

Phonon interference in single-molecule junctions

P. M. Martinez^{1,2}, Sai C. Yelishala³, Yunxuan Zhu³, Hongxuan Chen³, Mohammad Habibi³, Giacomo Prampolini⁴, Wei Zhang³, Longji Cui³, J. C. Cuevas¹, J. G. Vilhena²

¹Universidad Autónoma de Madrid, UAM, Spain

²Instituto de Ciencia de Materiales de Madrid, ICM, Spain

³University of Colorado Boulder, Colorado, USA

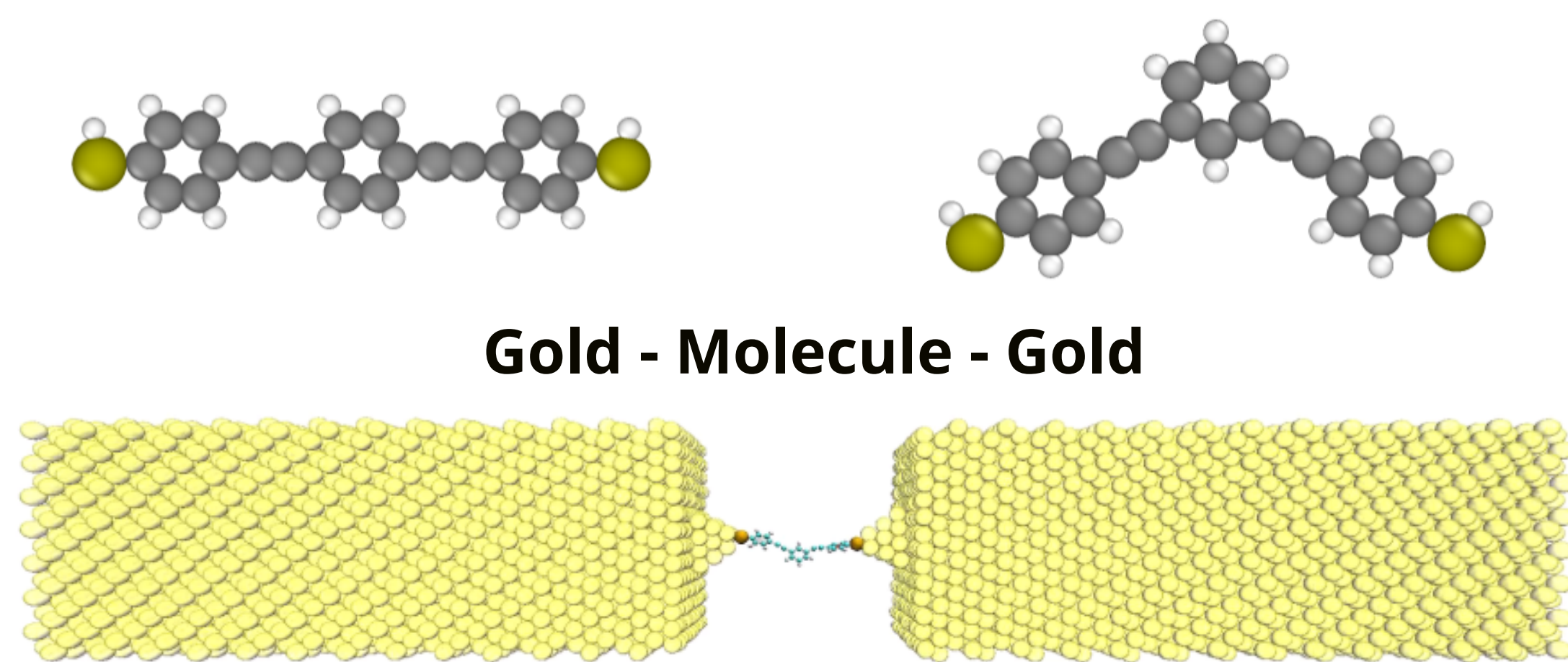
⁴Istituto di Chimica dei Composti Organometallici, CNR, Italy

1. Molecular Junctions

Ideal testbed to probe fundamental physics and chemically tunable. We investigate the effect of vibrational interferences [1].

para-OPE3

meta-OPE3

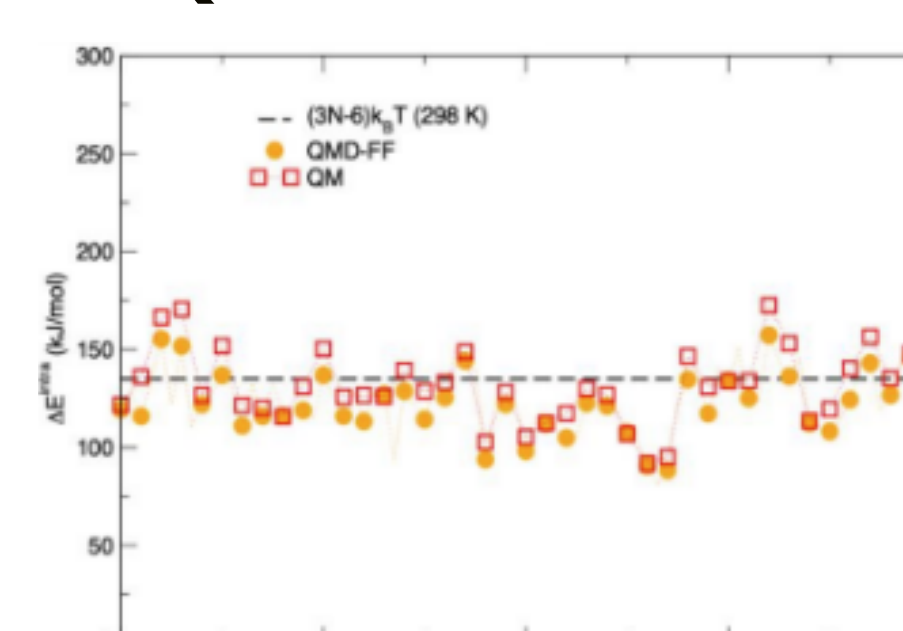


2. QM-accurate Force Fields

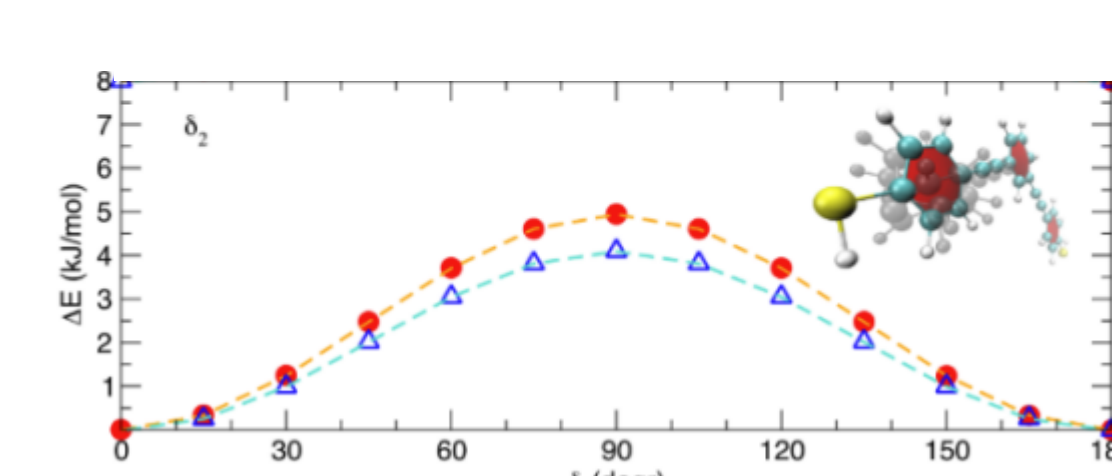
Our force fields are sourced from DFT data. The end result are trajectories that map the QM potential energy surface (PES).

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

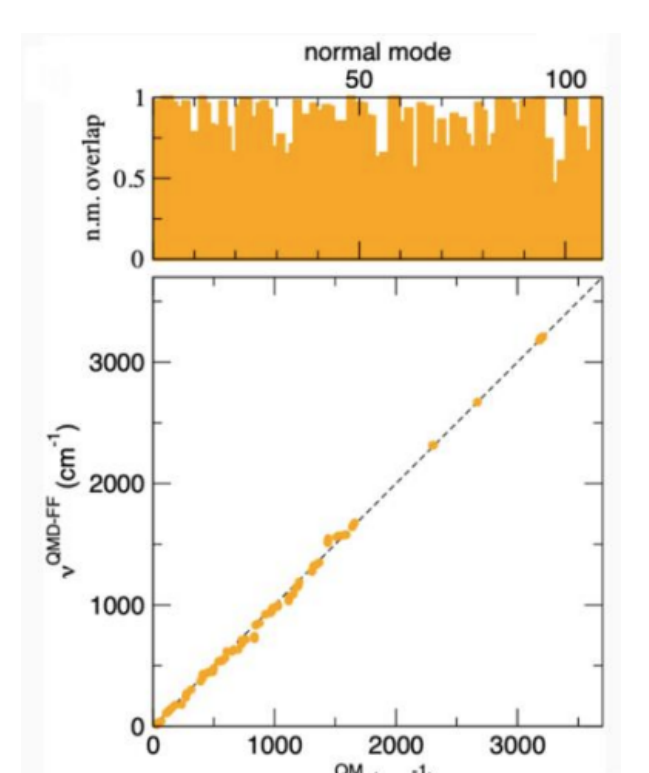
QM-accurate PES



DFT Torsional Scans

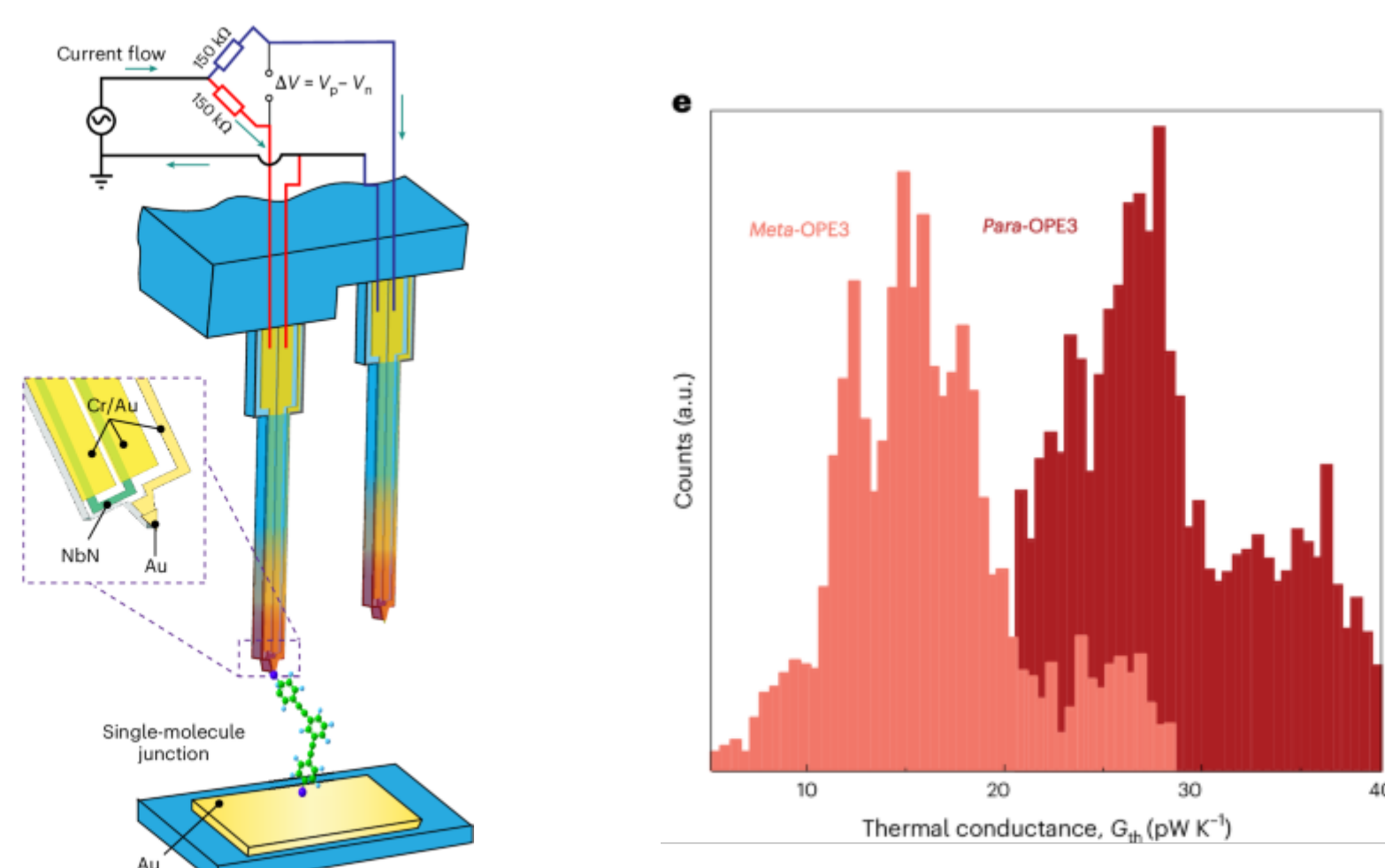


DFT Hessian



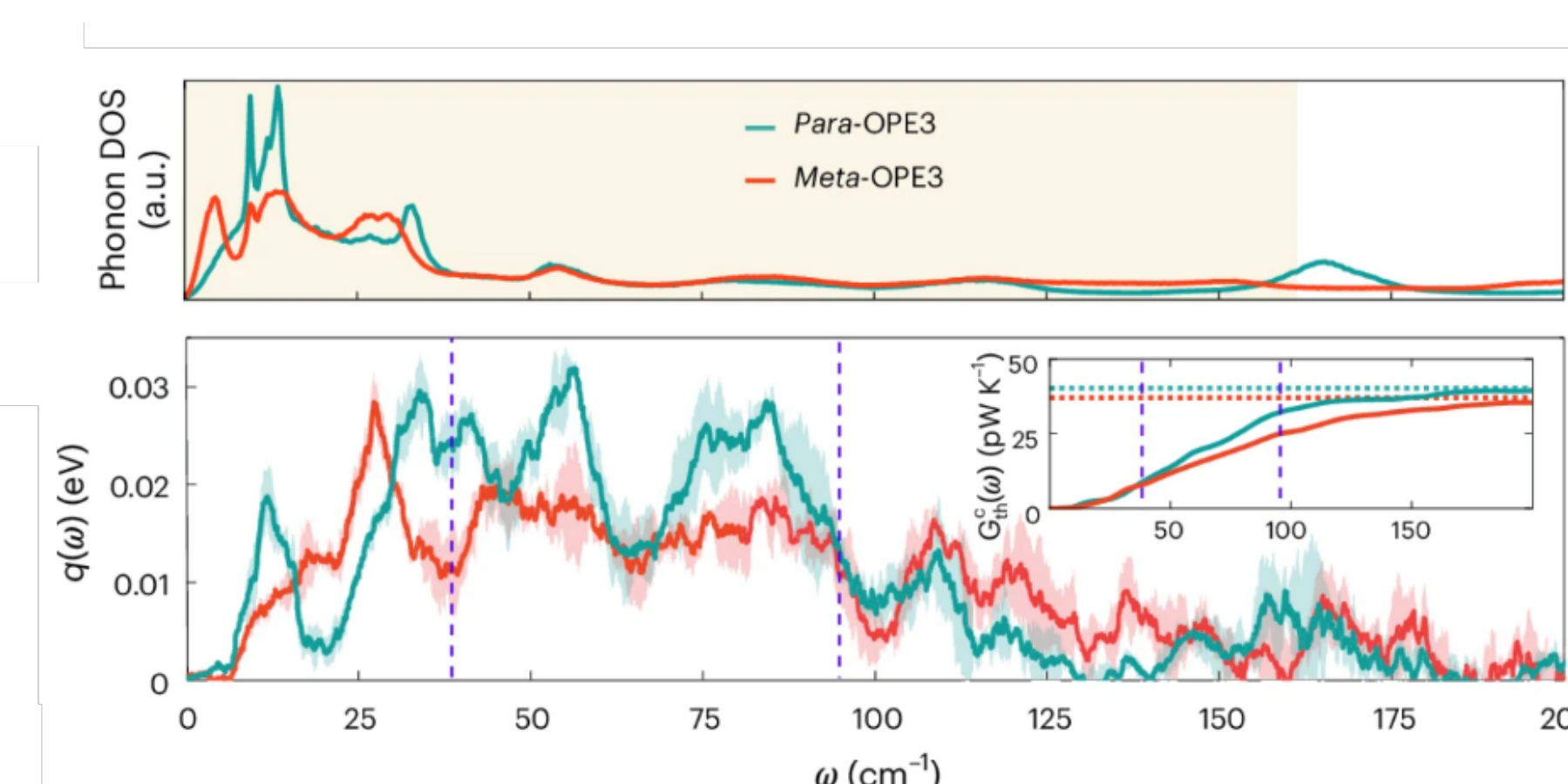
3. Heat reduced by 40%

Novel SThM twin probes measure thermal conductance through both isomeric OPE3 molecules

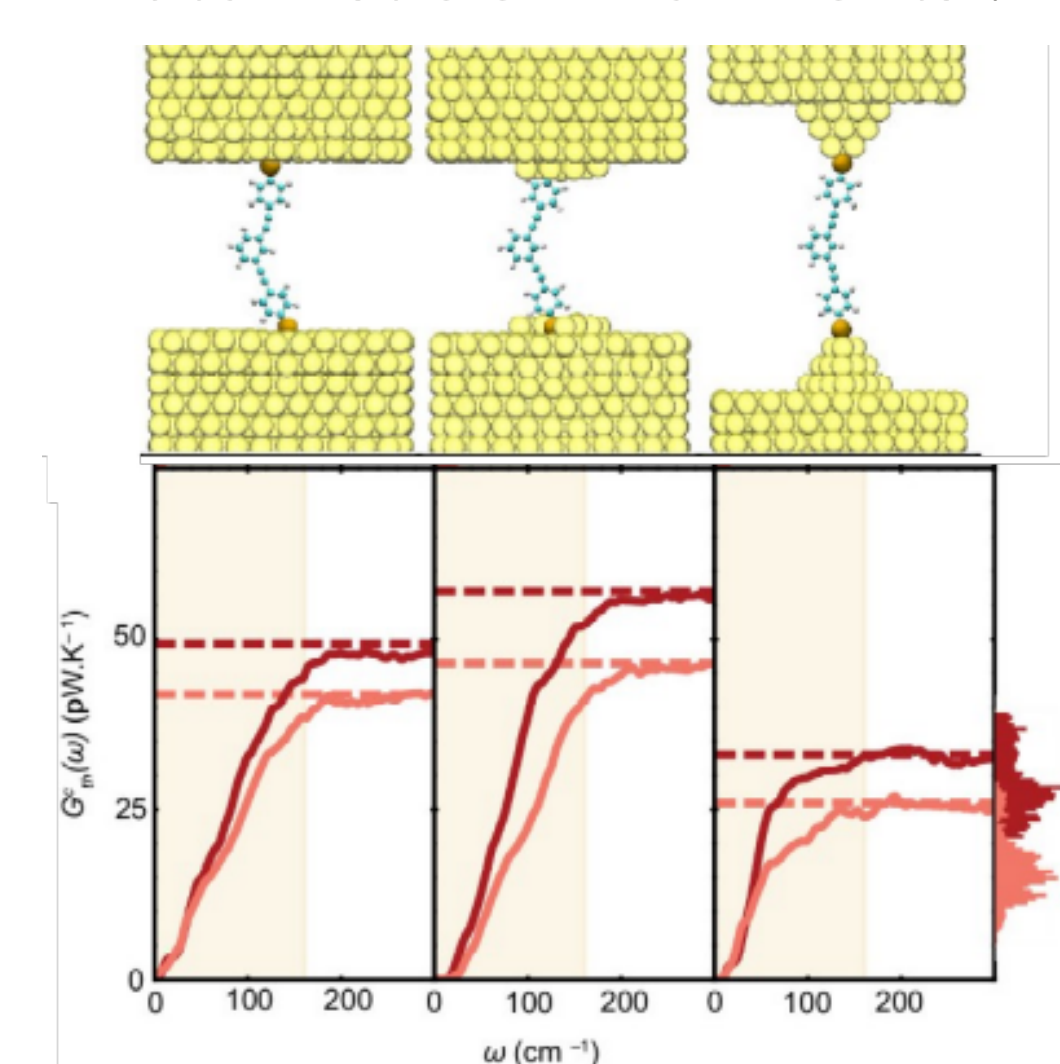


4. Classical MD reveal phonon suppression

We found normal modes are similarly populated but carry different energy $q(\omega)$ in each isomer.



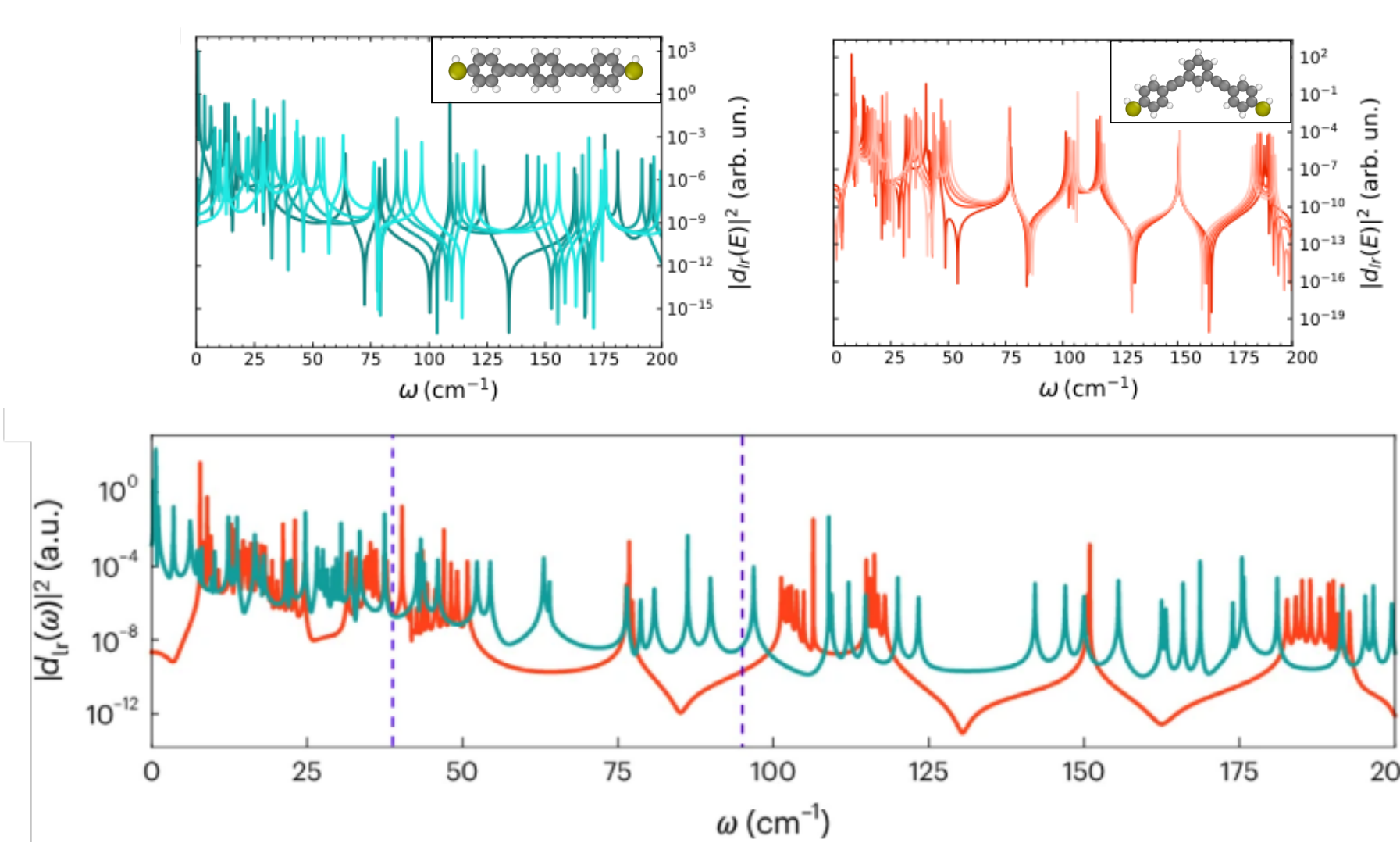
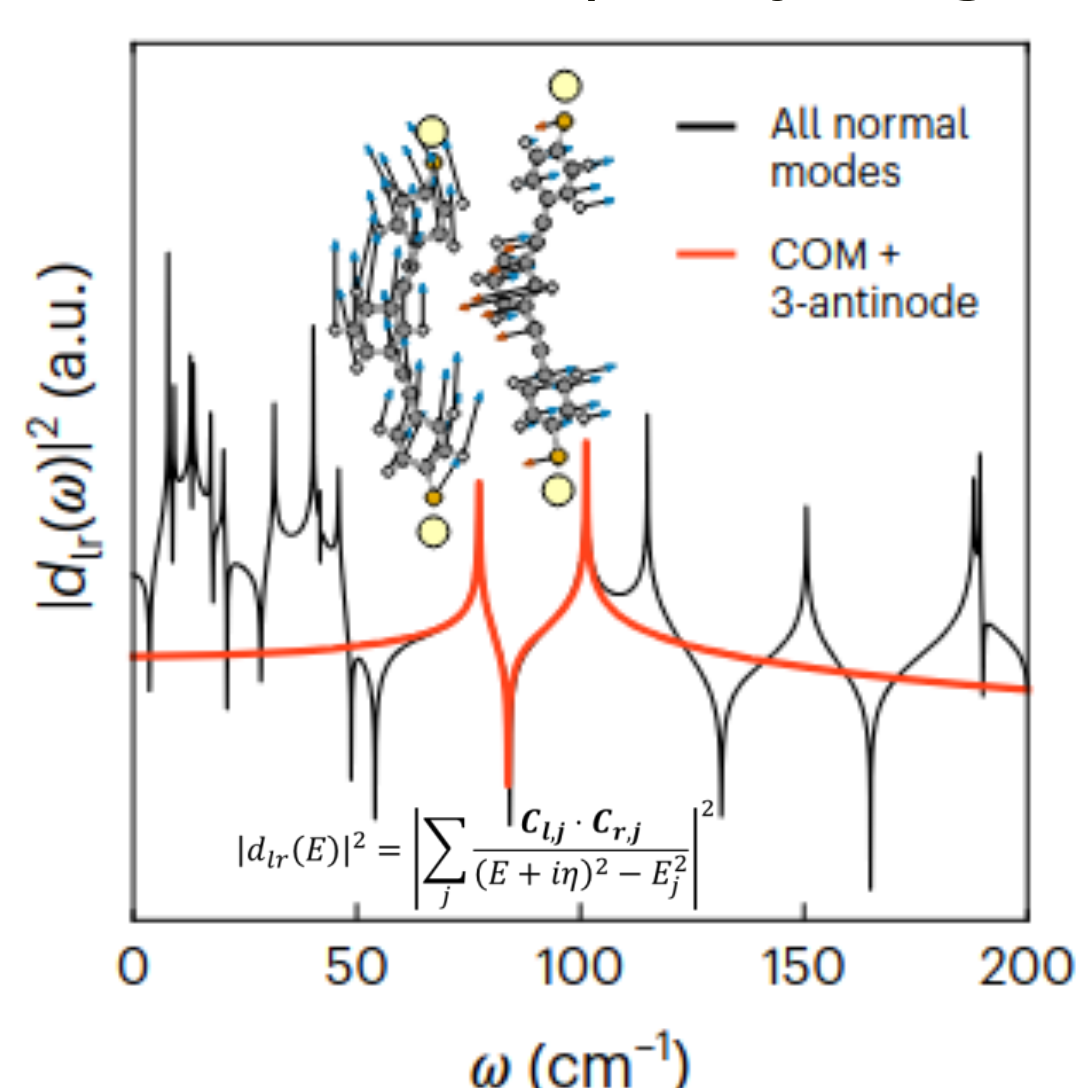
The difference in thermal conductance is found in several atomistic environments.



5. Normal mode destructive interference

Normal modes may interfere based on their parity. We find plenty within the frequency range.

Only one isomer shows consistent interferences at every geometry explored in the MD trajectory.



6. Conclusions

Heat transport was chemically tuned with a 40% reduction in conductance.

Normal modes can interfere based on their parity.

Thermal fluctuations alter the mechanical coupling at room temperature, potentially quenching interferences.

Softer degrees of freedom help pinning interferences in molecular junctions.

References and acknowledgments

[1] S.C. Yelishala, Y. Zhu, P.M. Martinez et al. Phonon interference in single-molecule junctions. Nat. Mater. **24**, 1258–1264 (2025).

[2] S. Giannini et al. J. Chem. Theory Comput. **21**, 3156–3175 (2025)

The project that gave rise to these results received the support of a fellowship from the Spanish Ministry of Education within the FPU grant program number EST25/00227.

