

Optically Switchable Diarylethene Junctions: Assessing Heat Transport Modulation

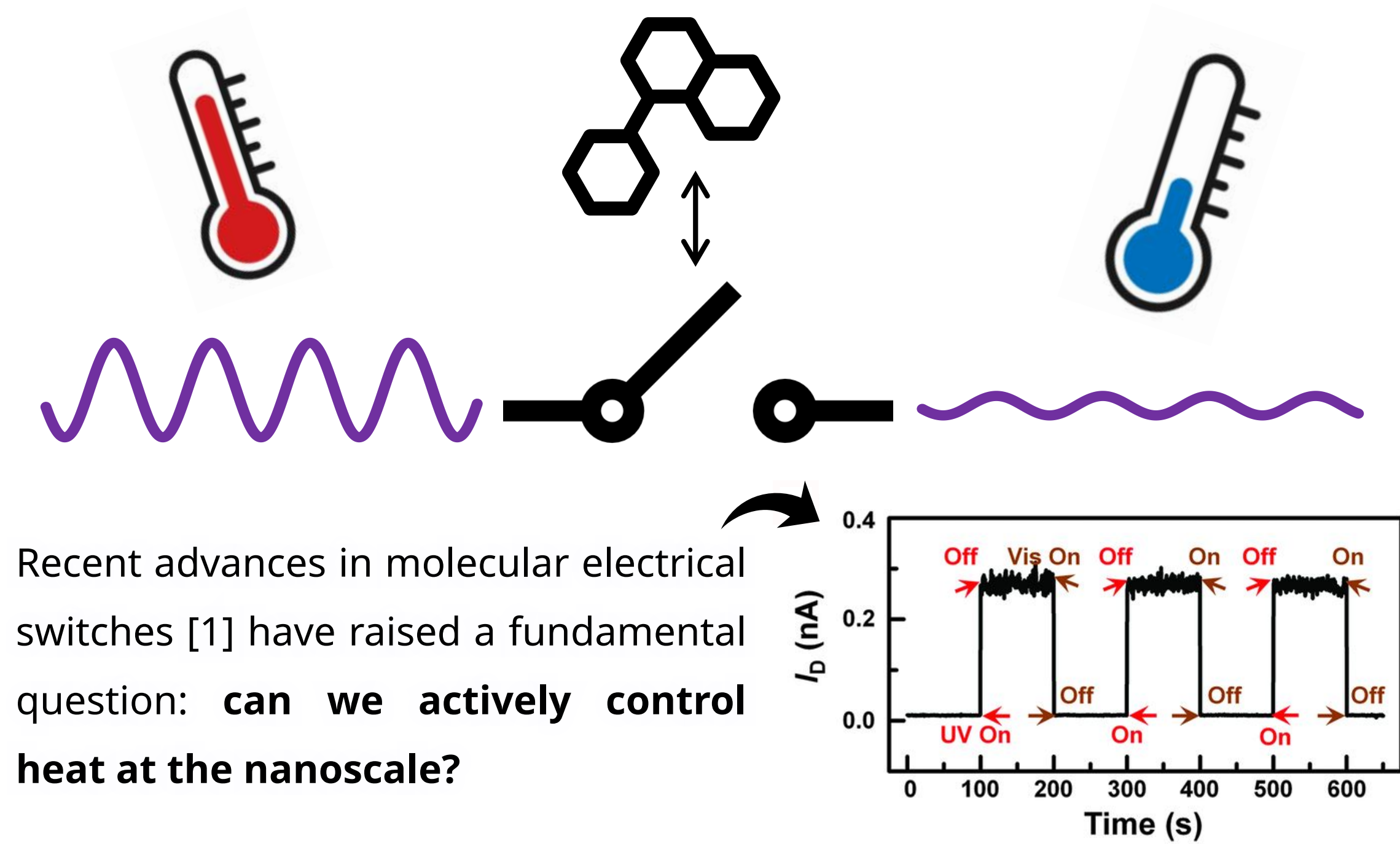
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Can we build a thermal switch?



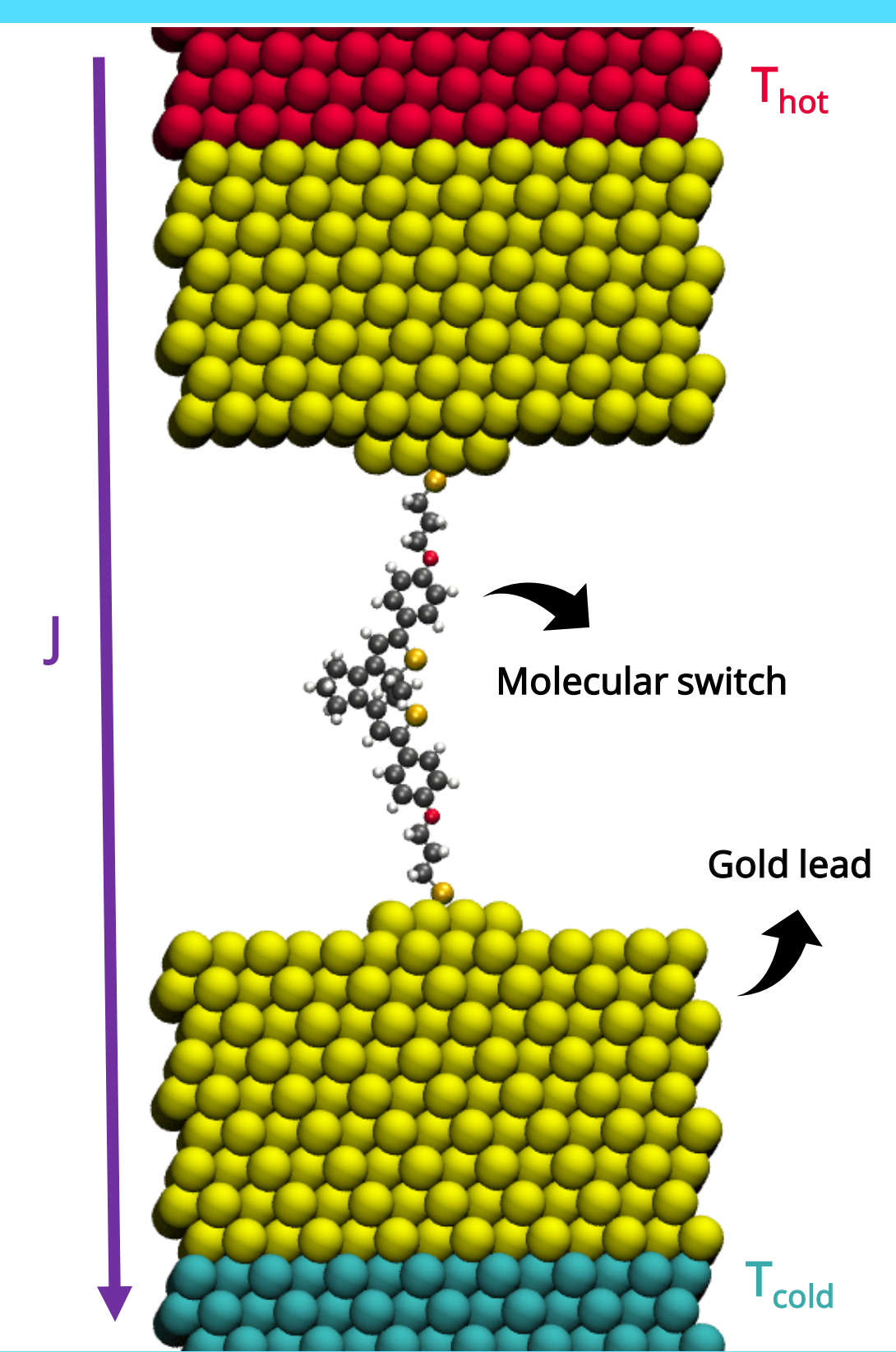
Methods

- Quantum mechanical interatomic potentials [2].

- Non-equilibrium molecular dynamics.

- Computing thermal conductance (G_{th}): how much energy (J) does it take to keep the temperature gradient (ΔT)?

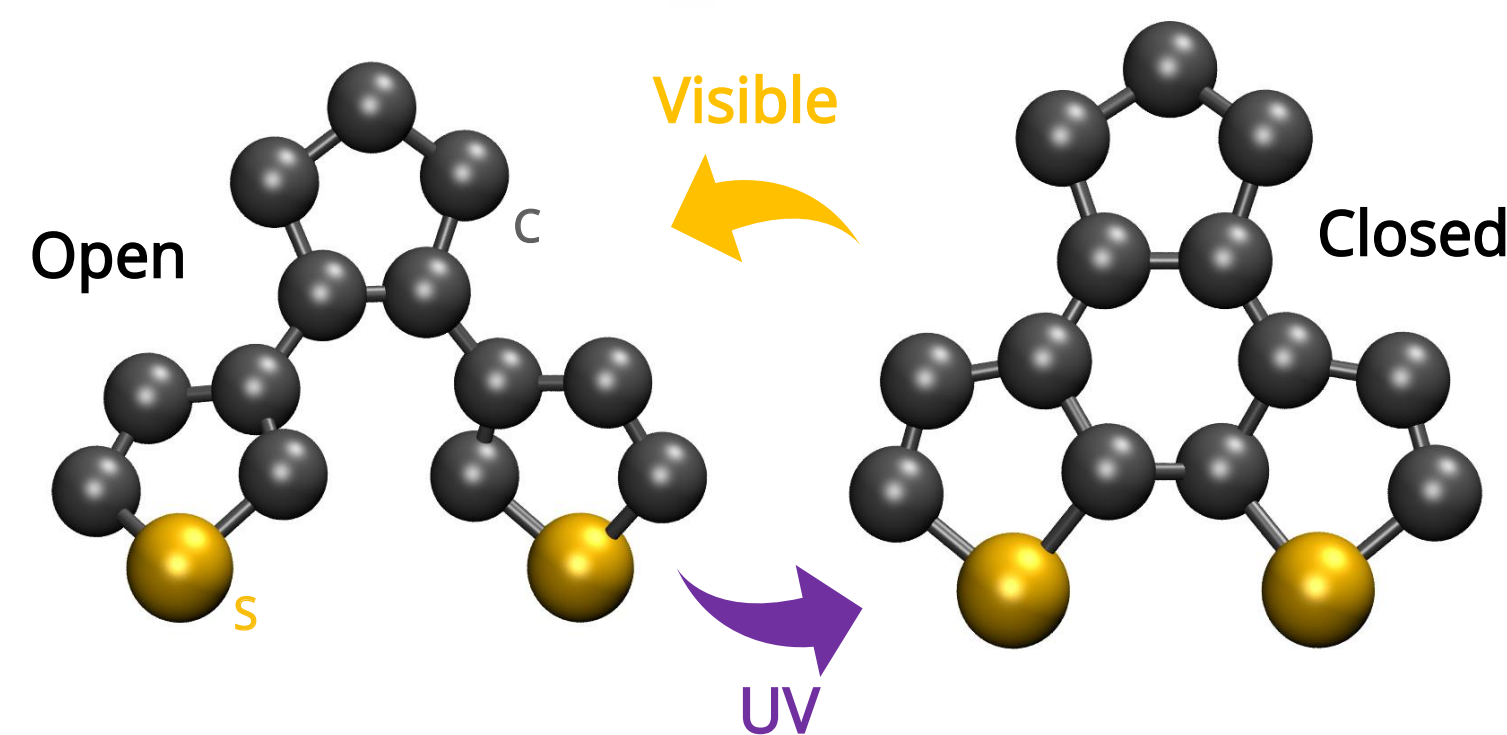
$$G_{th} = J/\Delta T$$



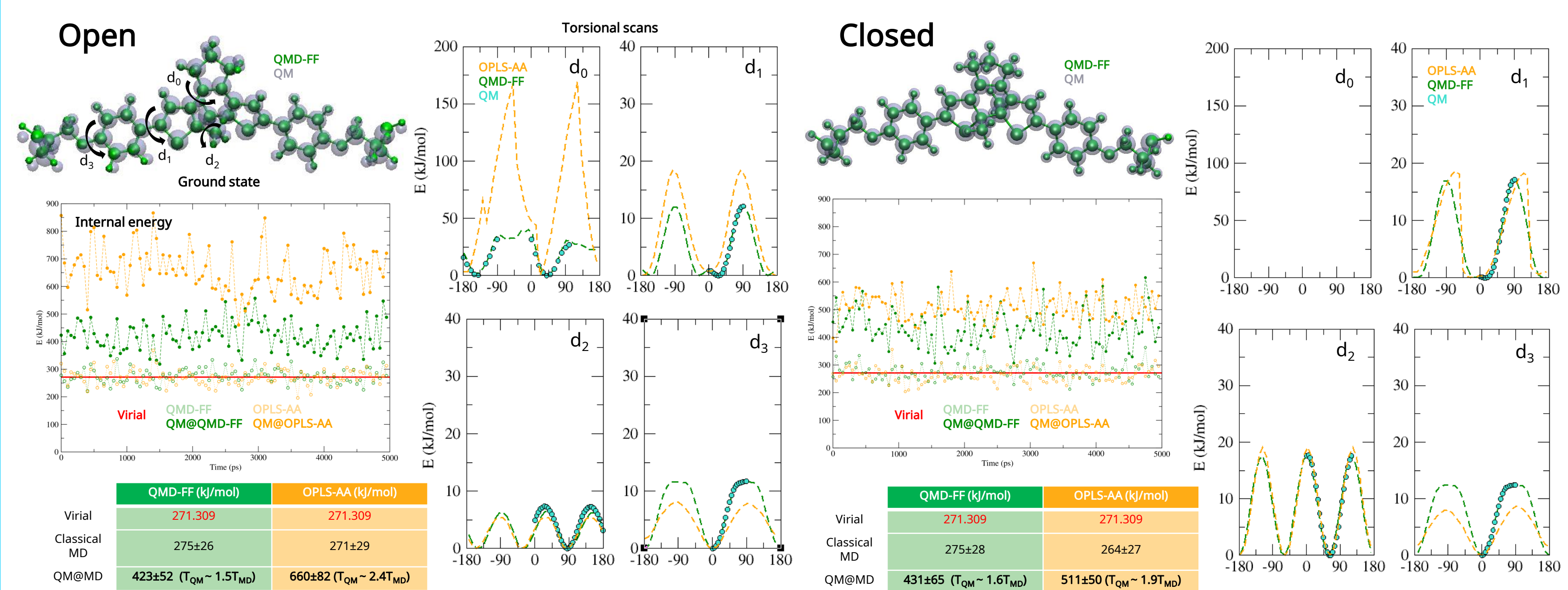
The switch

Diarylethenes (DAE) are optically-active photochromic molecules **featuring two long-lived isomers** [3]:

- Distinct phonon pathways.
- Modified vibrational spectra.



Interatomic Potentials (QM-FF)

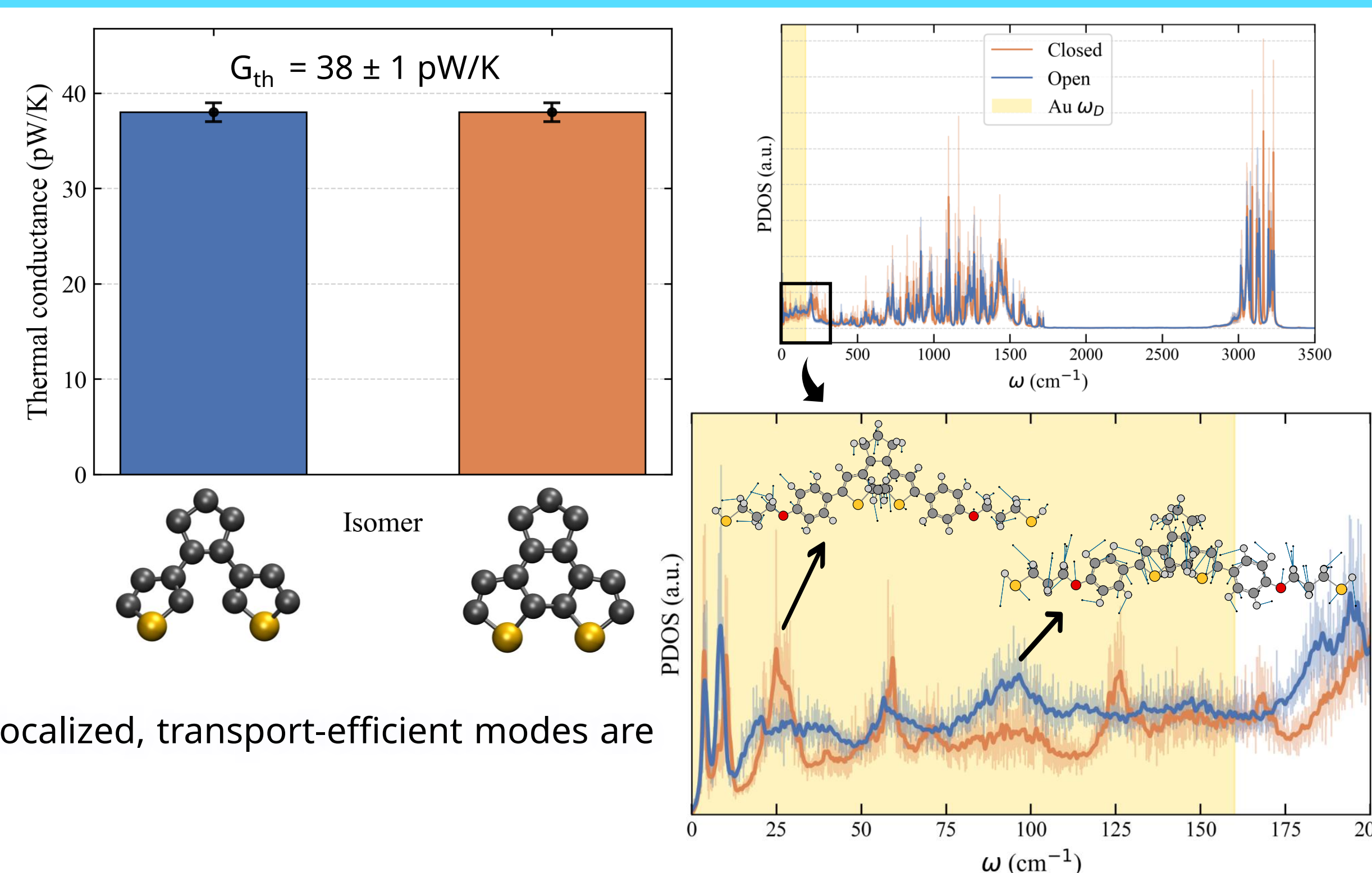


Results

- Both isomers exhibit the **same thermal conductance**.

- Vibrational density of states shows **no significant differences** ($\omega \leq 160 \text{ cm}^{-1}$).

- Population imbalances of delocalized, transport-efficient modes are ultimately compensated.



Outlook

- Inefficient thermal switch:

$$\Delta G_{th}^{DAE} \approx 1 \text{ pW/K}$$

$$\Delta G_{ele}^{DAE} \approx 100 \text{ pW/V}^2$$

- Optical switching is unable to alter vibrational modes.

- Possible candidates for thermoelectric switches:

$$zT = \frac{\sigma S^2 T}{\kappa}$$

- Accessing a broader vibrational frequency window (e.g. by changing electrodes) may reveal isomer-dependent thermal transport.

References and acknowledgments

[1] C. Jia *et al.* *Science* **352** 1443-1445 (2016)

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

[3] M. Irie *et al.* *Chem. Rev.* **114** 12174-12277 (2014)

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