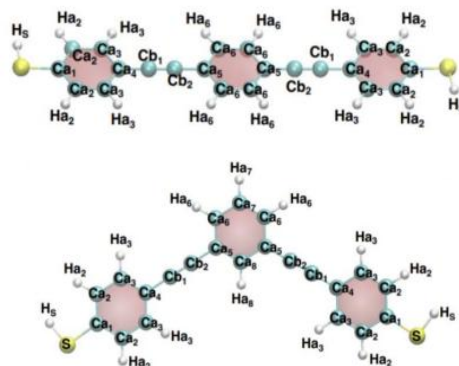
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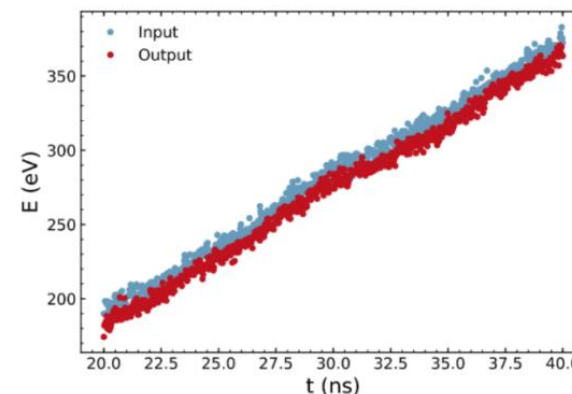
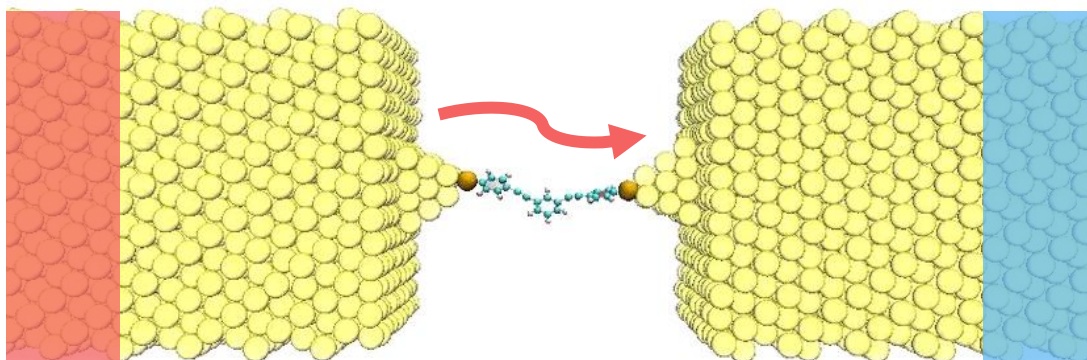
G. Prampolini



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- How to measure heat in MD?



NEMD simulations with QM-derived force fields

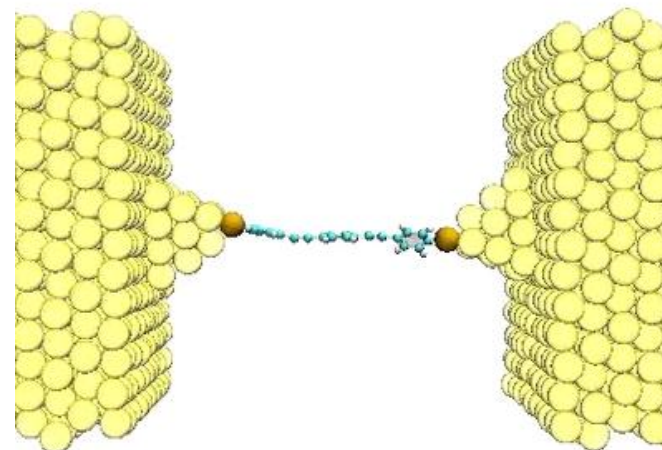
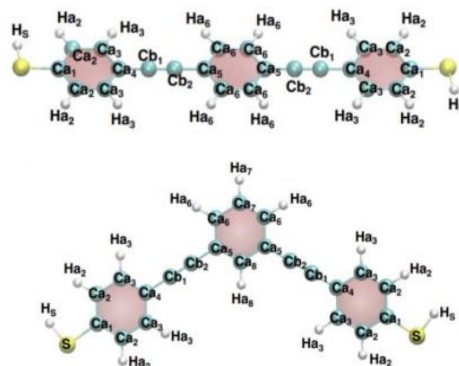
- Intramolecular force field sourced from QM data



G. Prampolini

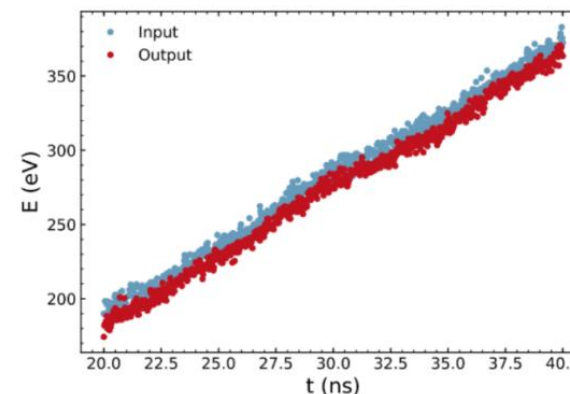
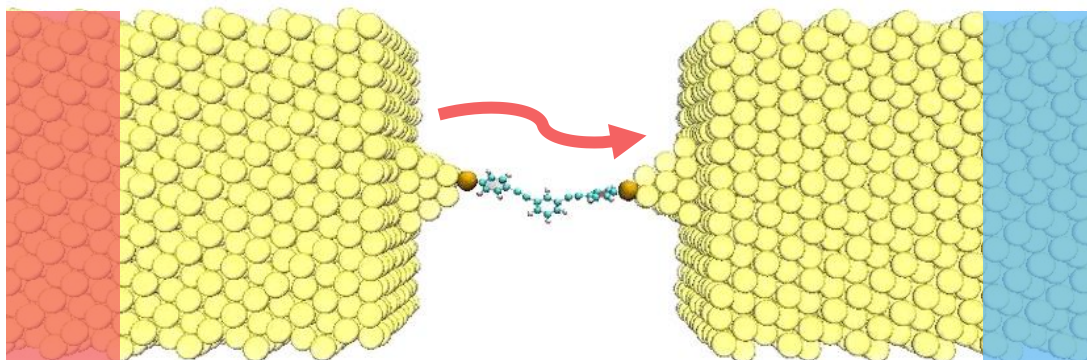


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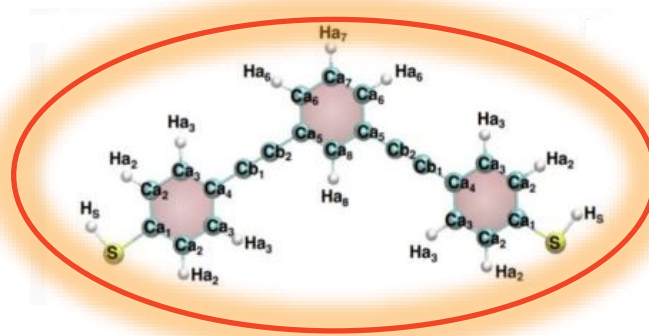
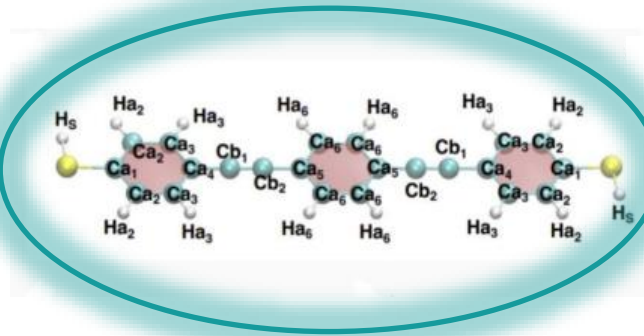
- How to measure heat in MD?

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



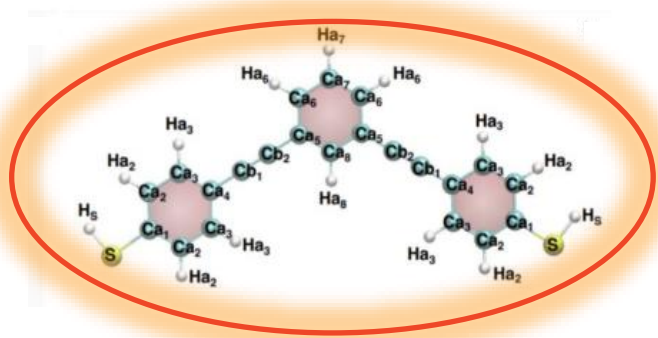
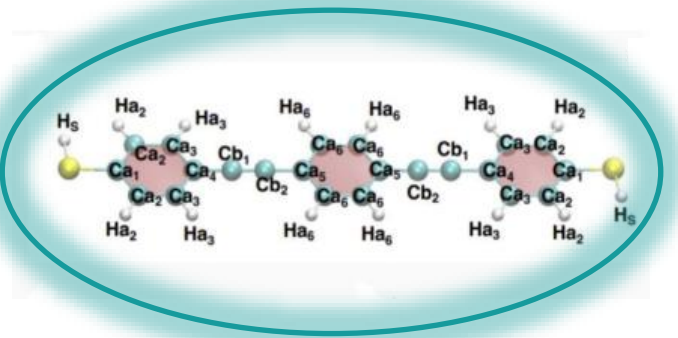
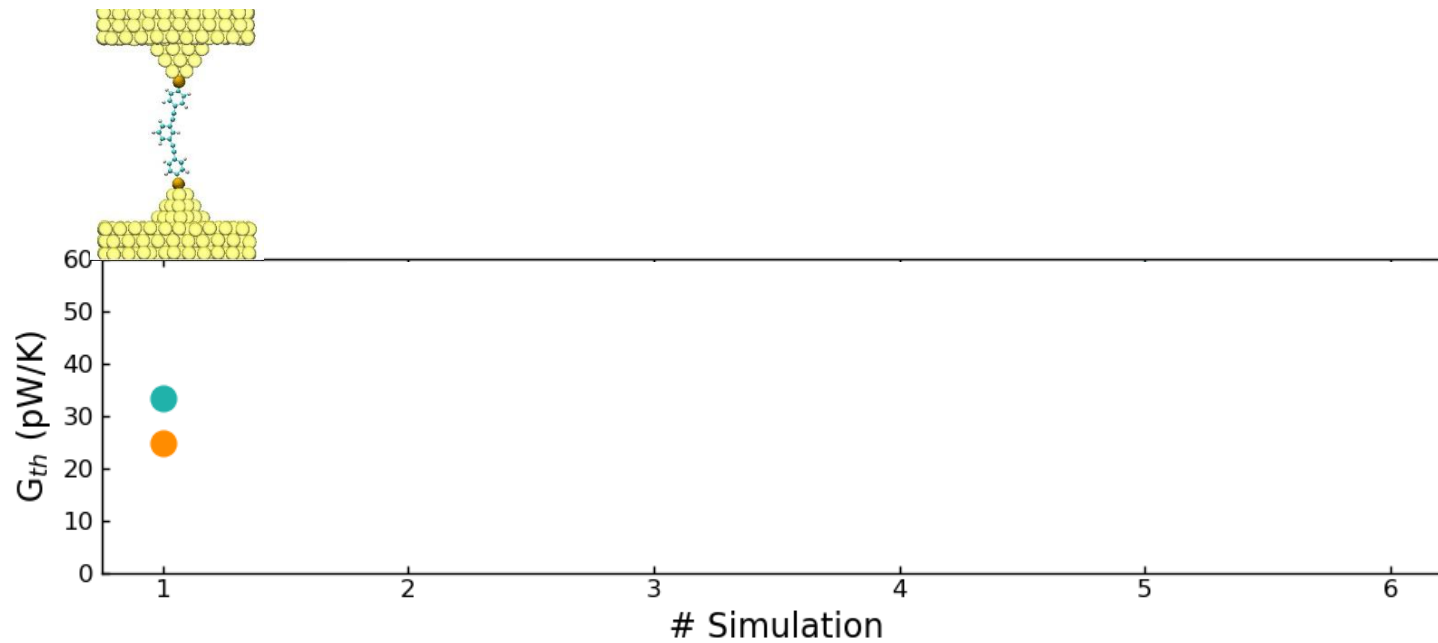
NEMD thermal conductance

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



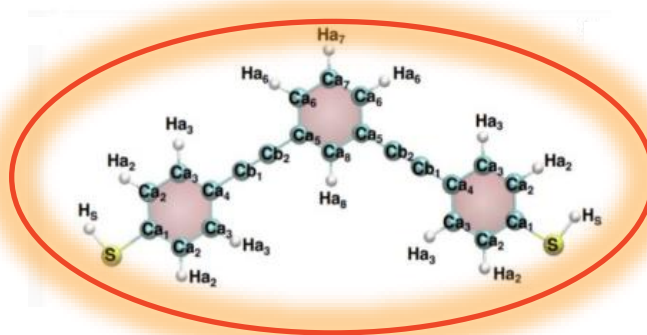
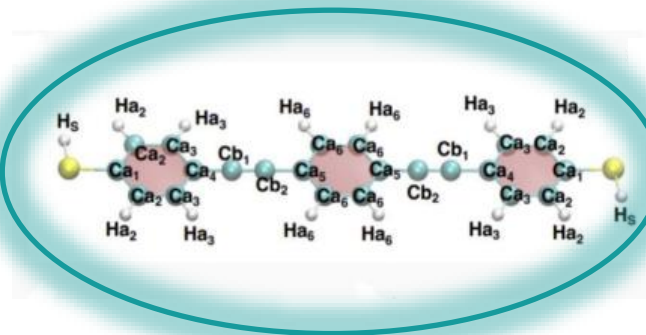
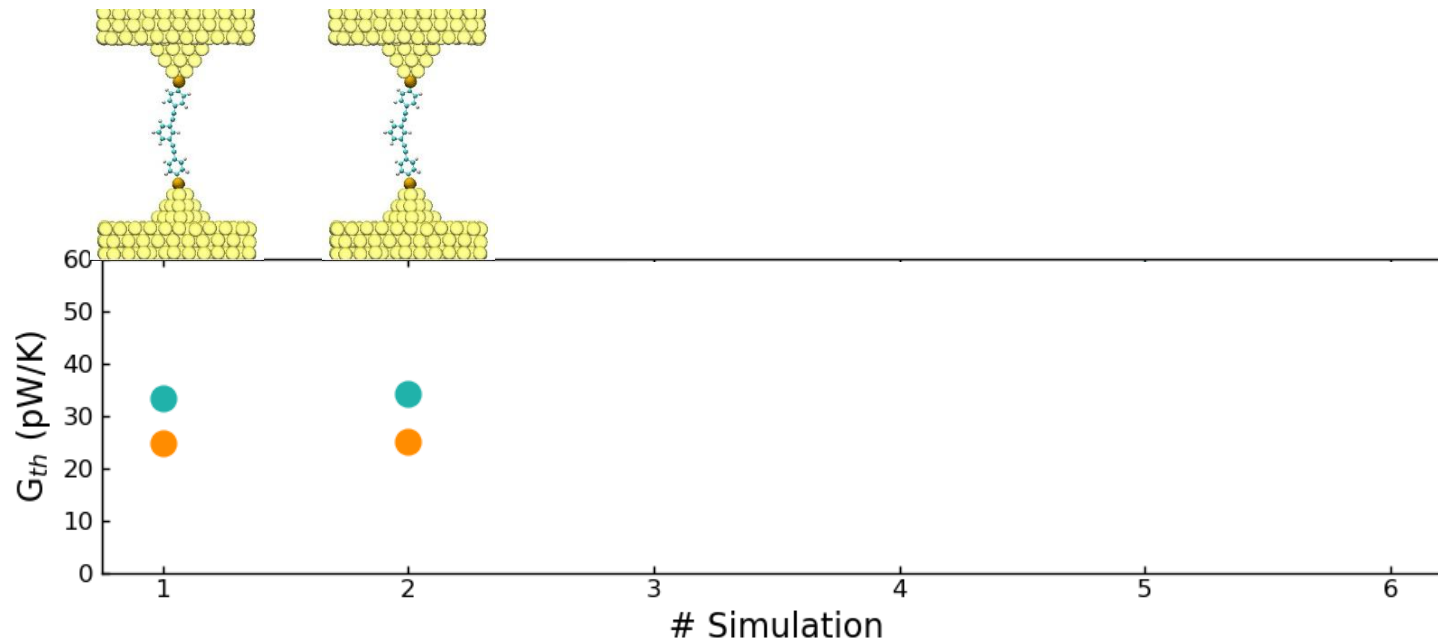
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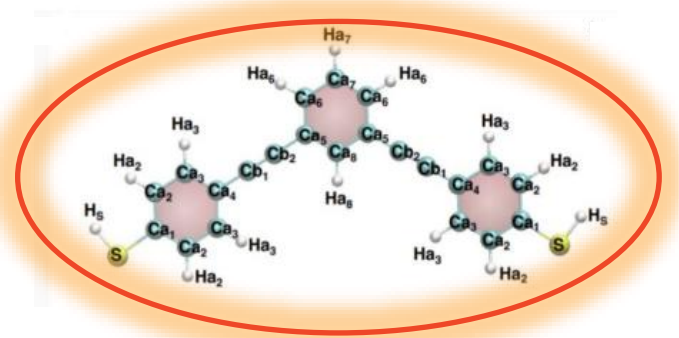
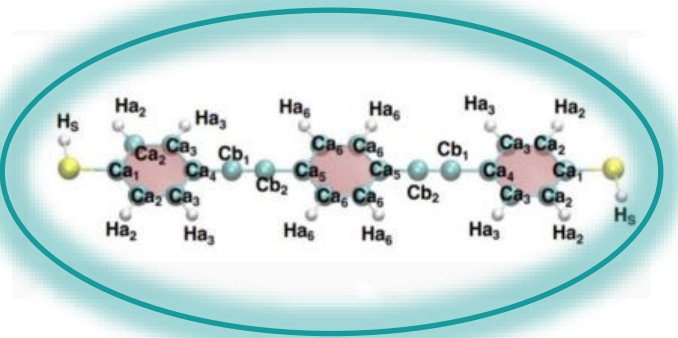
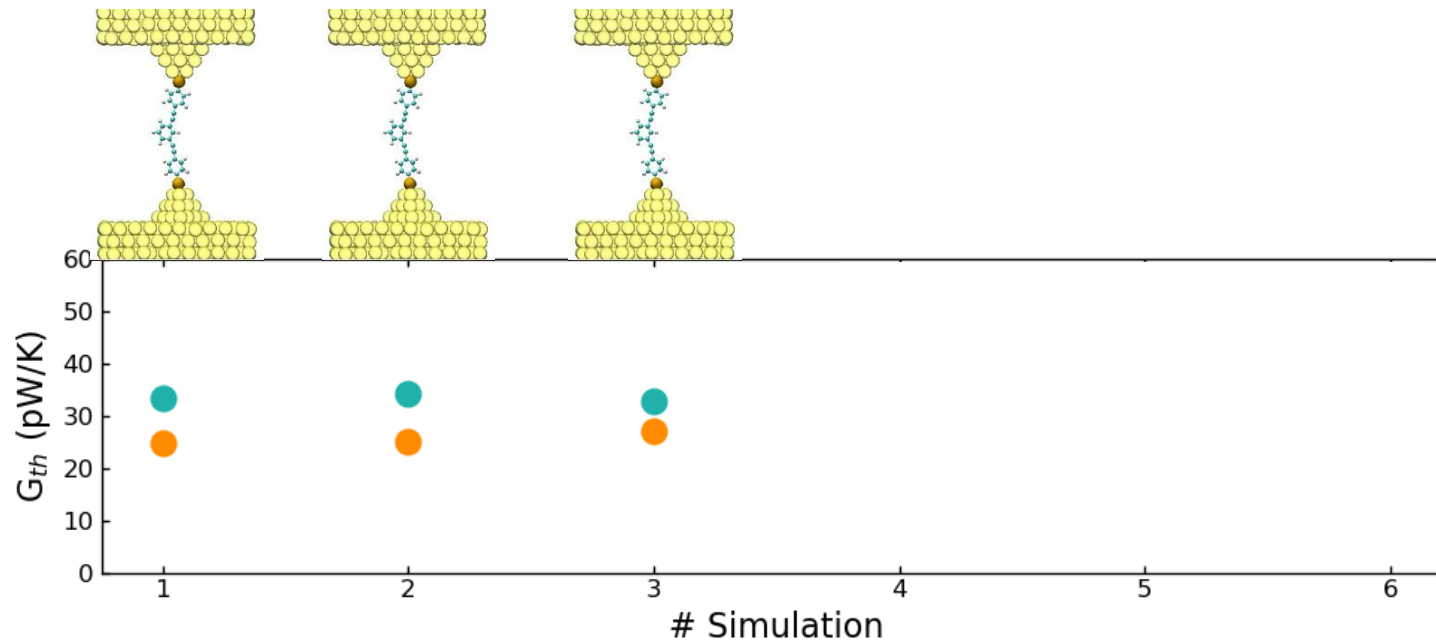
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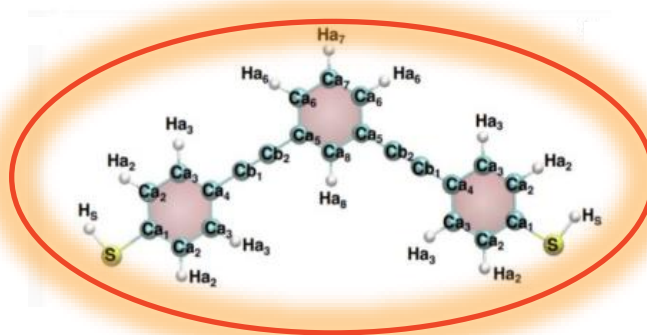
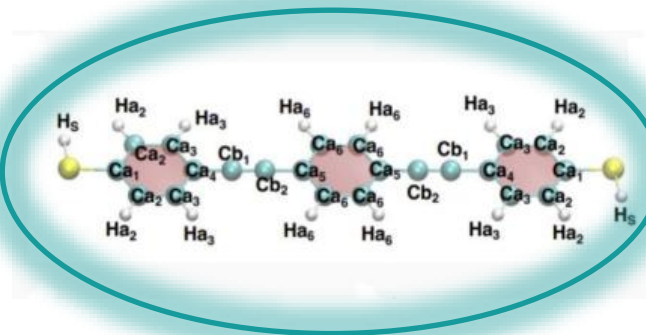
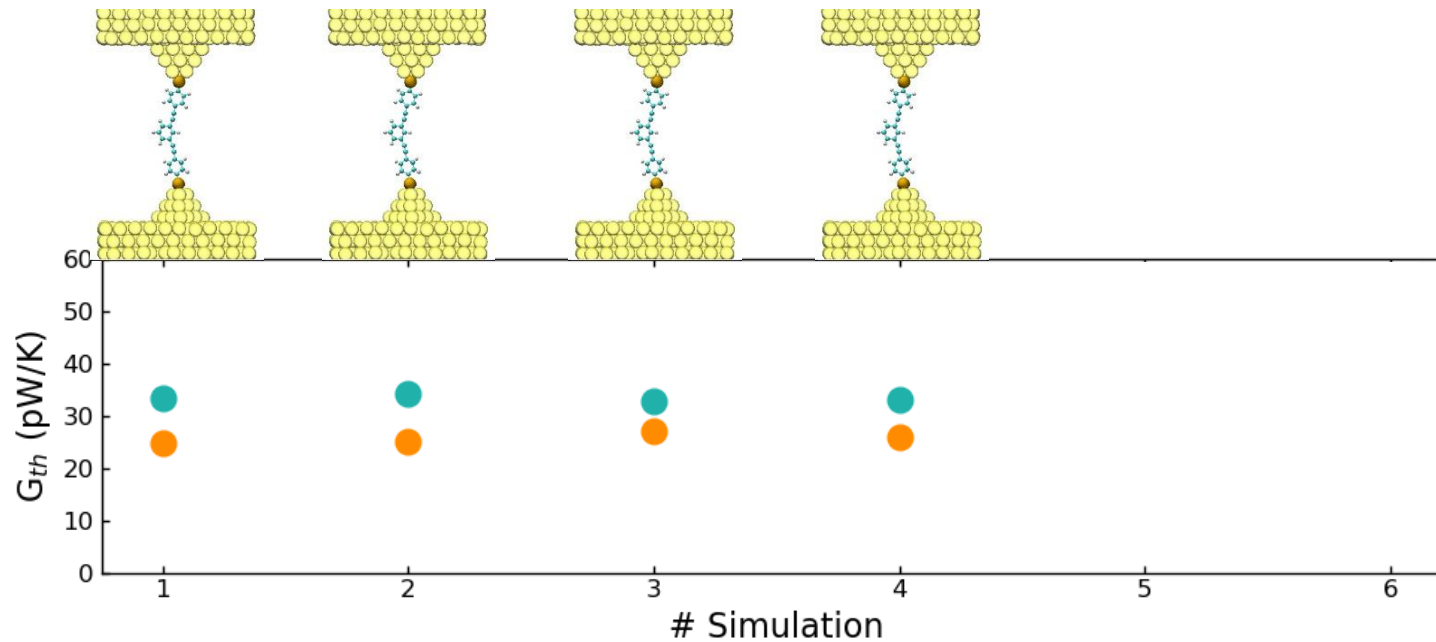
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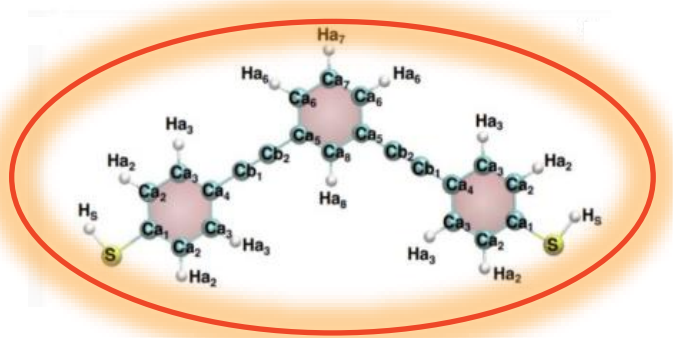
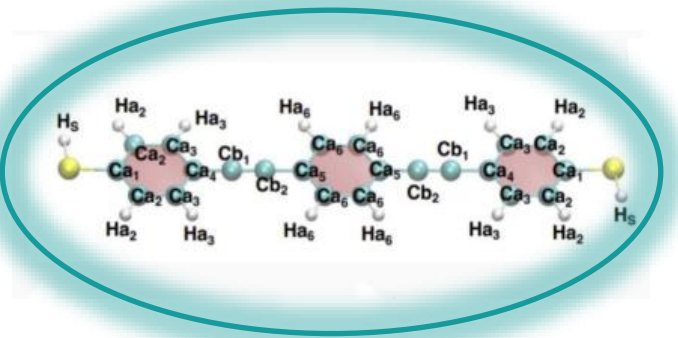
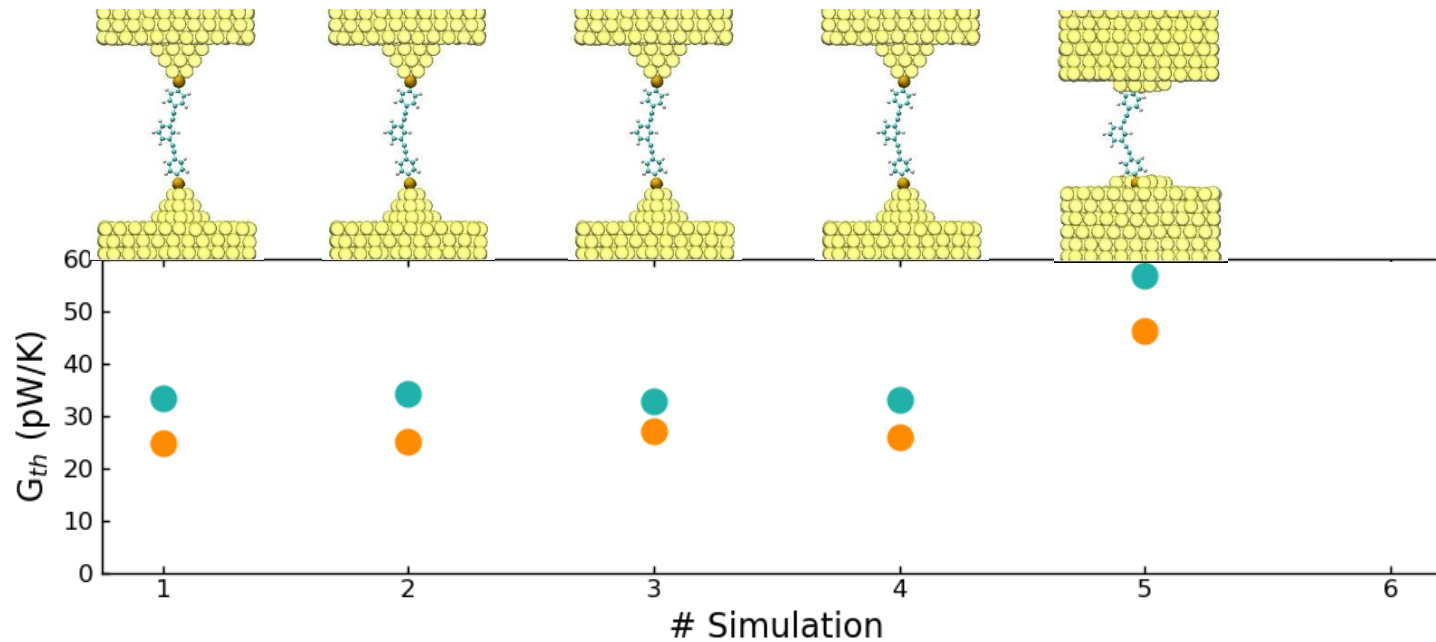
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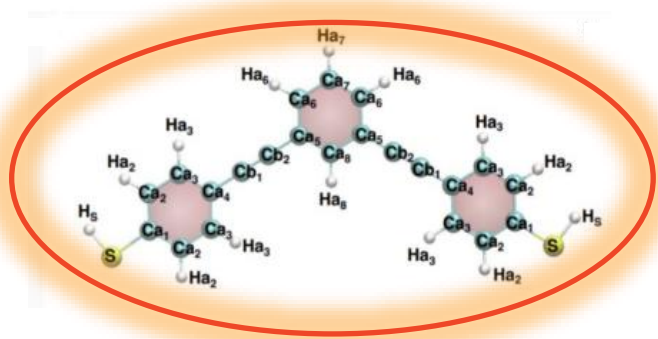
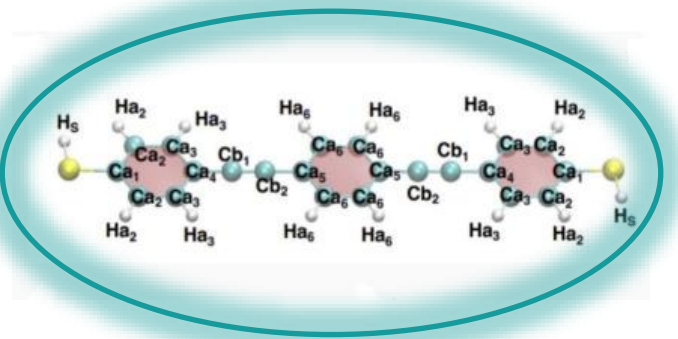
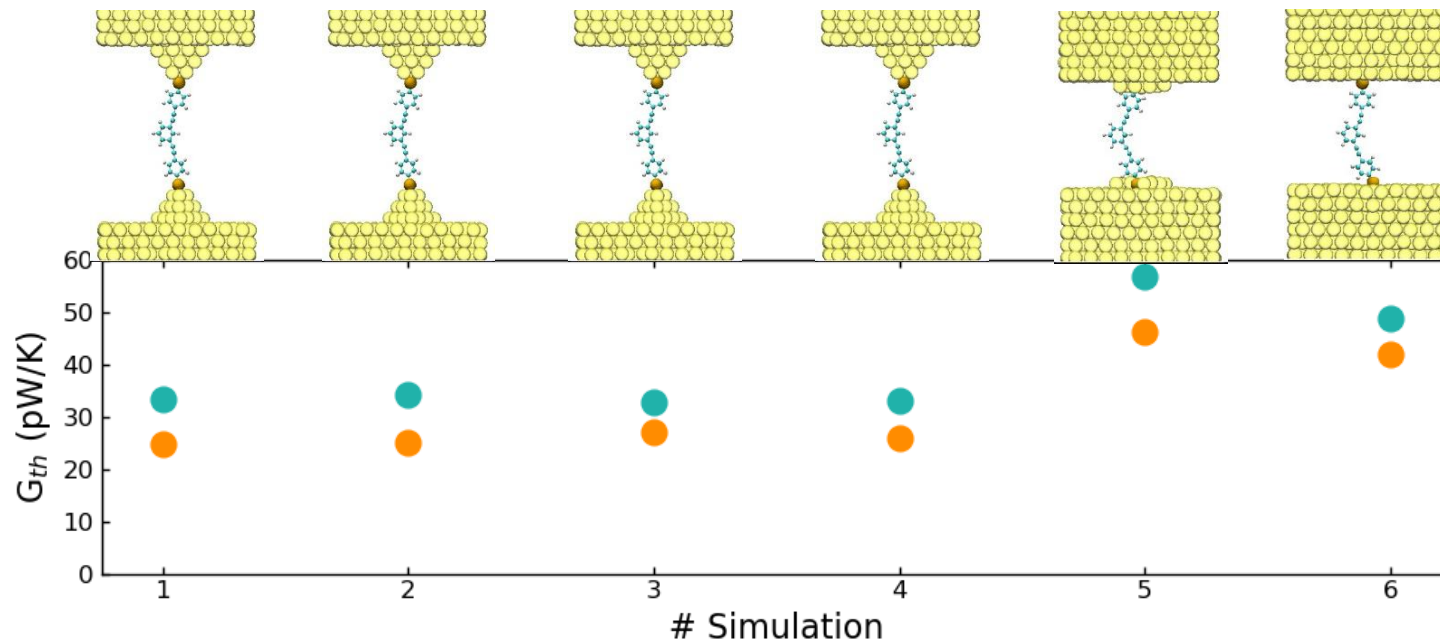
NEMD thermal conductance

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

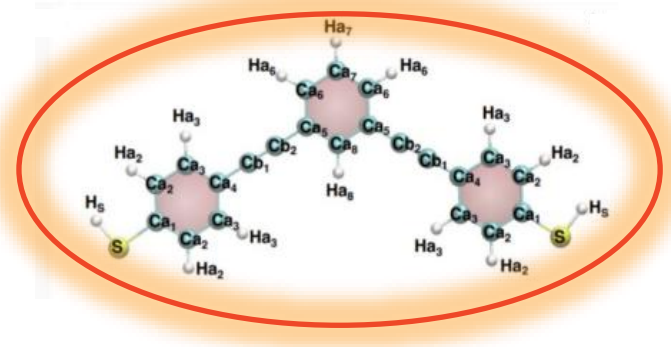
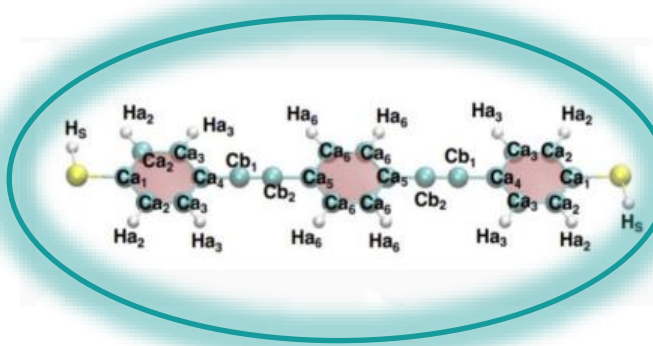


NEMD thermal conductance

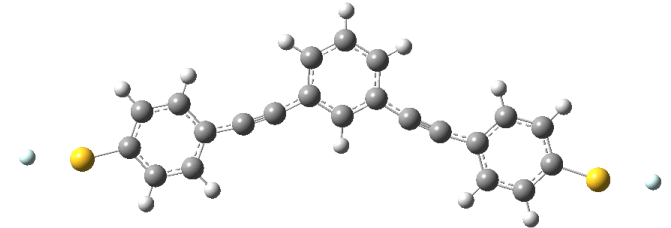
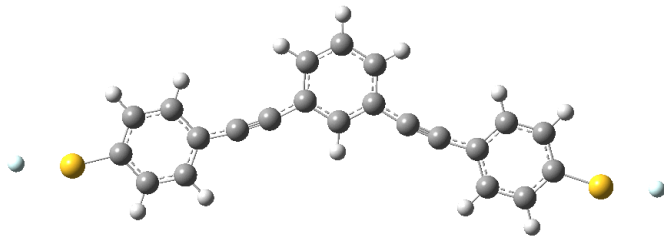
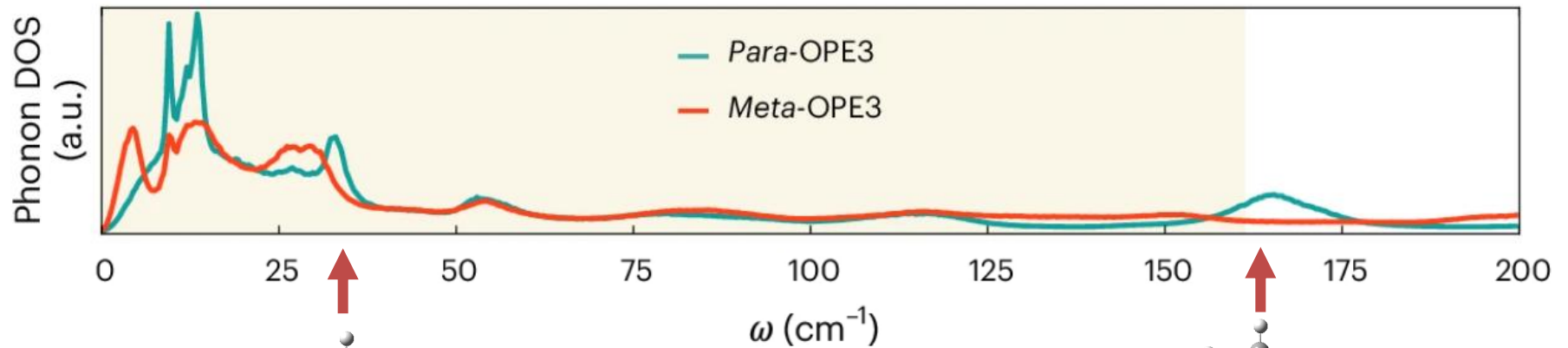
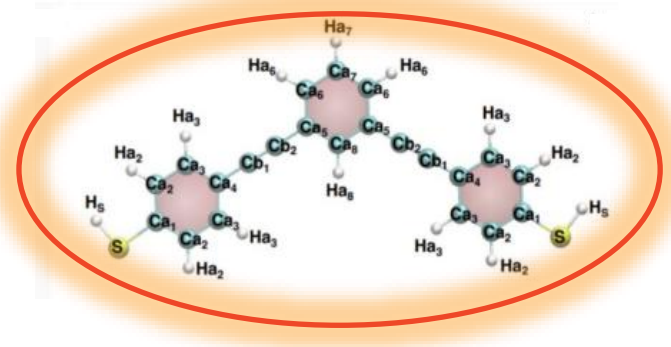
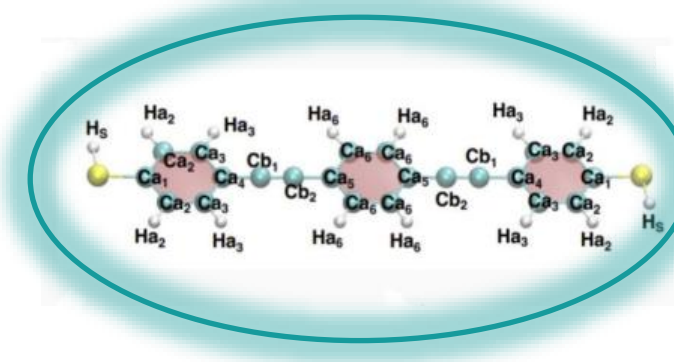
NPT → Pulling (0.35 nN) → Thermal Bias (40 K) → Production (30 ns)



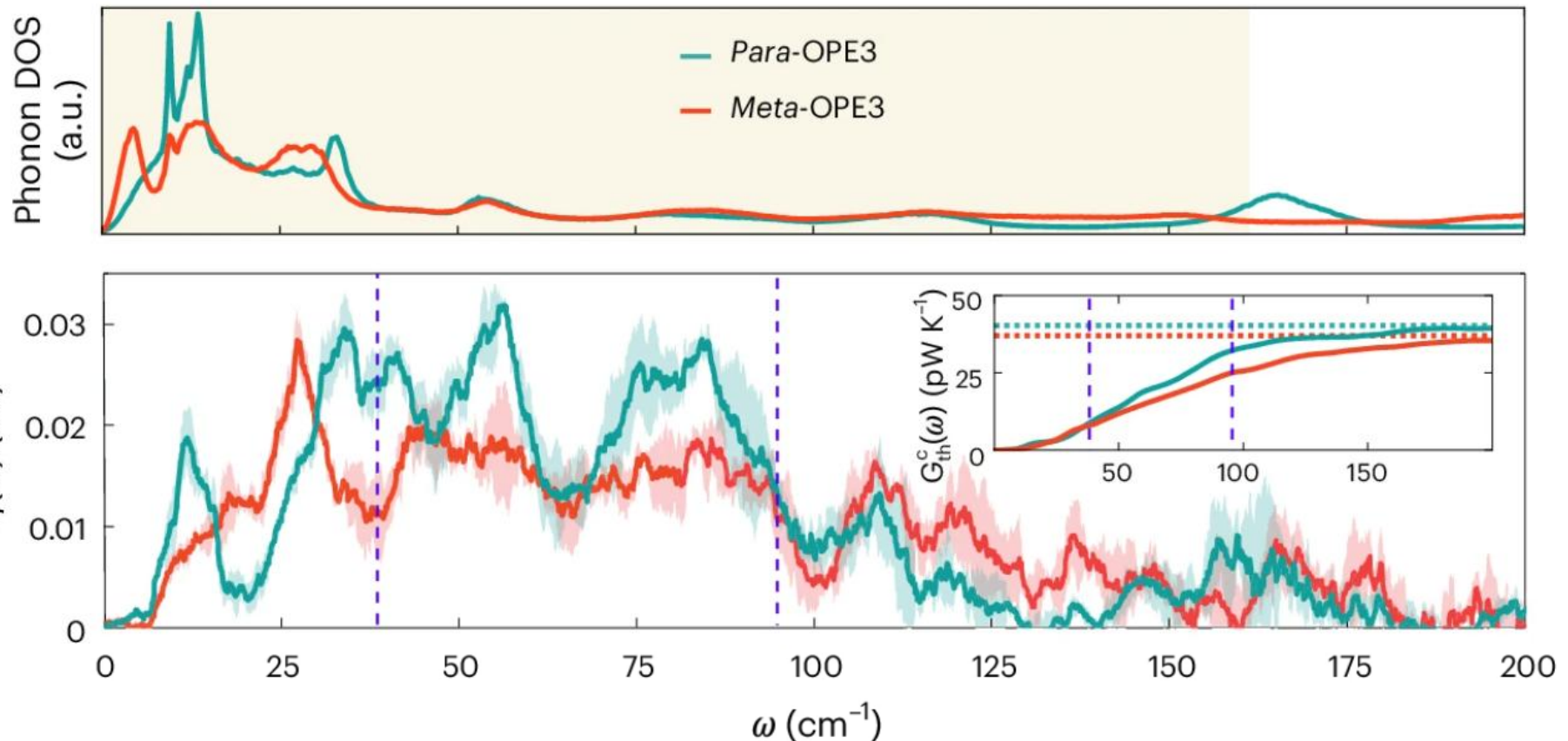
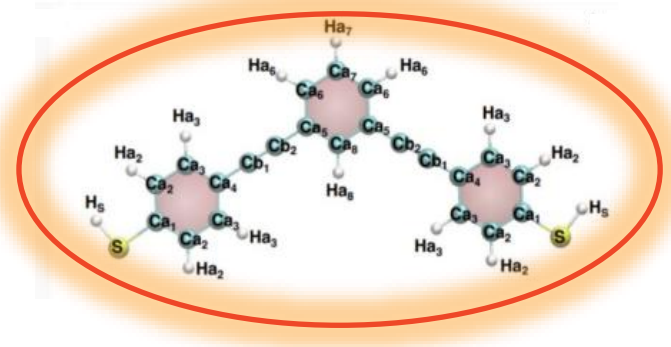
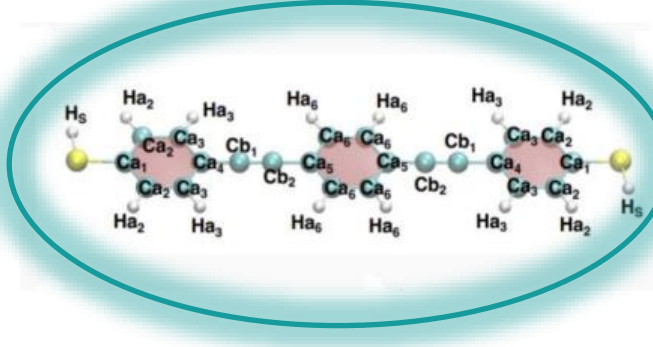
Spectral conductance and vibrational occupation



Spectral conductance and vibrational occupation

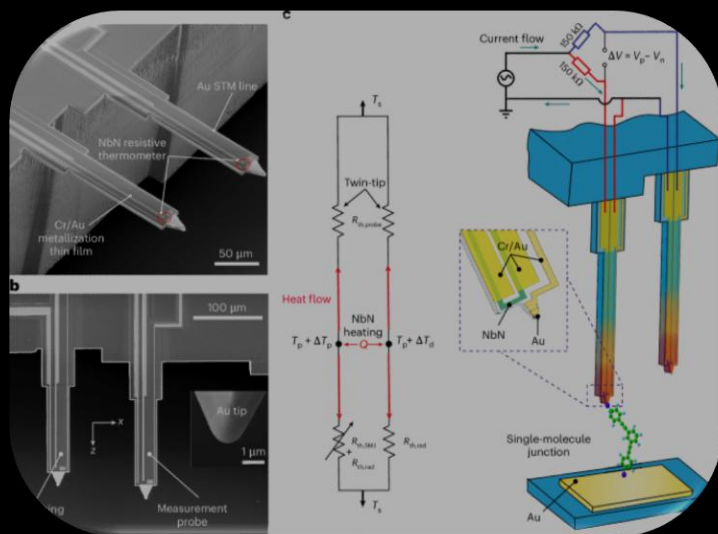


Spectral conductance and vibrational occupation

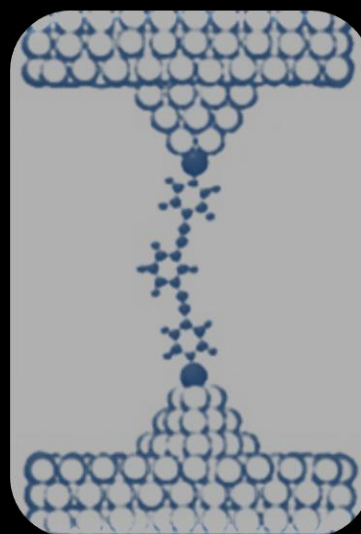


Results

Measurements



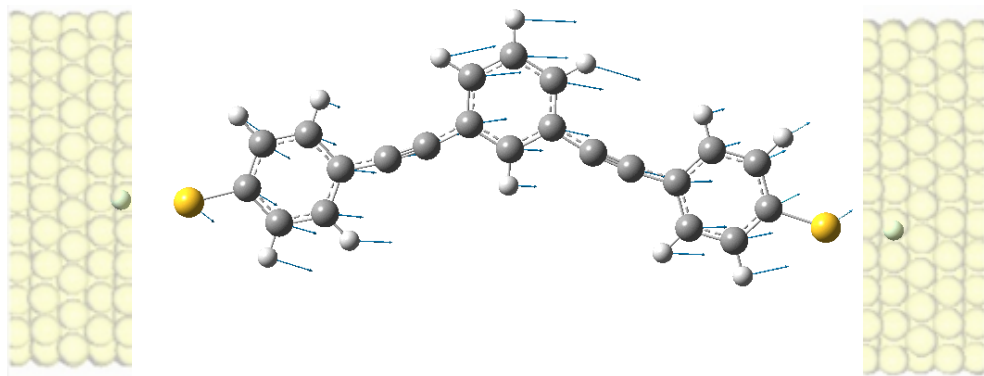
MD simulation



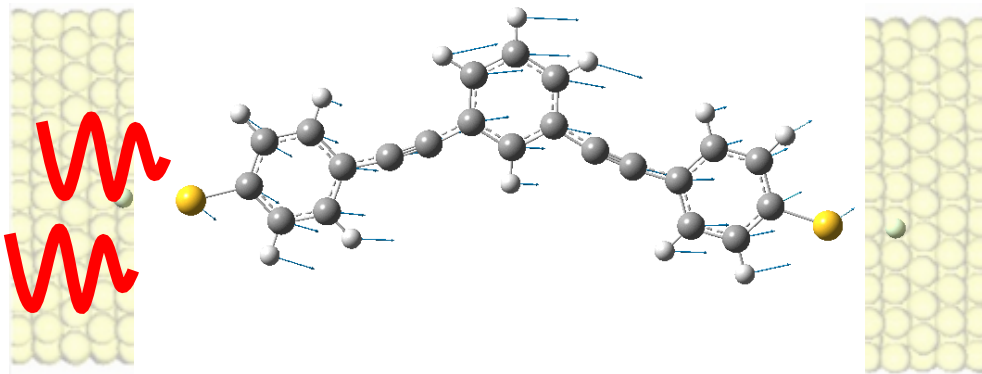
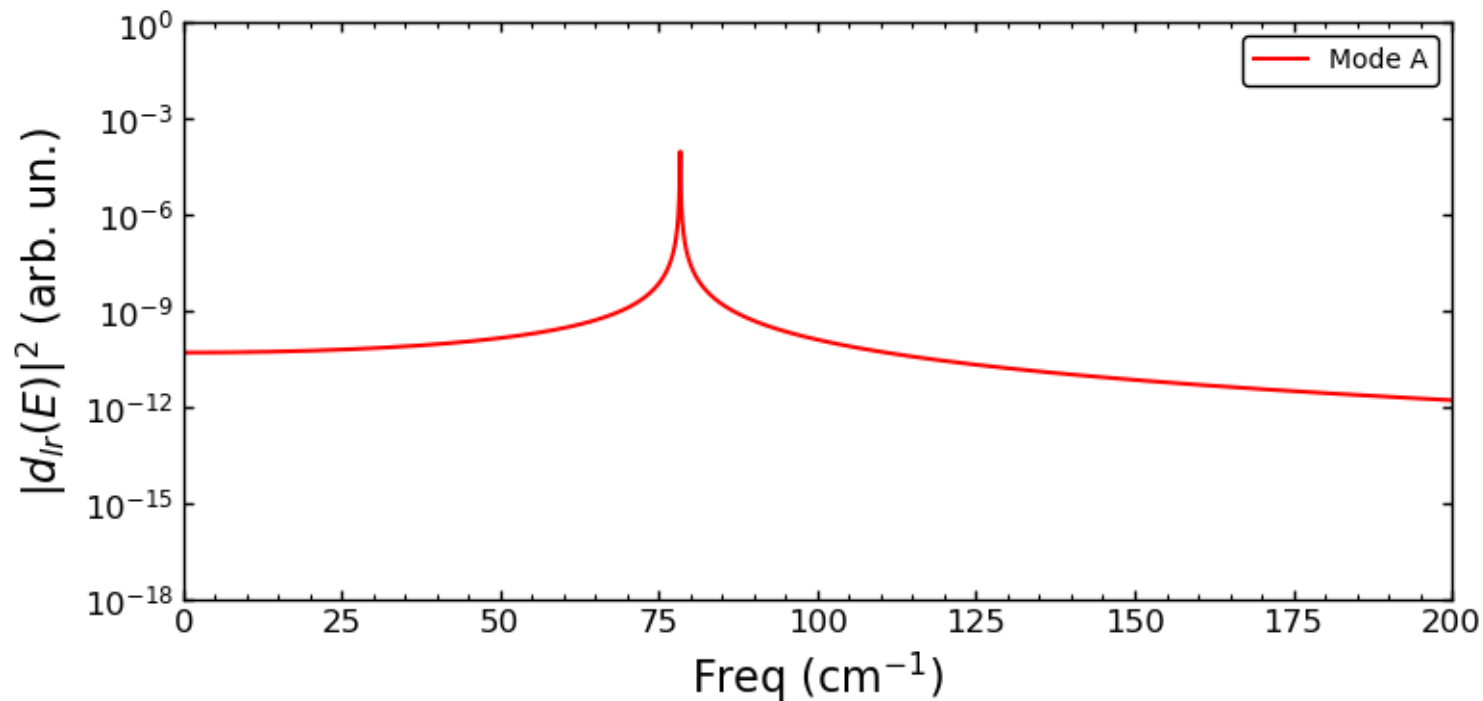
Interference



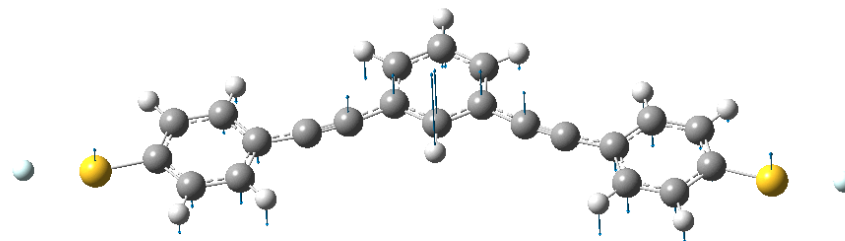
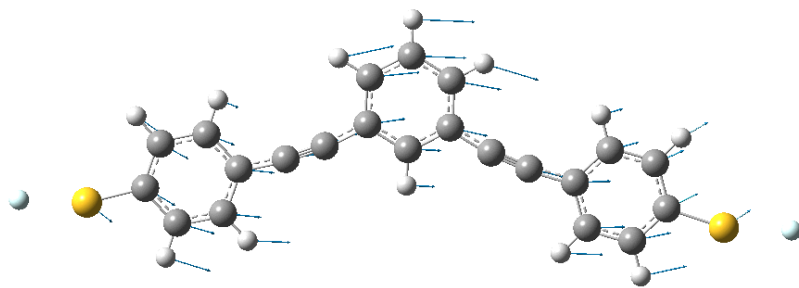
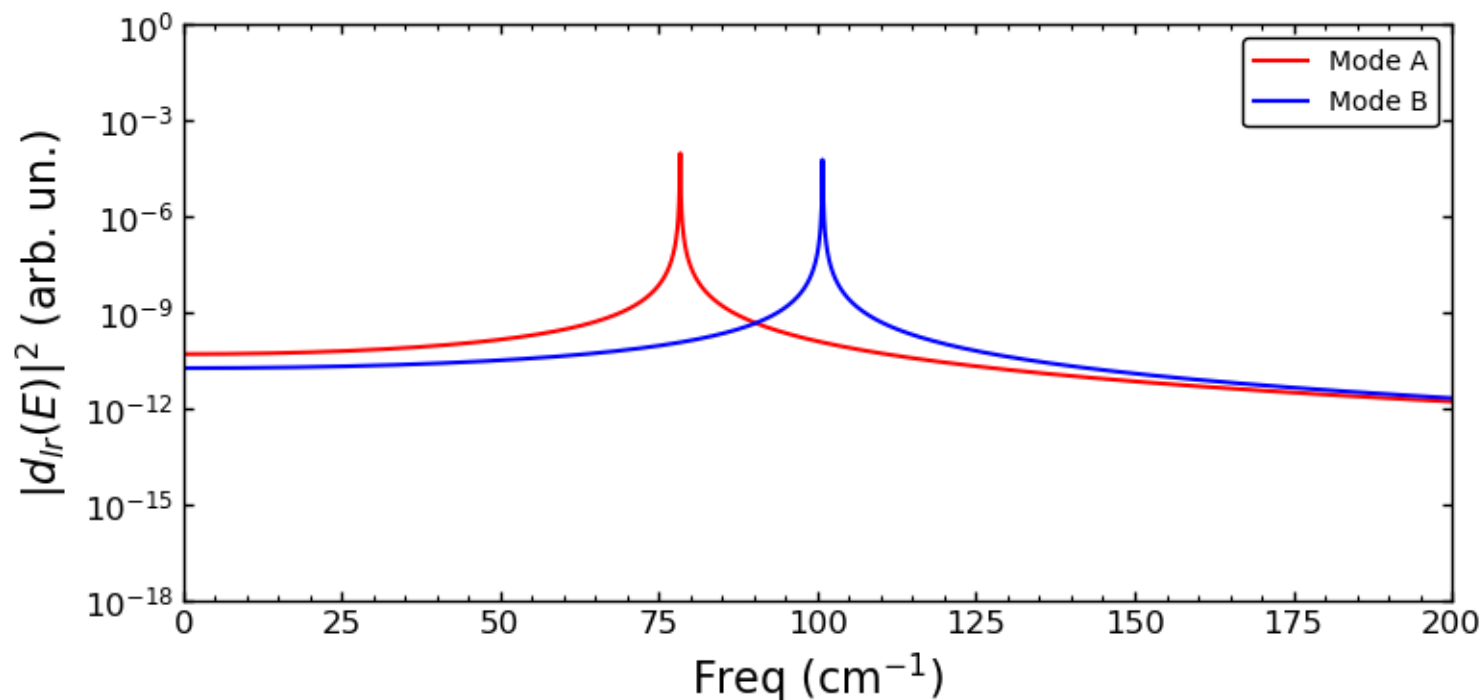
Vibrational interference: two-mode antiresonance



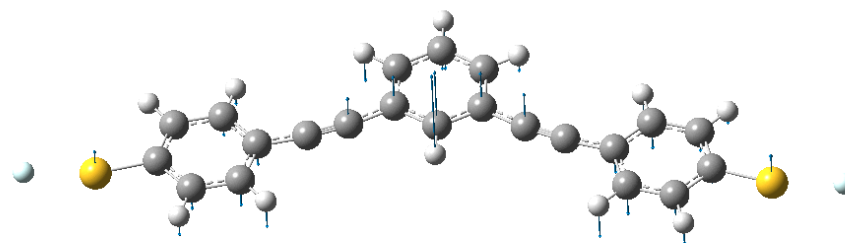
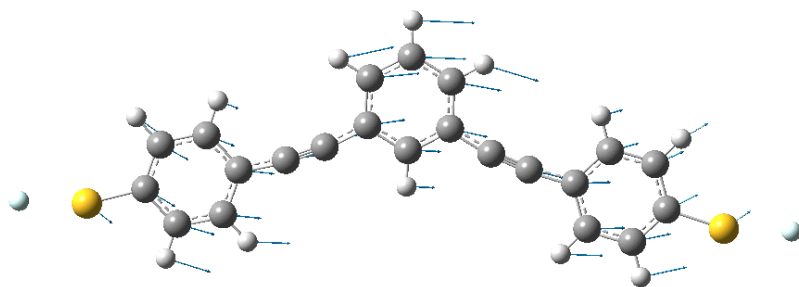
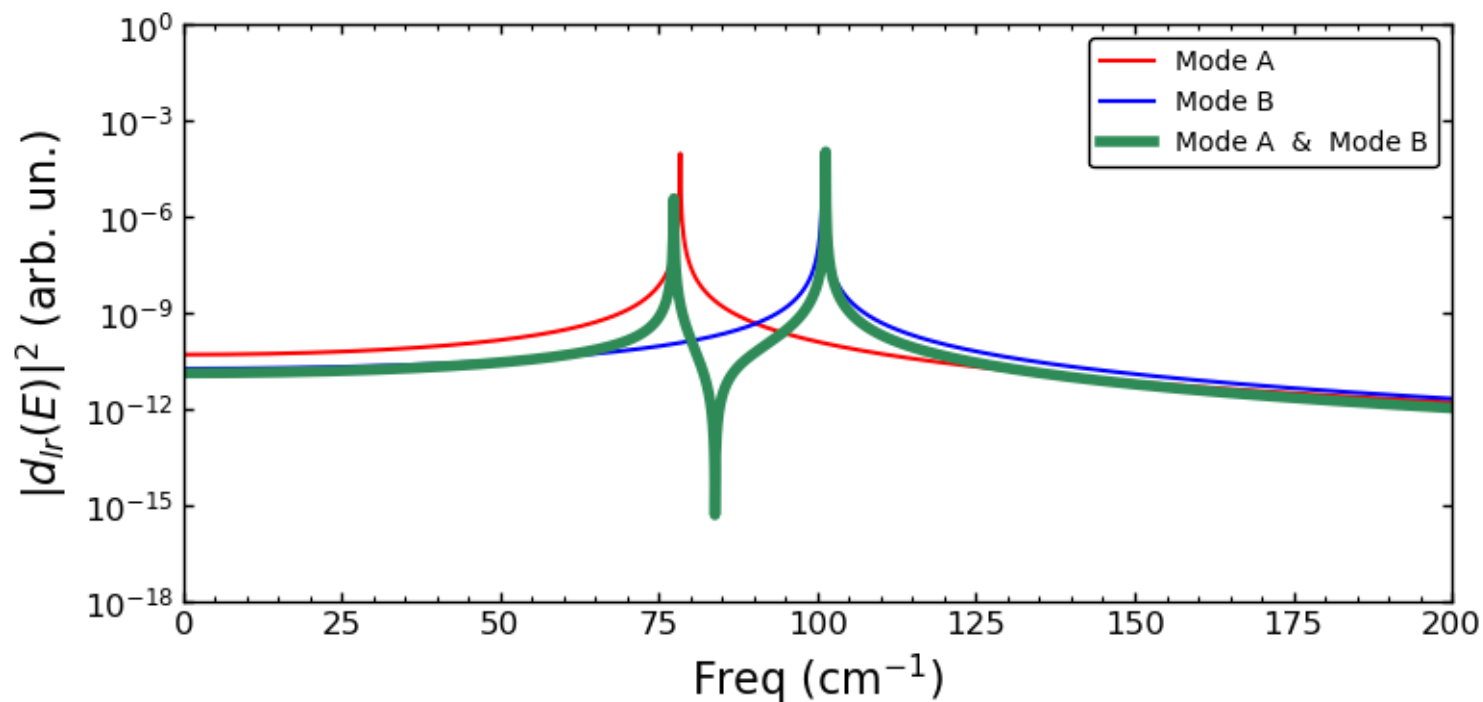
Vibrational interference: two-mode antiresonance



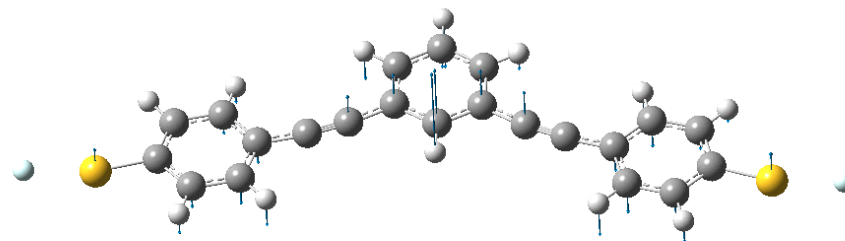
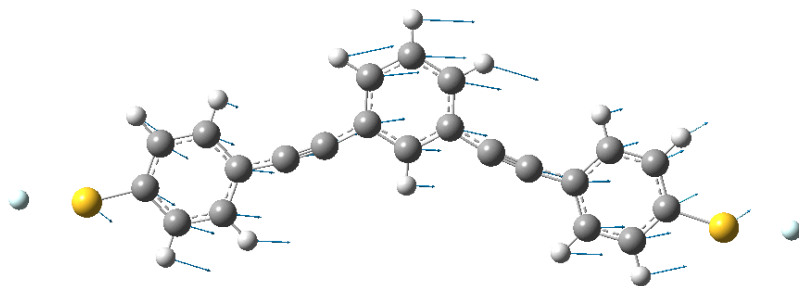
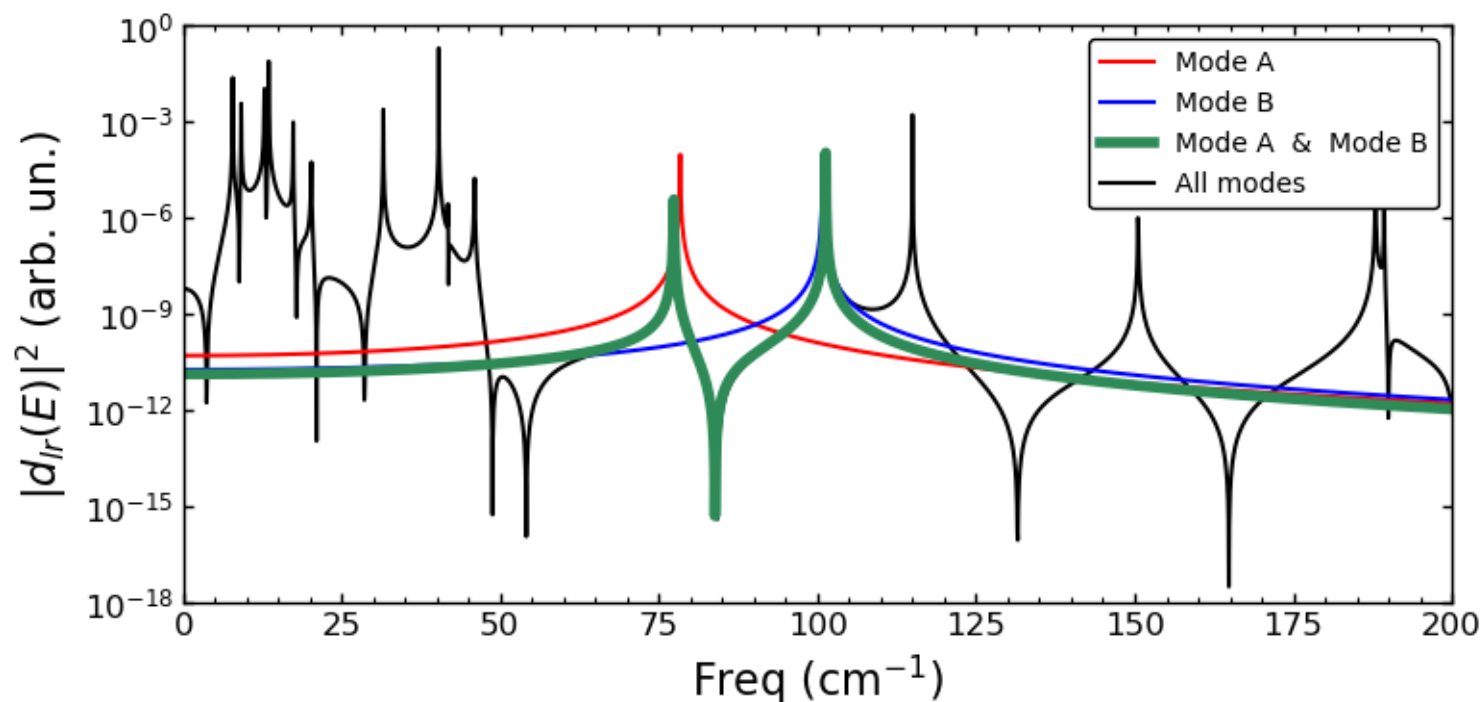
Vibrational interference: two-mode antiresonance



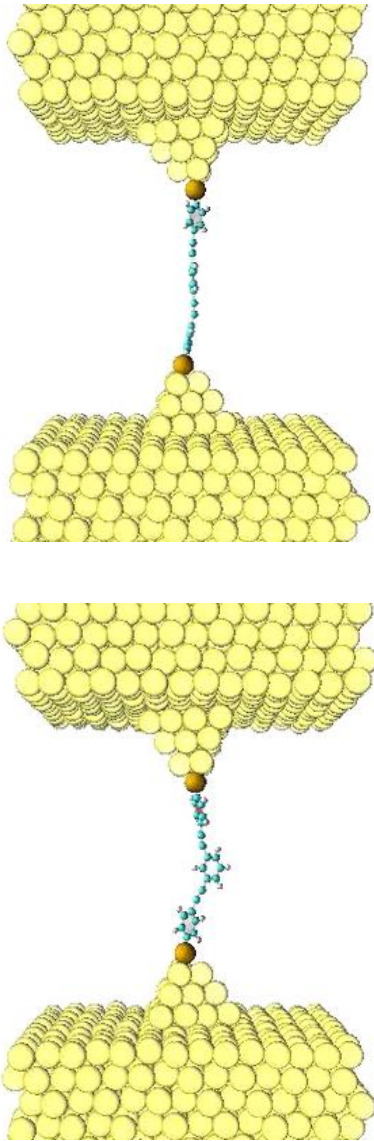
Vibrational interference: two-mode antiresonance



Vibrational interference: two-mode antiresonance



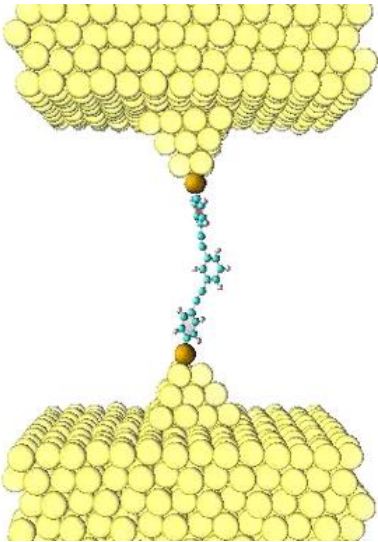
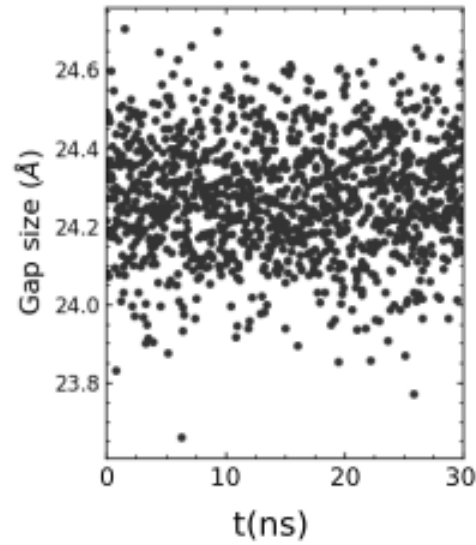
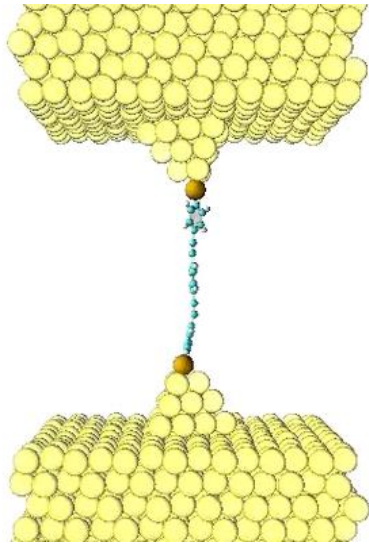
Vibrational interference: accounting for temperature



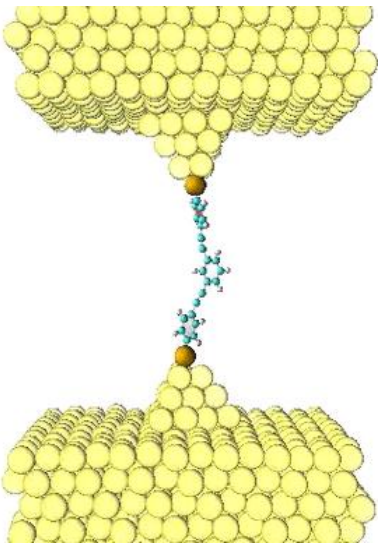
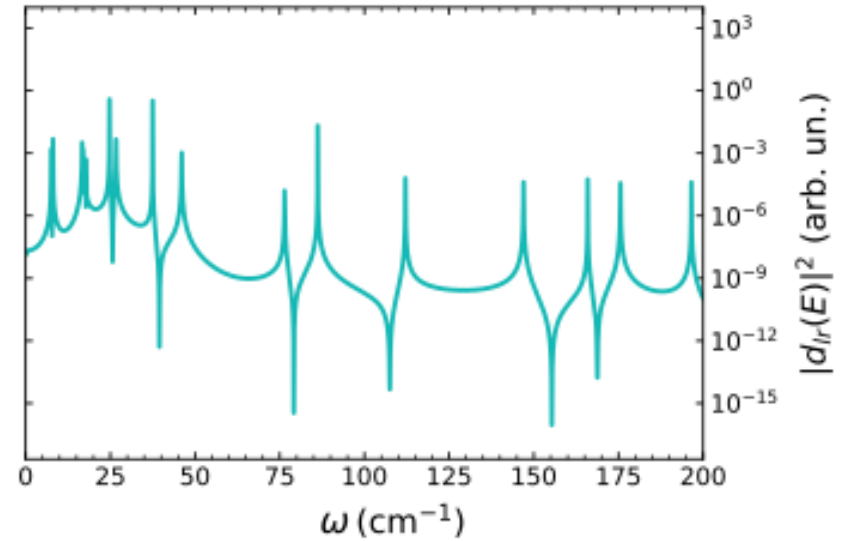
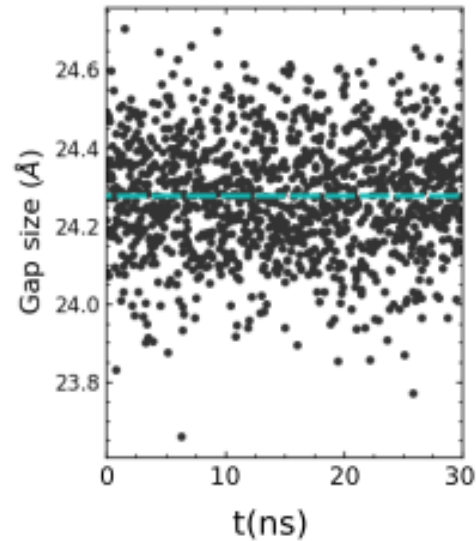
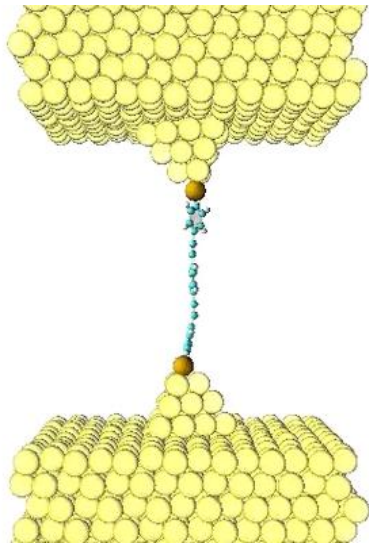
Vibrational interference: accounting for temperature



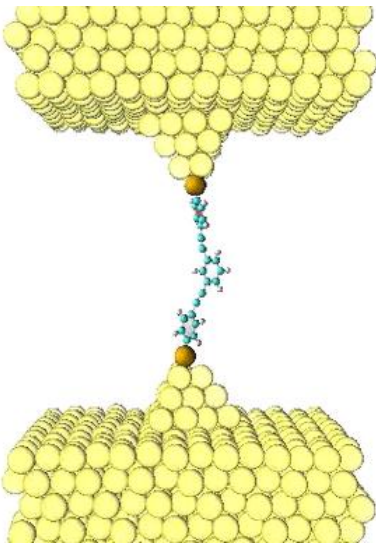
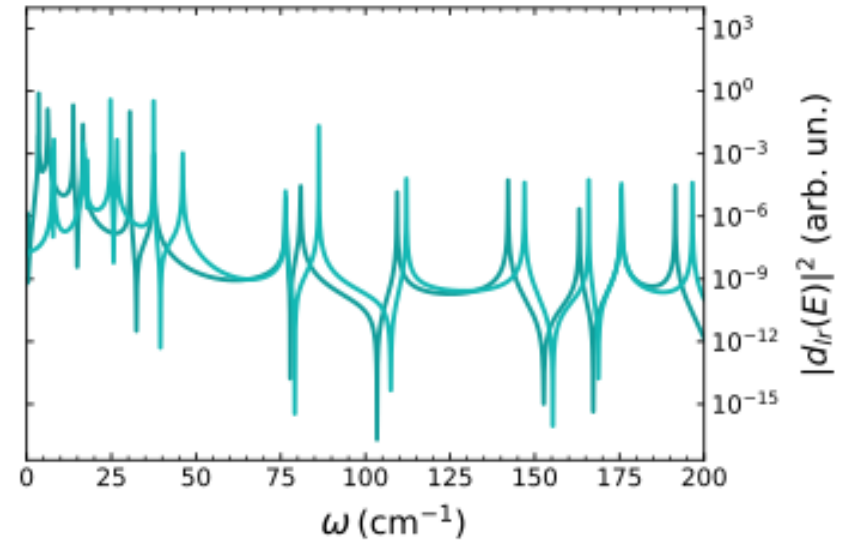
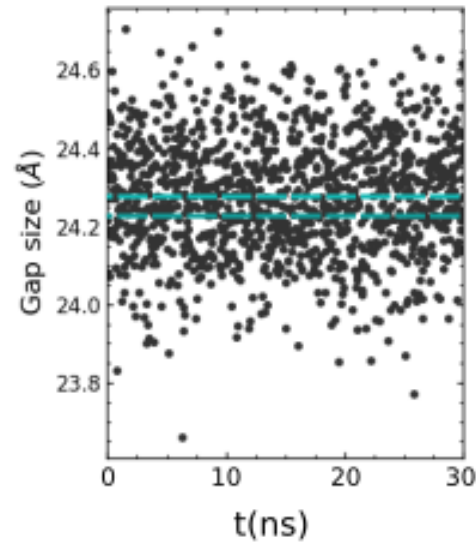
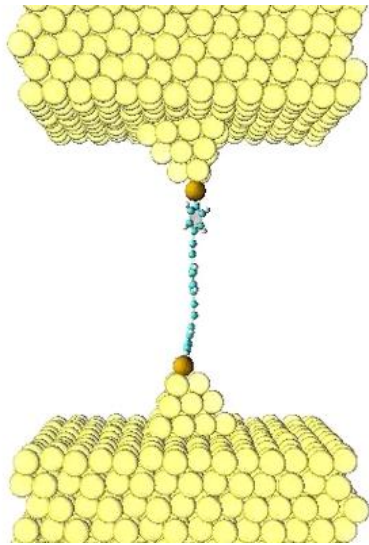
J. Cerezo



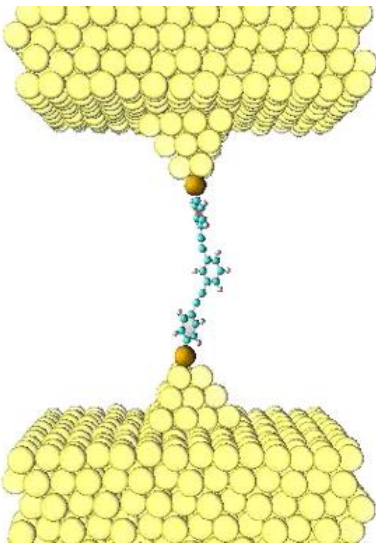
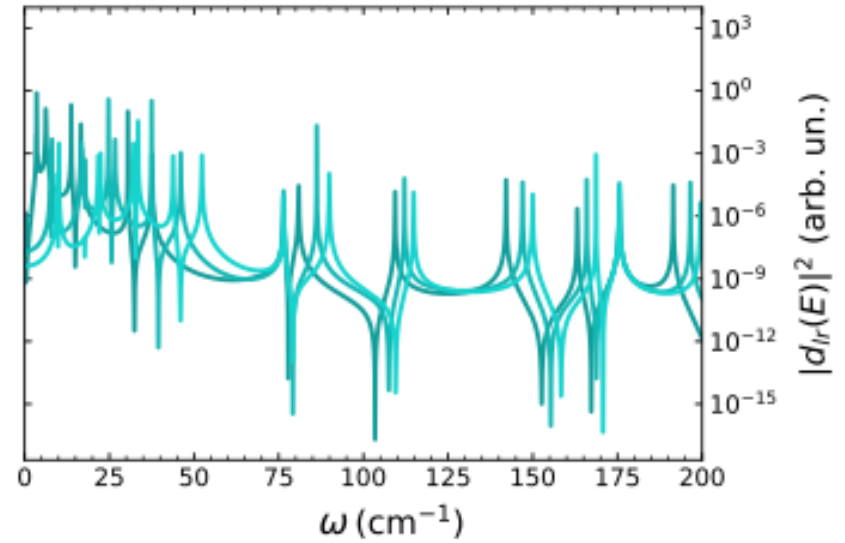
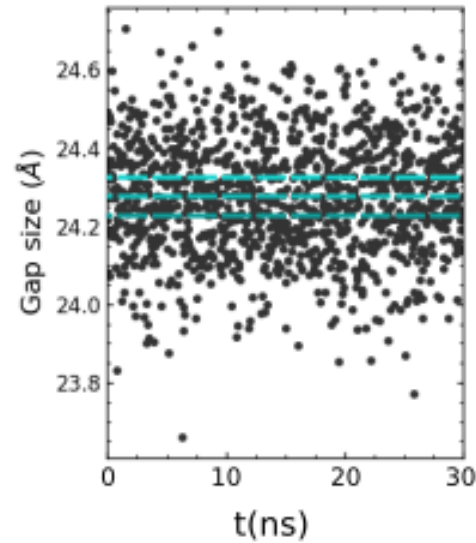
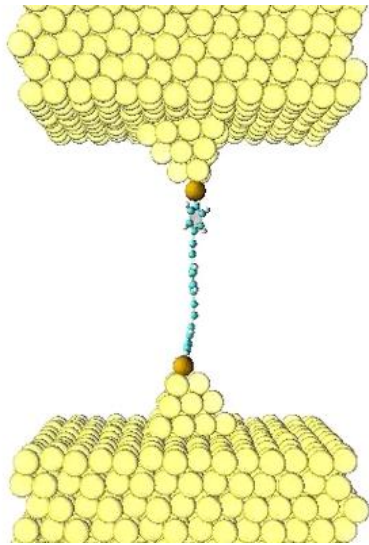
Vibrational interference: accounting for temperature



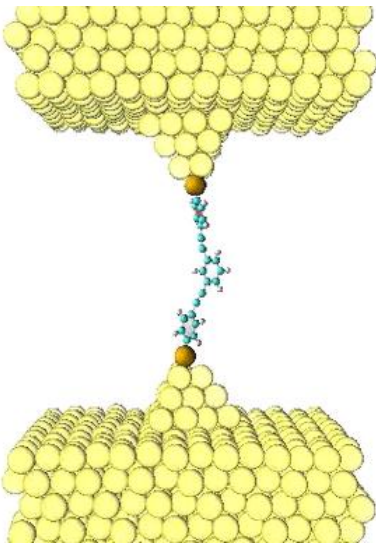
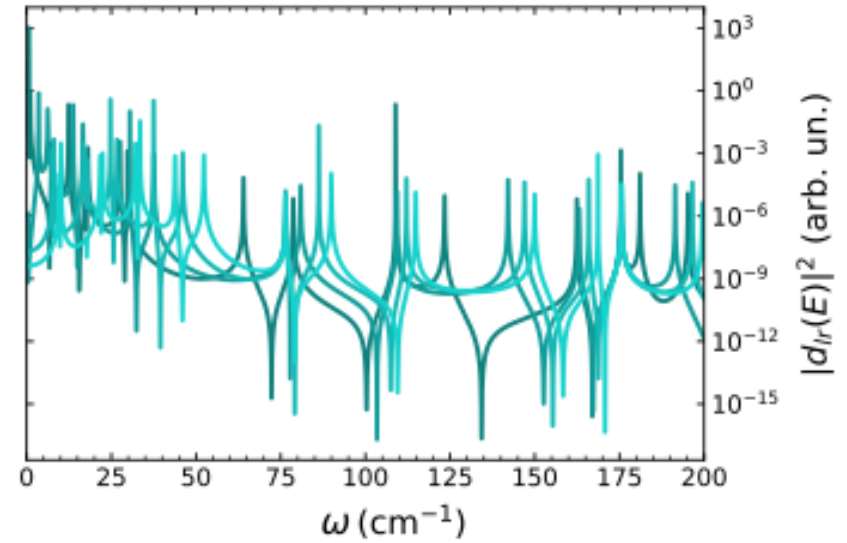
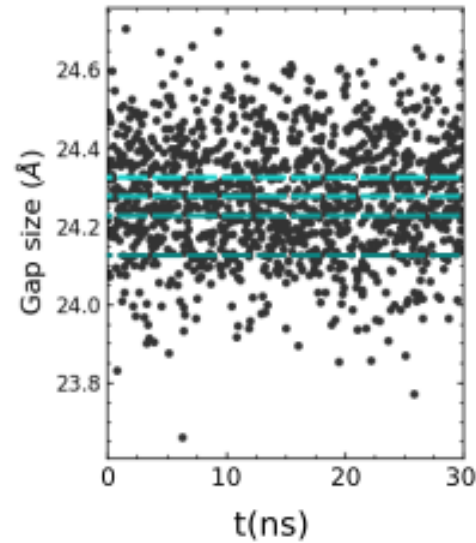
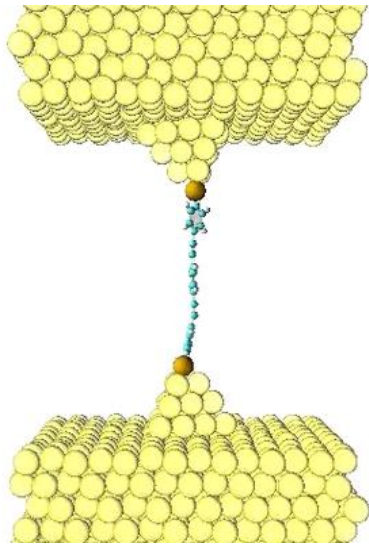
Vibrational interference: accounting for temperature



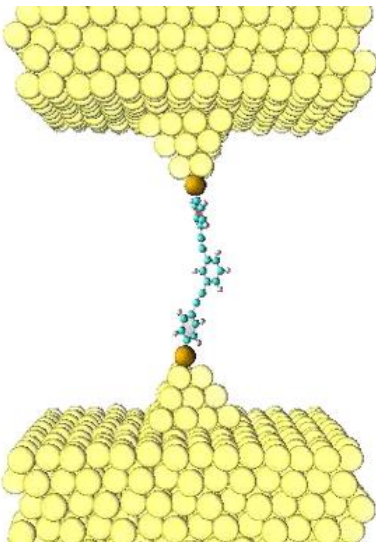
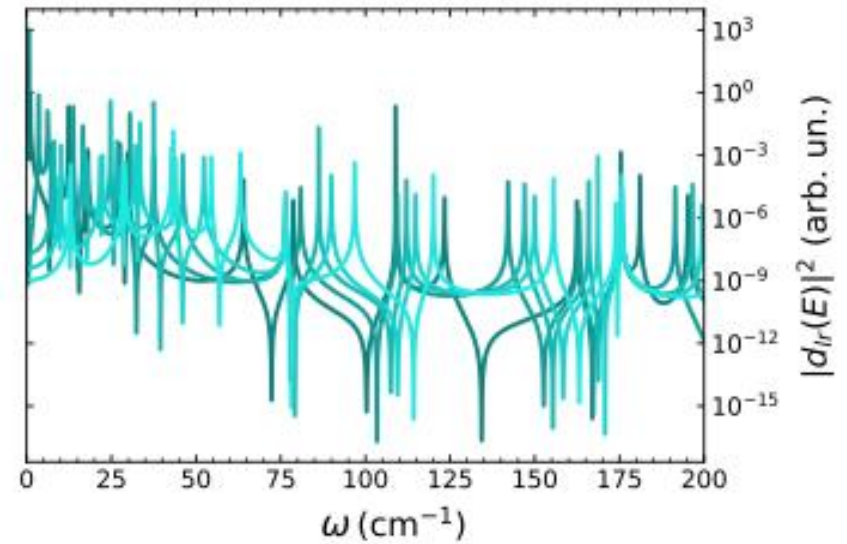
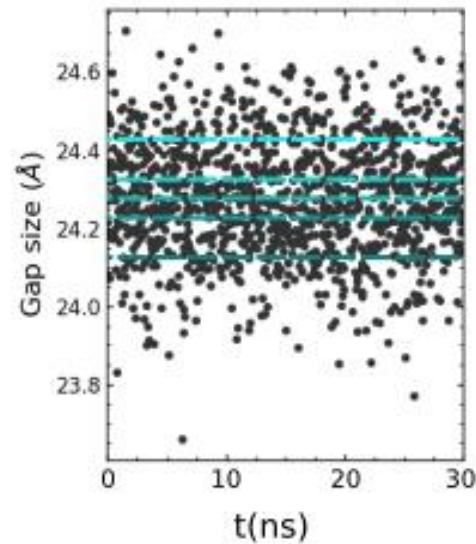
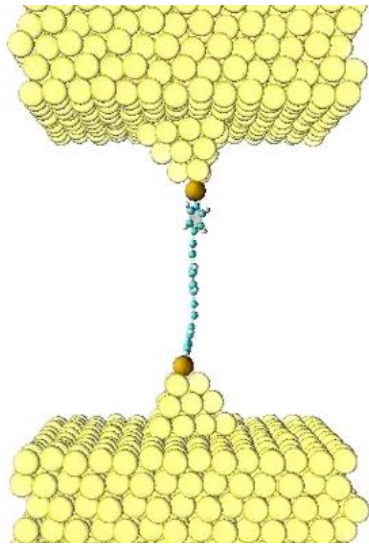
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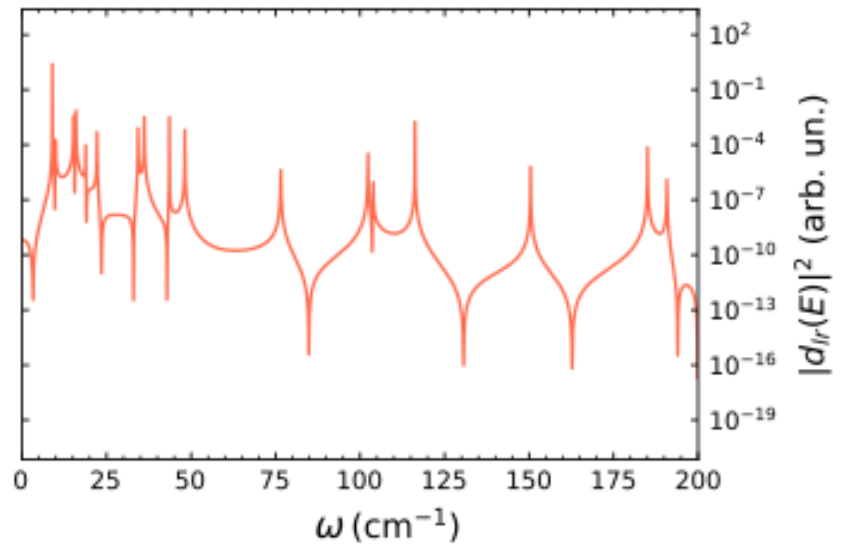
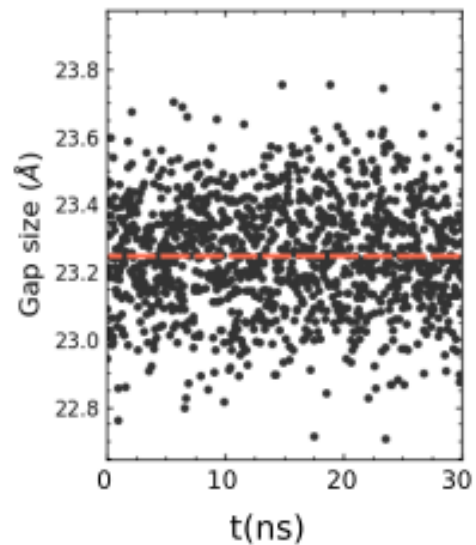
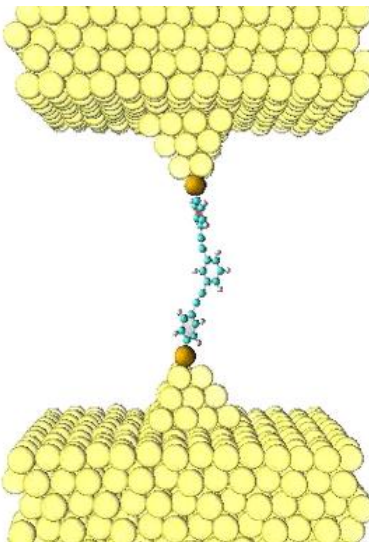
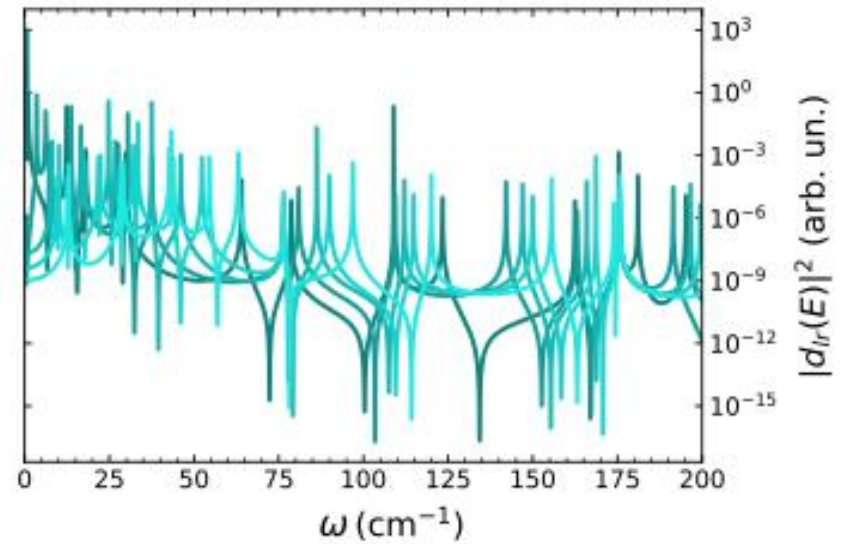
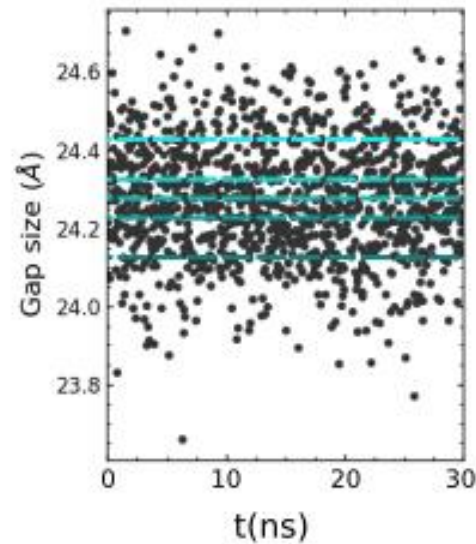
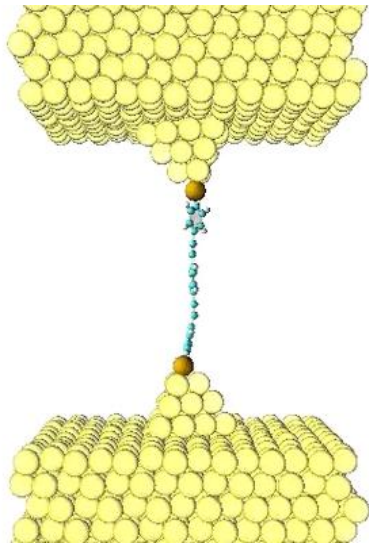
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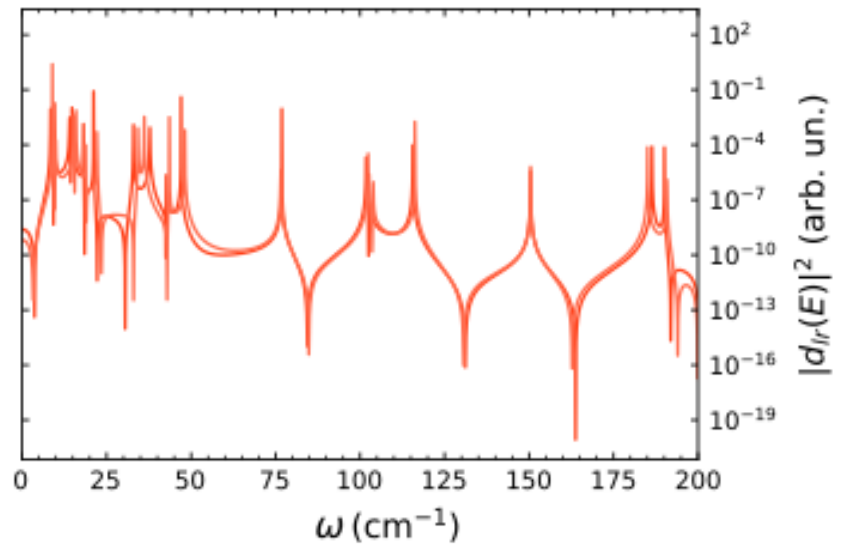
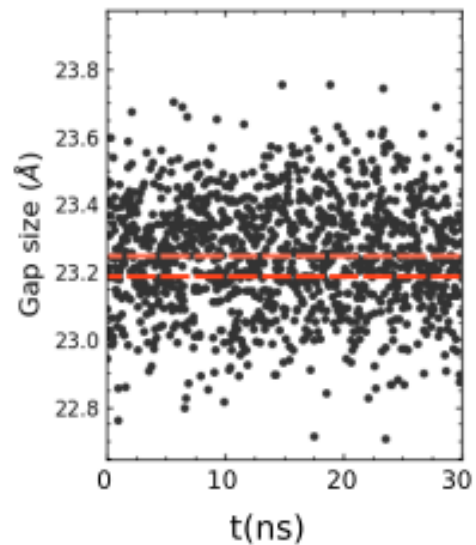
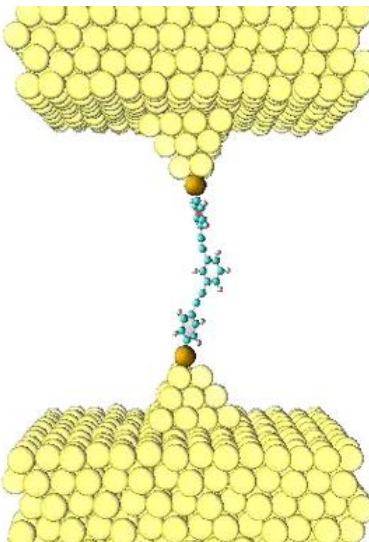
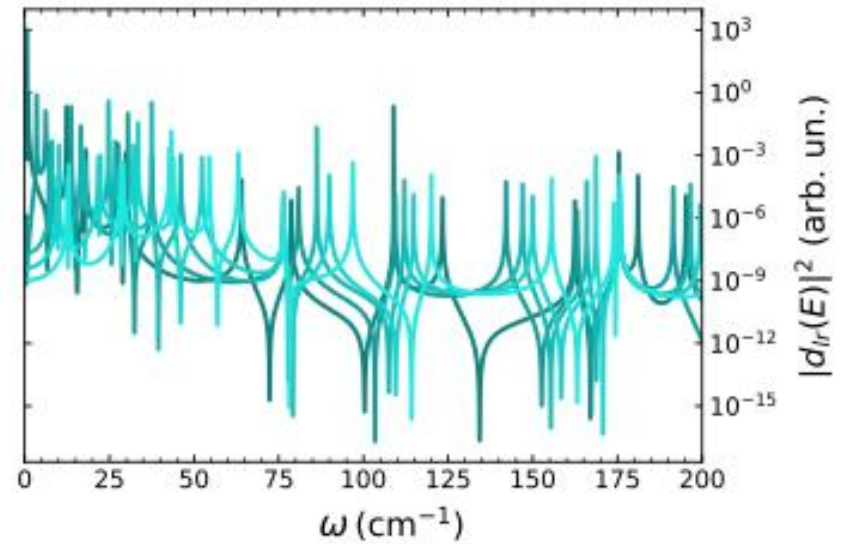
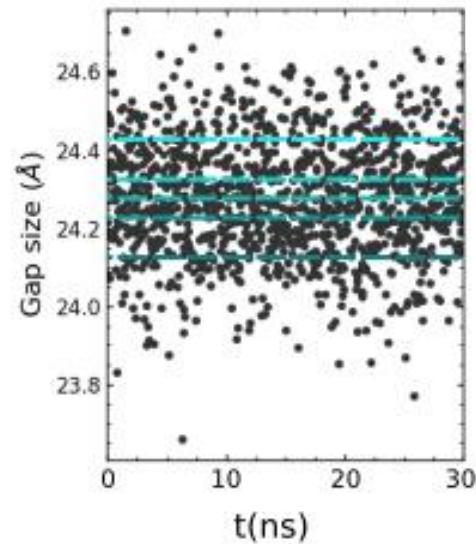
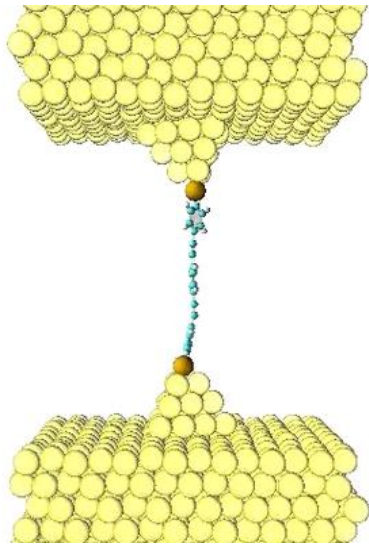
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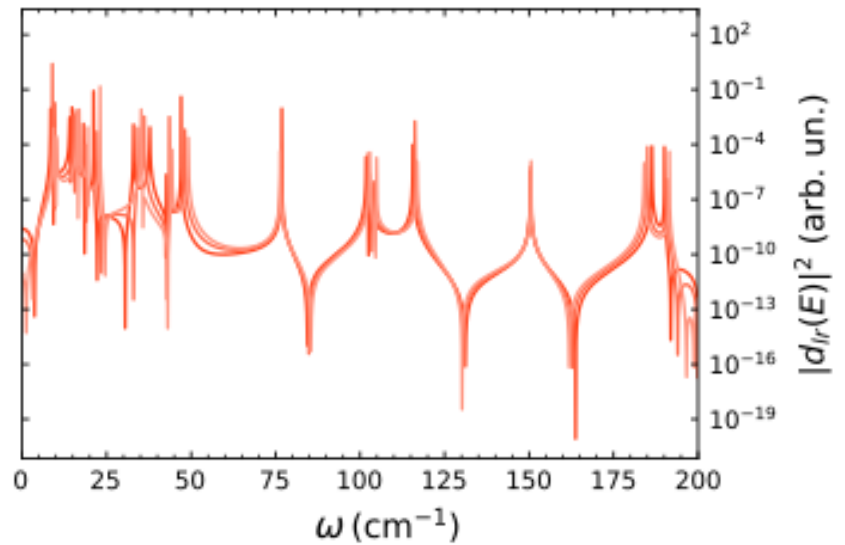
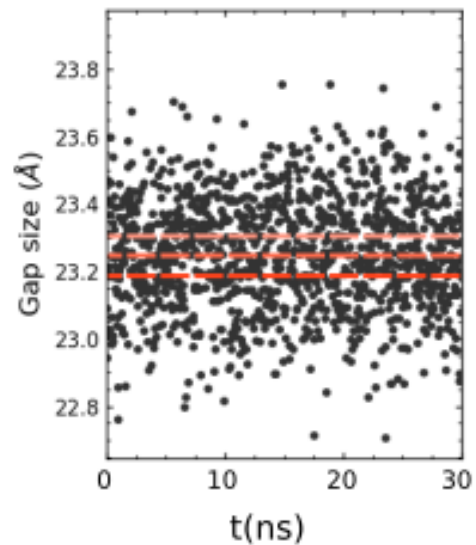
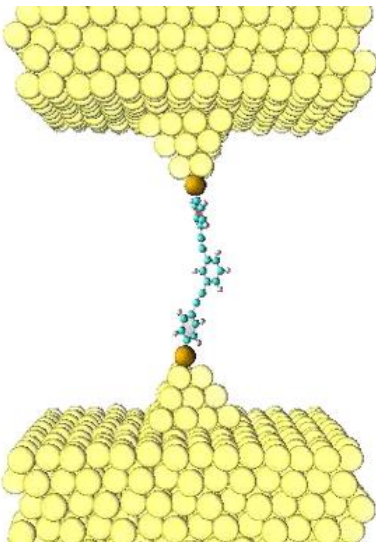
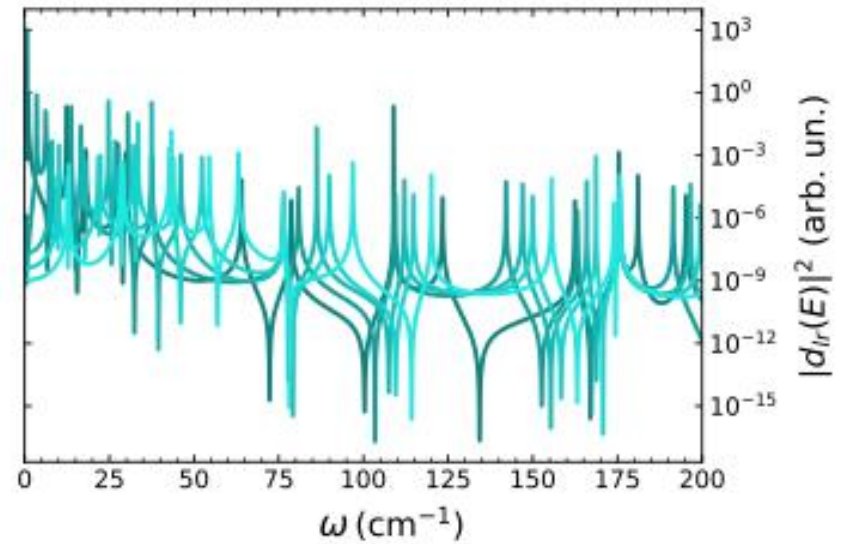
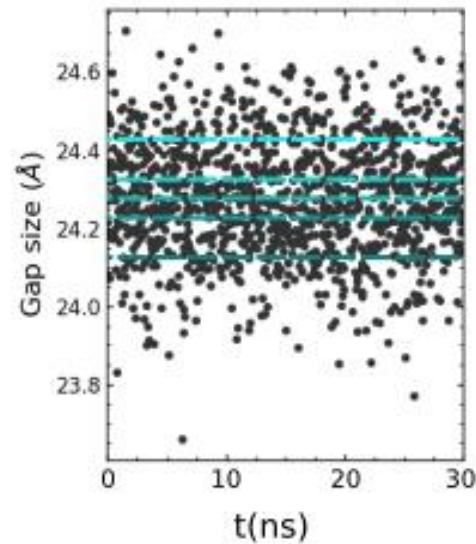
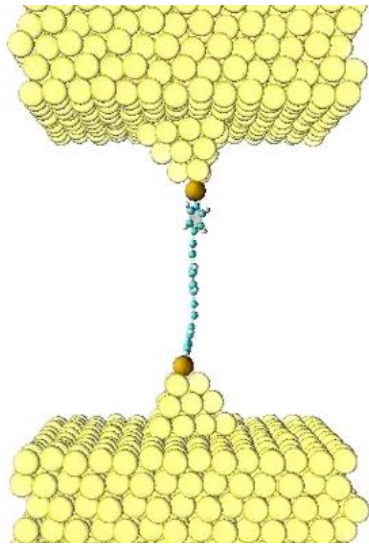
Vibrational interference: accounting for temperature



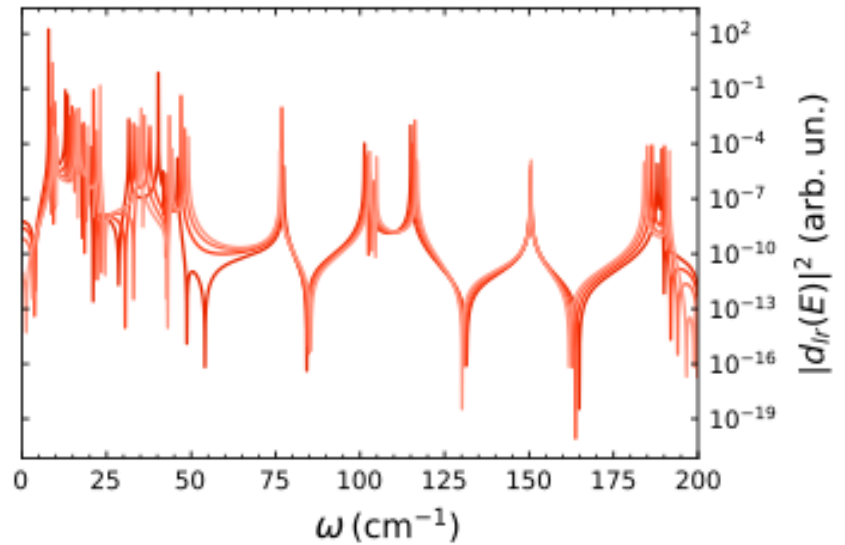
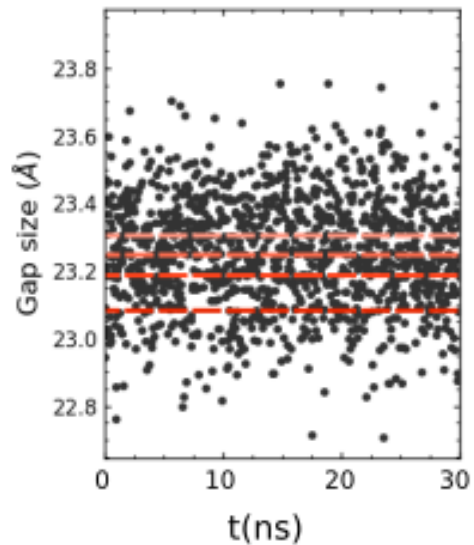
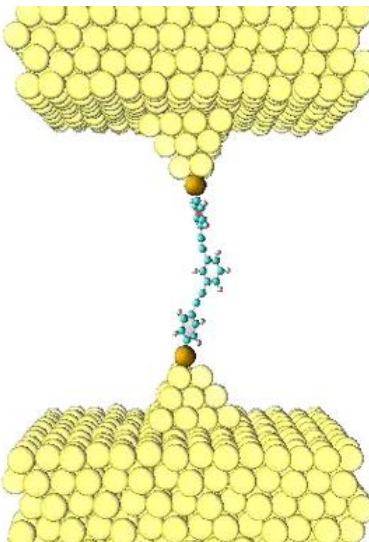
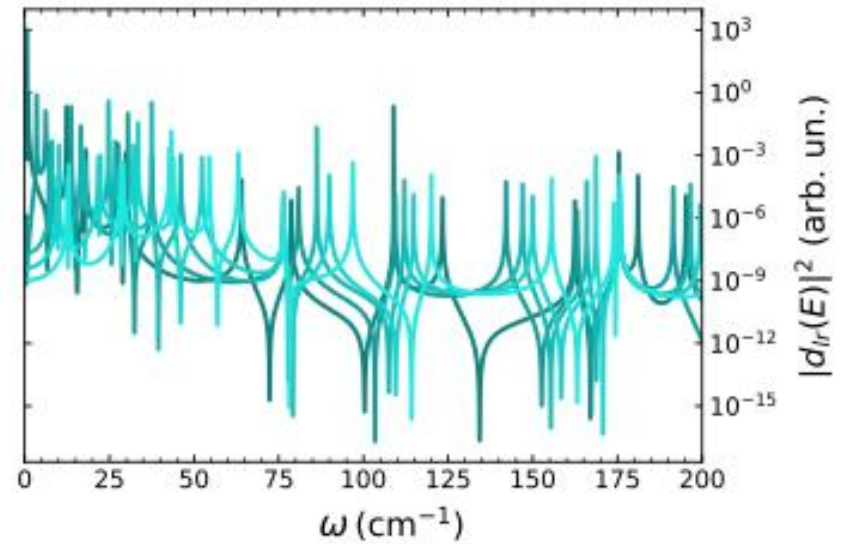
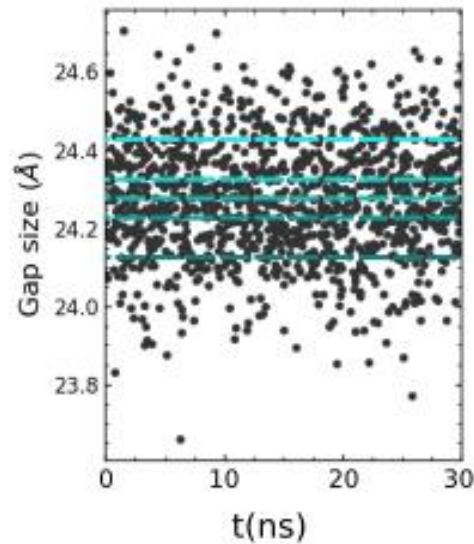
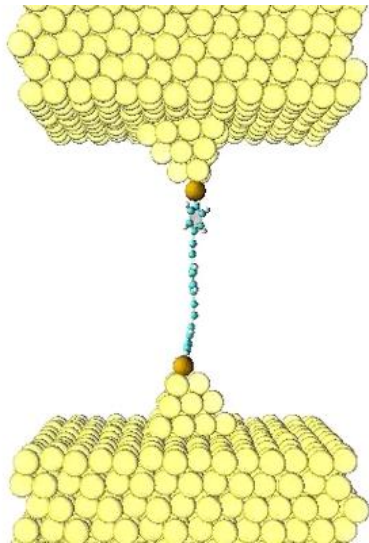
Vibrational interference: accounting for temperature



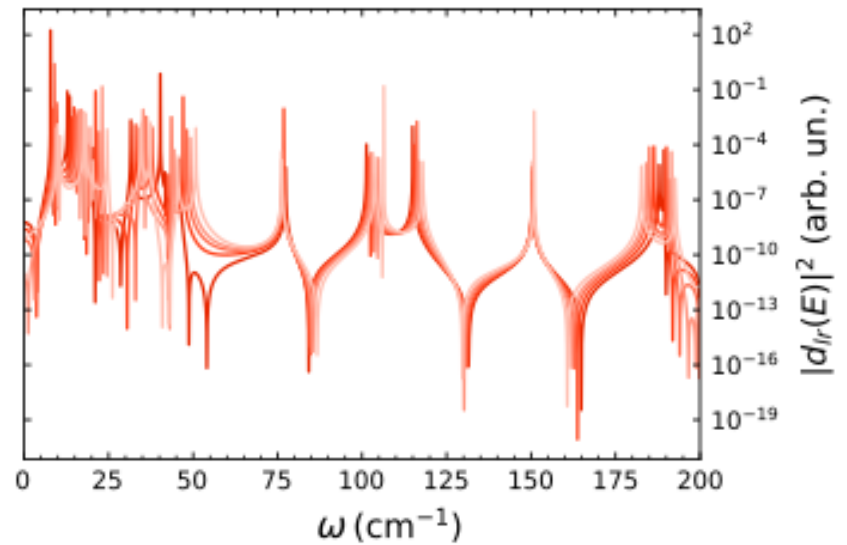
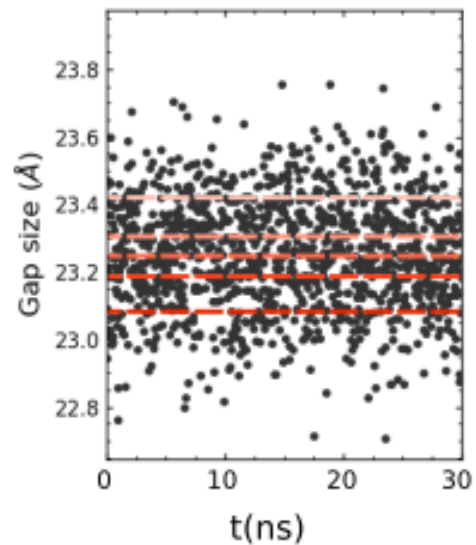
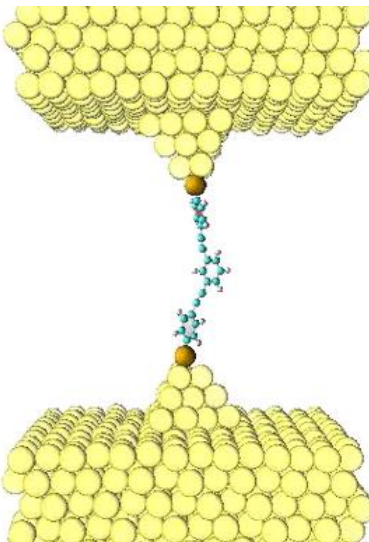
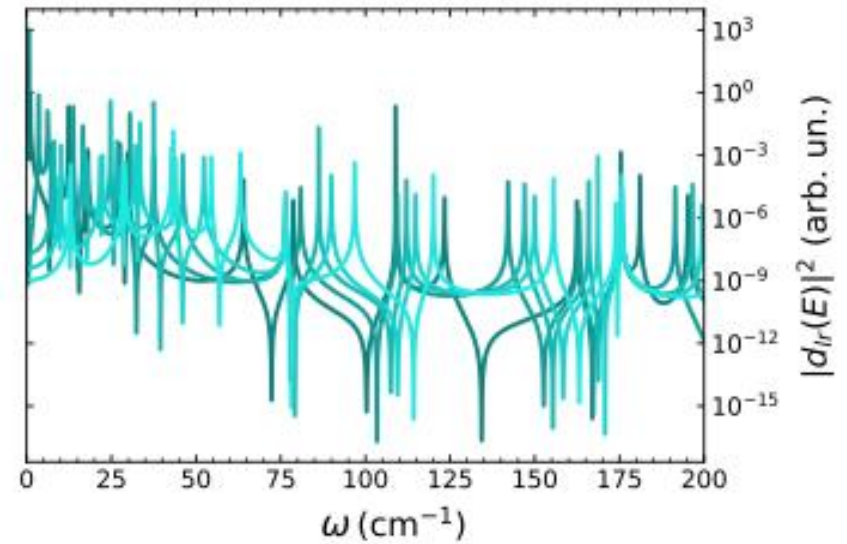
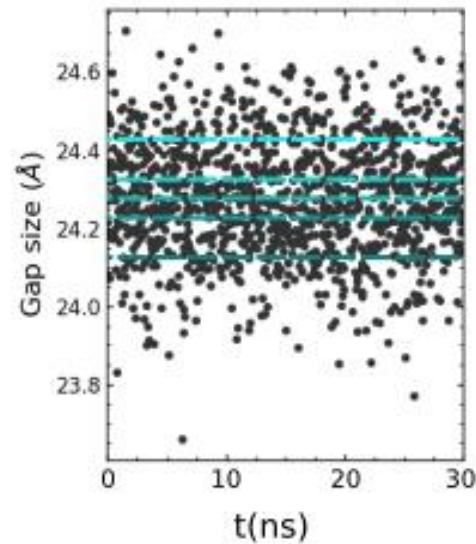
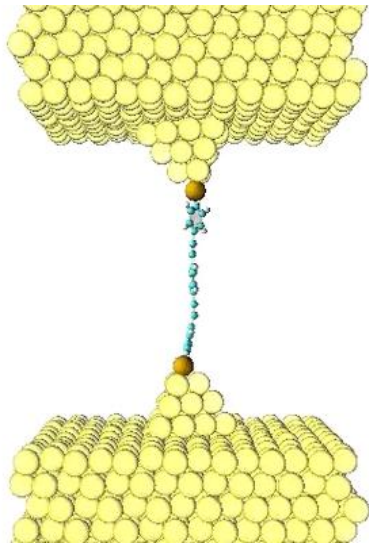
Vibrational interference: accounting for temperature



Vibrational interference: accounting for temperature



Vibrational interference: accounting for temperature

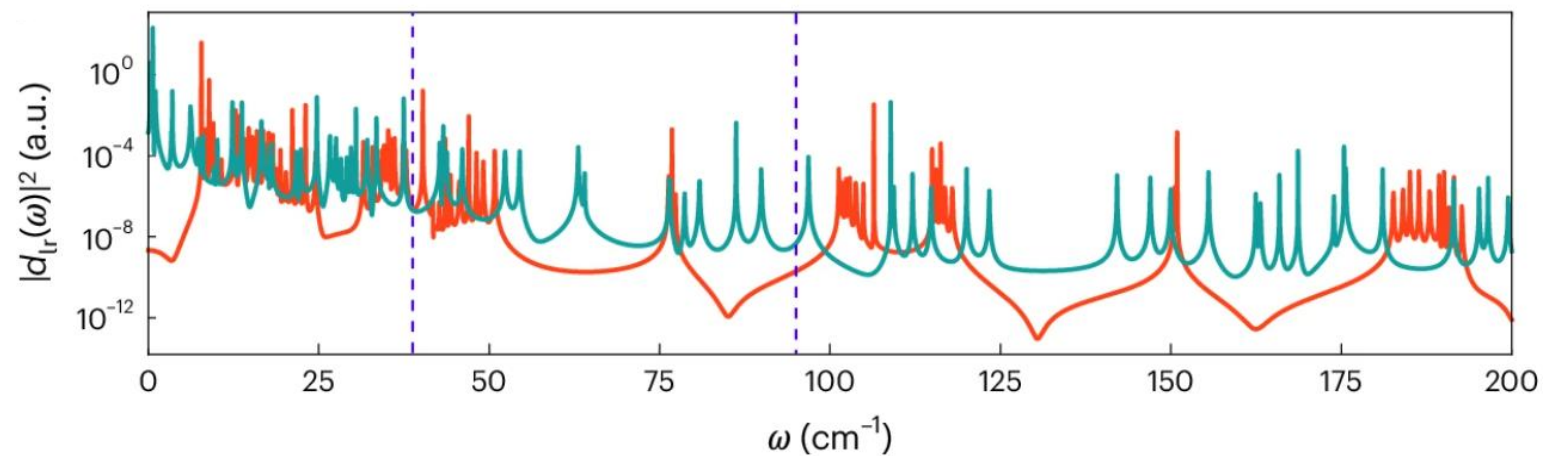
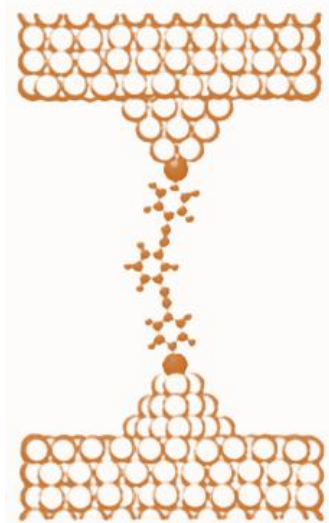


Vibrational interference: accounting for temperature

para-OPE3

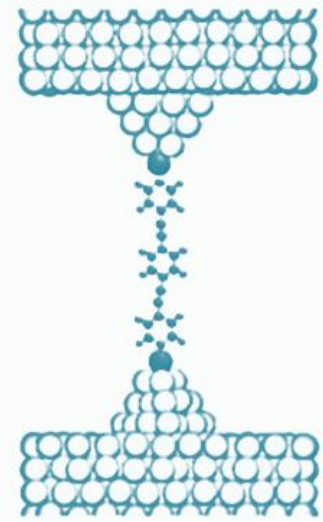


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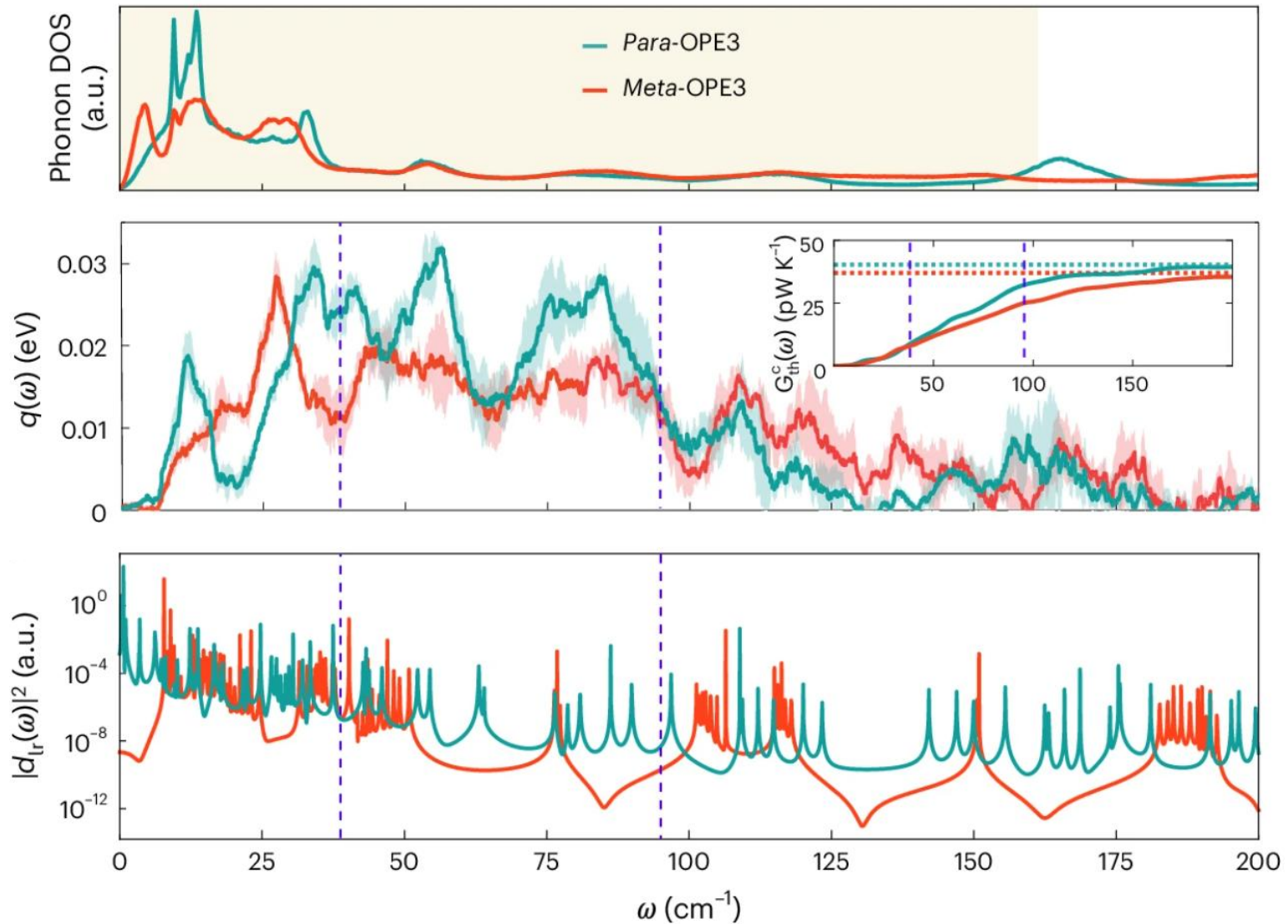


Vibrational interference: accounting for temperature

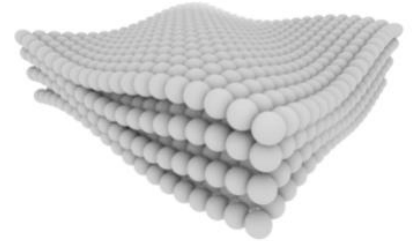
para-OPE3



meta-OPE3



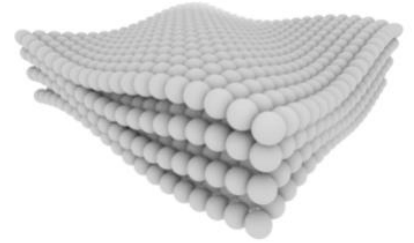
Takeaways



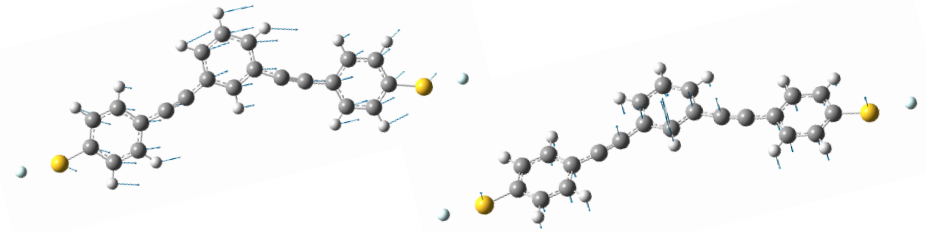
✓ Heat is wave-like at the nanoscale ($L < 100 \text{ nm}$)

Takeaways

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



✓ Normal modes can interfere

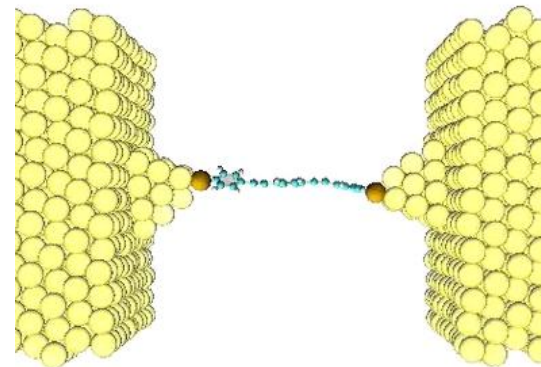
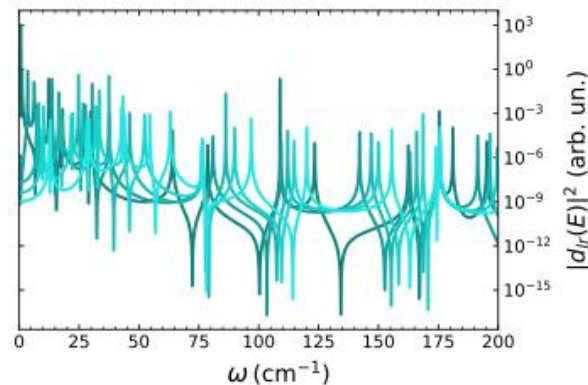
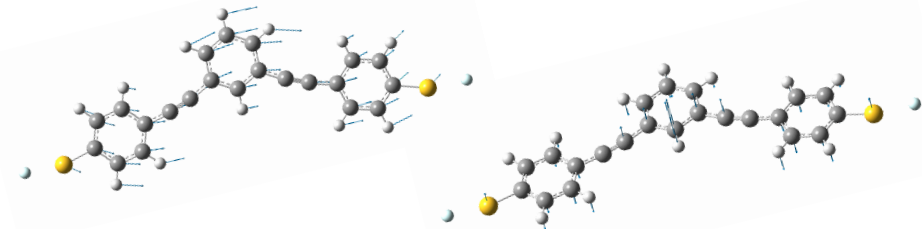
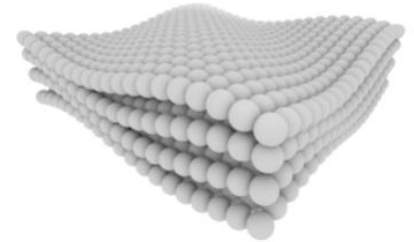


Takeaways

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

✓ Normal modes can interfere

✓ Finite temperature matters



Acknowledgements



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J.C. Cuevas



G. Prampolini

Thank you for
your attention!

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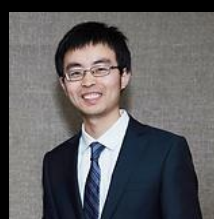
S.C. Yelishala



X. Zhu



M. Habibi



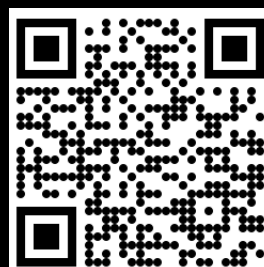
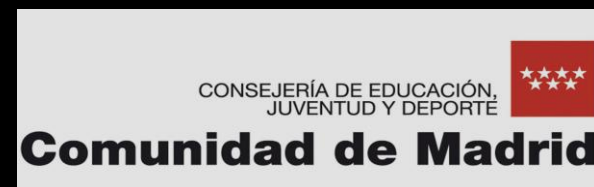
L. Cui



W. Zhang

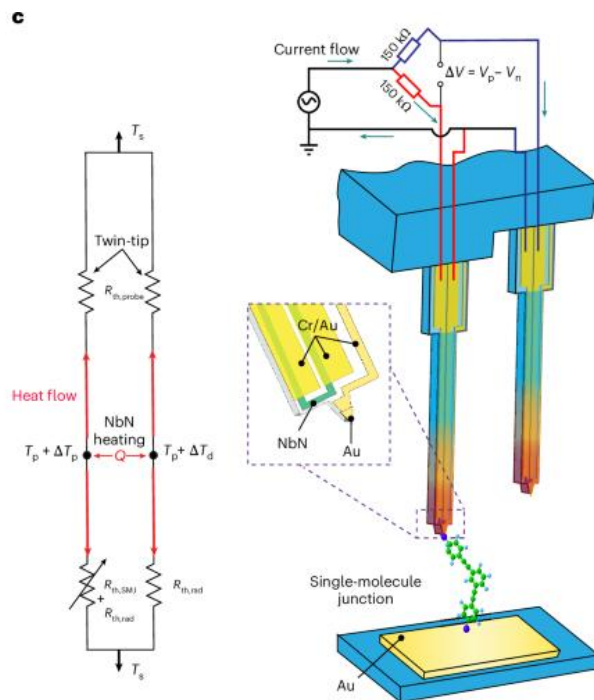
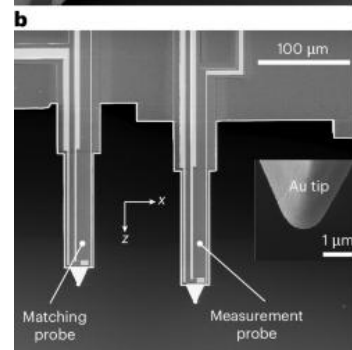
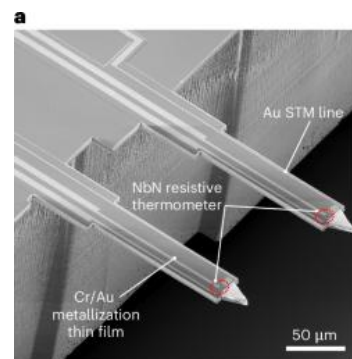
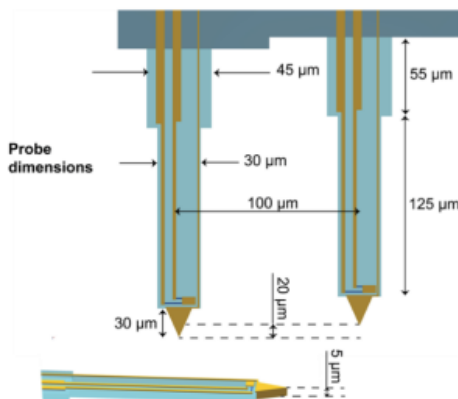
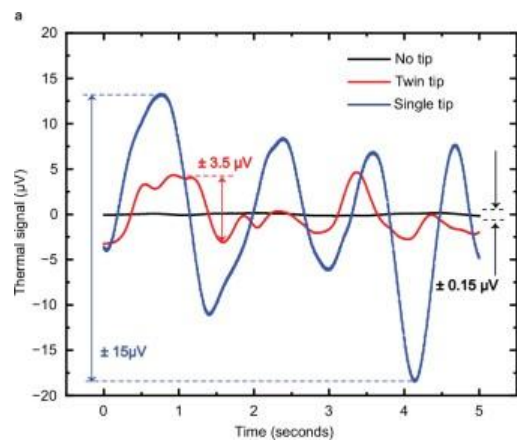


H. Chen

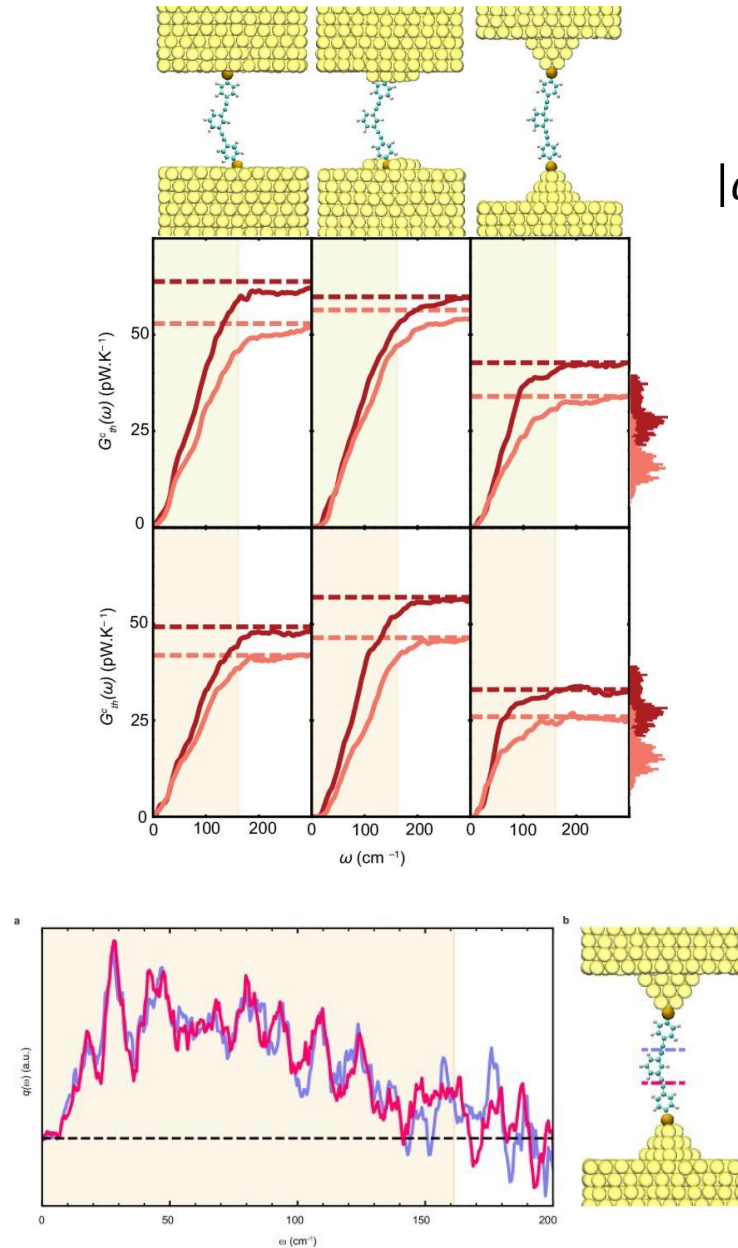
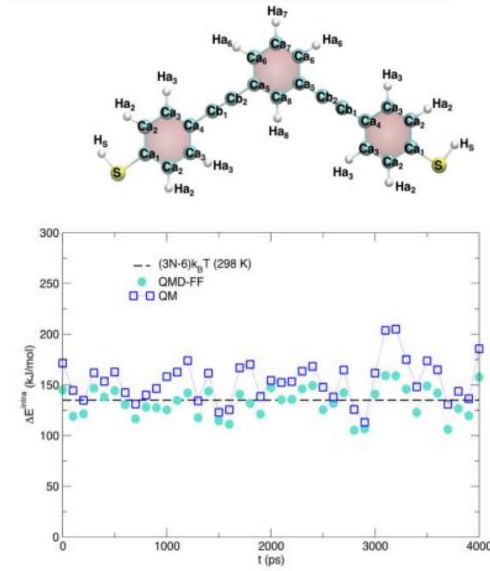
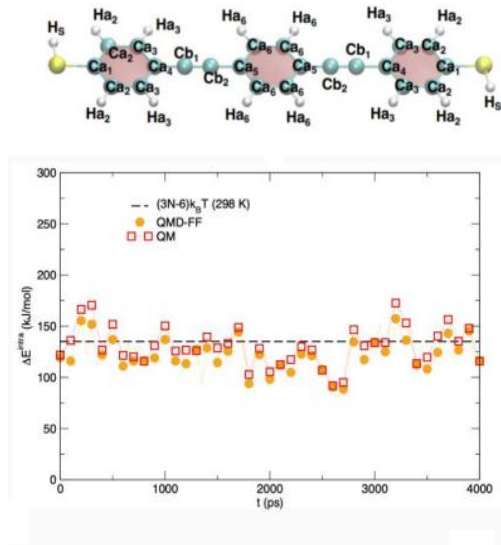


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Extra figures – Experiments



Extra figures – Theory



Kernel of transmission

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