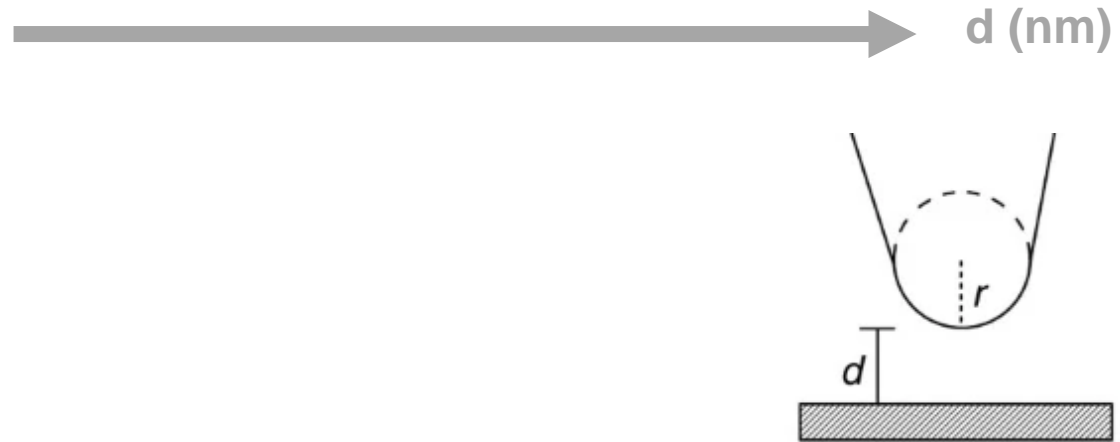


HEAT TRANSFER ACROSS NANOMETER-SIZED GAPS

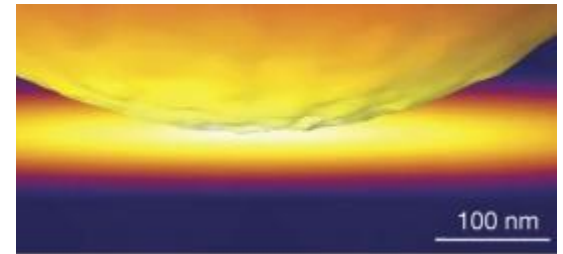
O. Mateos-Lopez, R. Lopez-Nebreda, P. M. Martinez, N. Agrait,
J. G. Vilhena, J. C. Cuevas

Heat Transfer in the Crossover Regime

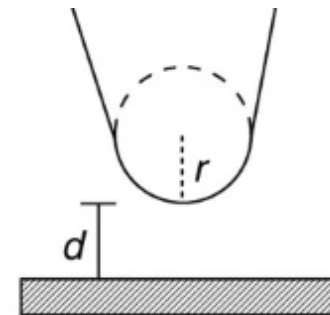


Heat Transfer in the Crossover Regime

photons

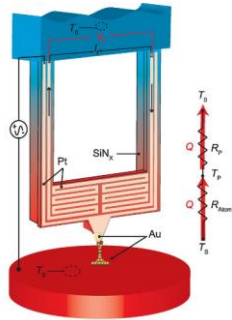


Reddy *et al*, Nature, **528**, 387-391 (2015)



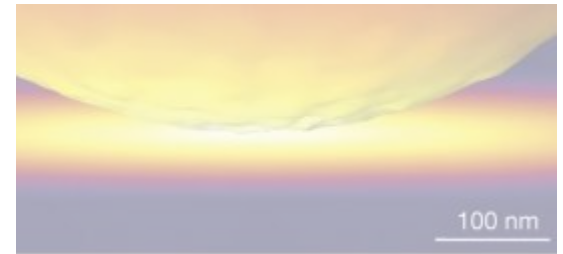
Heat Transfer in the Crossover Regime

electrons



Cui *et al*, Science, **355**, 6330 (2017)

photons

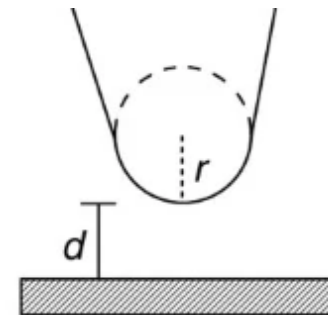


Reddy *et al*, Nature, **528**, 387-391 (2015)

in contact

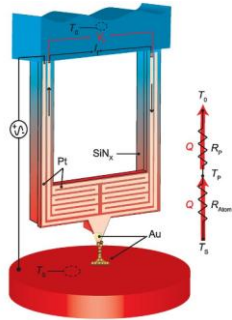
> 3 nm

d (nm)



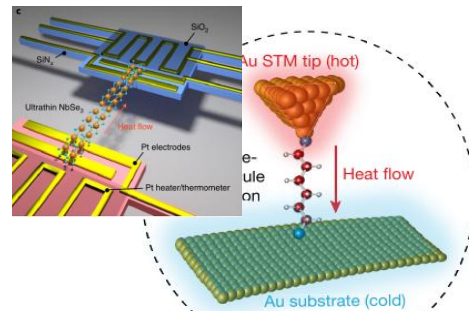
Heat Transfer in the Crossover Regime

electrons



Cui *et al*, Science, **355**, 6330 (2017)

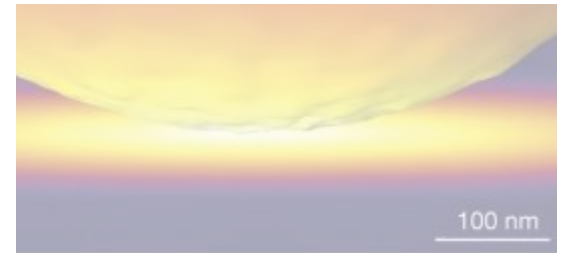
phonons



Yang *et al.*, Nat. Nano, **16**, p764(2021)

Cui *et al*, Nature, **572**, 628-633 (2019)

photons

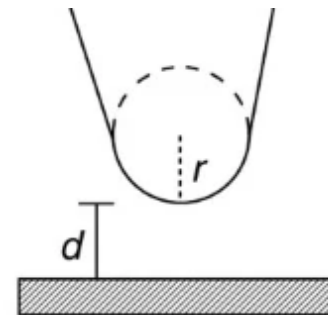


Reddy *et al*, Nature, **528**, 387-391 (2015)

in contact

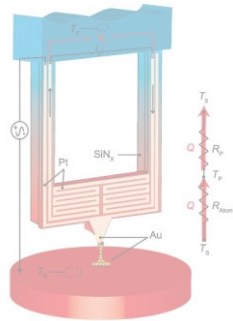
> 3 nm

d (nm)



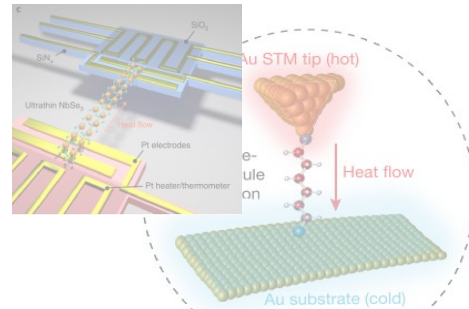
Heat Transfer in the Crossover Regime

electrons



Cui *et al*, Science, **355**, 6330 (2017)

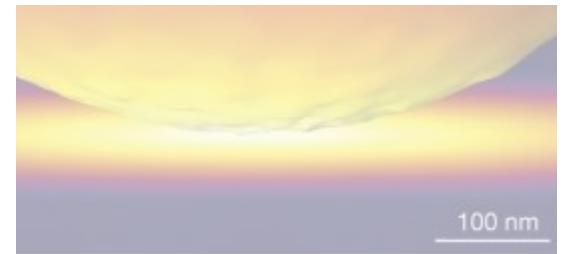
phonons



Yang *et al.*, Nat. Nano, **16**, p764(2021)

Cui *et al*, Nature, **572**, 628-633 (2019)

photons



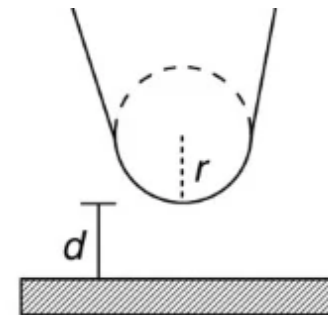
Reddy *et al*, Nature, **528**, 387-391 (2015)

?

in contact

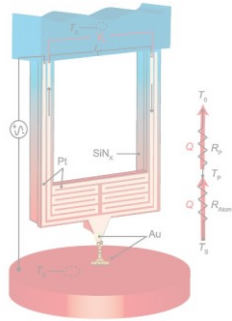
> 3 nm

d (nm)



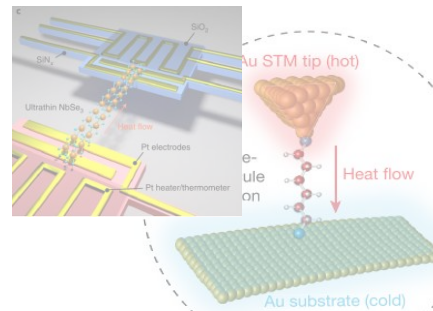
Heat Transfer in the Crossover Regime

electrons



Cui *et al*, Science, **355**, 6330 (2017)

phonons



Yang *et al.*, Nat. Nano, **16**, p764(2021)

Cui *et al*, Nature, **572**, 628-633 (2019)

photons



Reddy *et al*, Nature, **528**, 387-391 (2015)

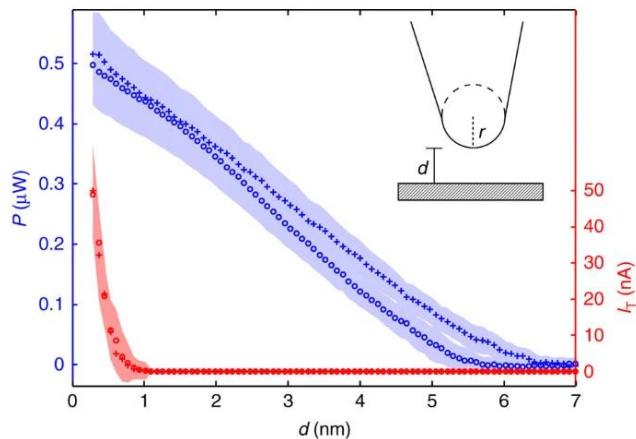
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in contact

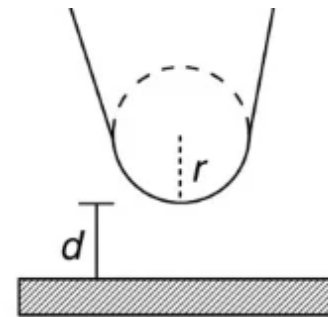
> 3 nm

d (nm)

Kloppstech *et al*, Nat. Comms, **8**, 14475 (2017)



Heat flux orders of magnitude larger than predicted!!!



Methods

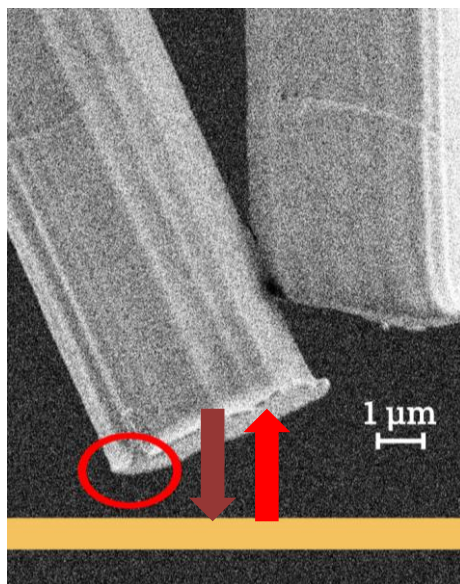
Methods: Experimental set-up



R. Lopez-Nebreda



N. Agraït



Custom STM setup (High-Vacuum E-6 mbar):

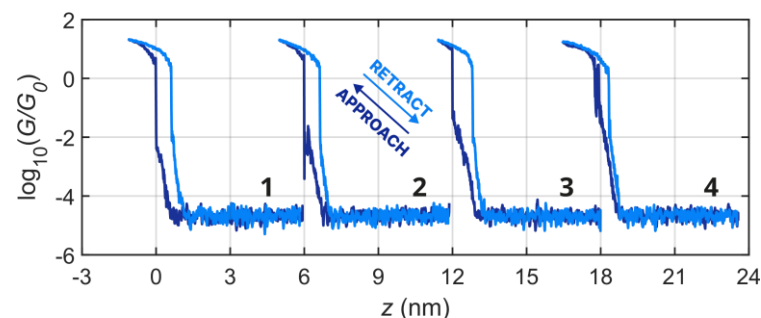
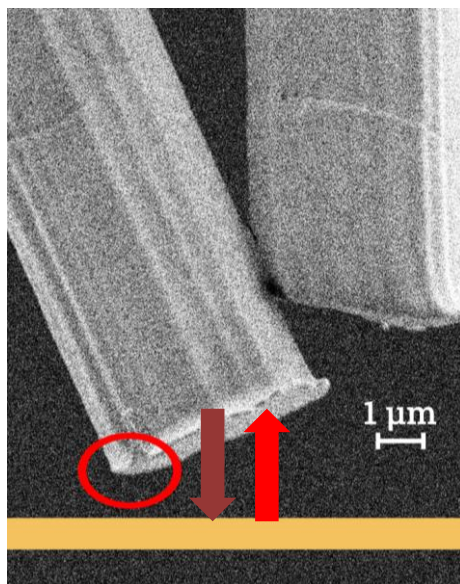
Methods: Experimental set-up



R. Lopez-Nebreda



N. Agraït



Custom STM setup (High-Vacuum E-6 mbar):

➤ Electrical Conductance (**G**)

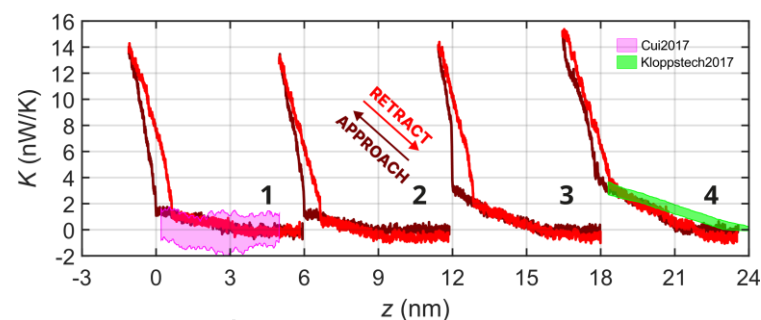
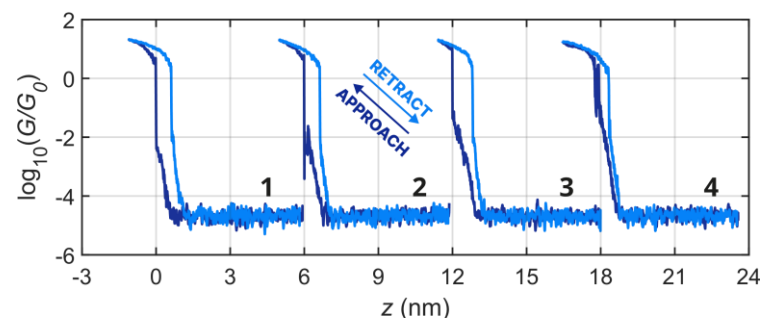
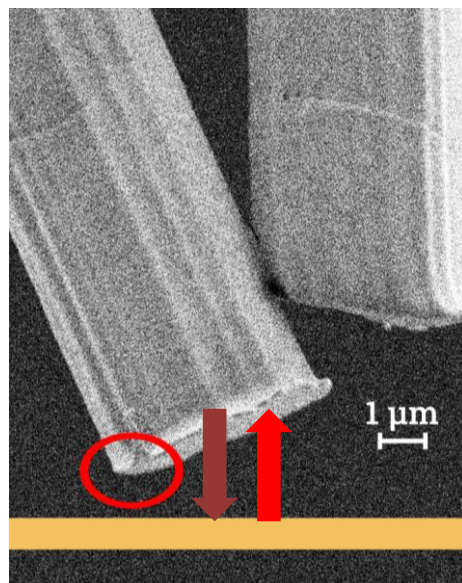
Methods: Experimental set-up



R. Lopez-Nebreda



N. Agraït

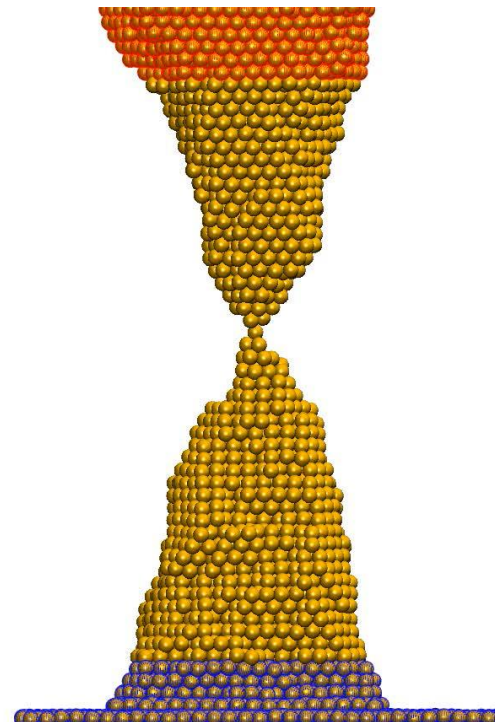


Custom STM setup (High-Vacuum E-6 mbar):

- Electrical Conductance (**G**)
- Thermal conductance (**K**) [using thermoelectric effect: $\Delta T \longrightarrow \Delta V$]

Methods: All-atom Molecular Dynamics simulations

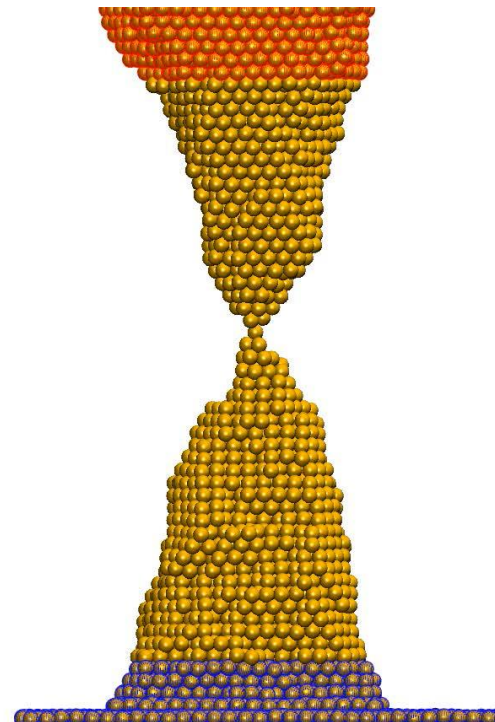
- All atoms included in the simulation.



Methods: All-atom Molecular Dynamics simulations

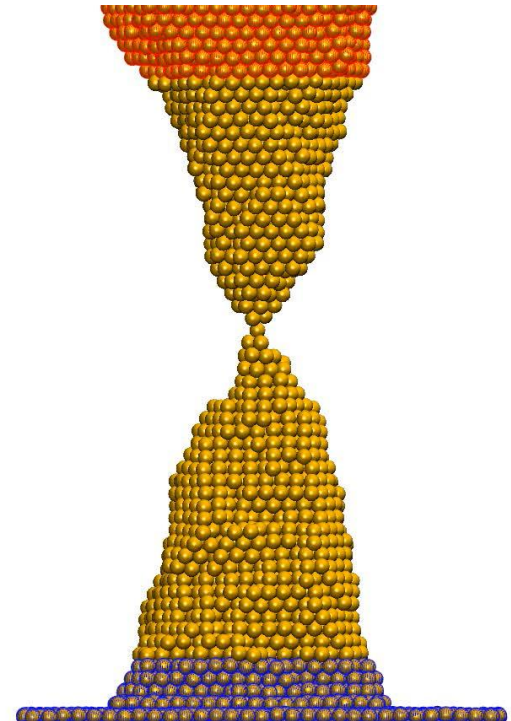
➤ All atoms included in the simulation.

➤ **Interaction:** classical force fields.



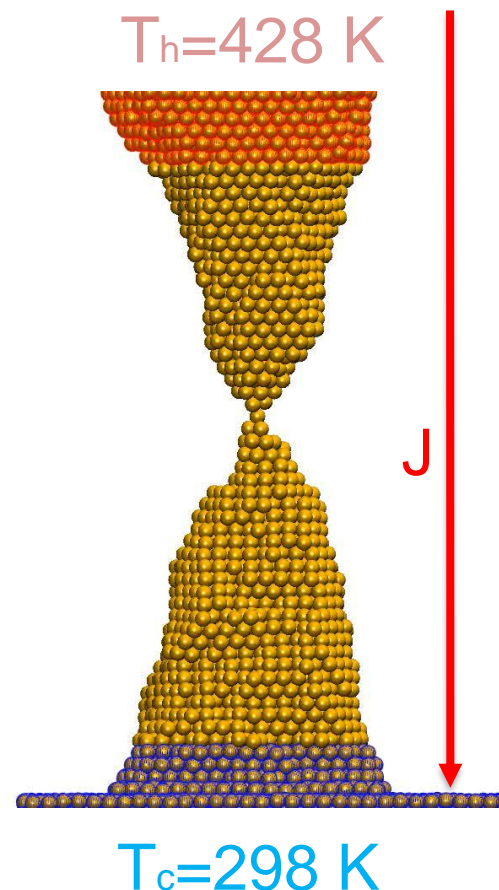
Methods: All-atom Molecular Dynamics simulations

- All atoms included in the simulation.
- **Interaction:** classical force fields.
- **Movement:** Newton's Equations.



Methods: All-atom Molecular Dynamics simulations

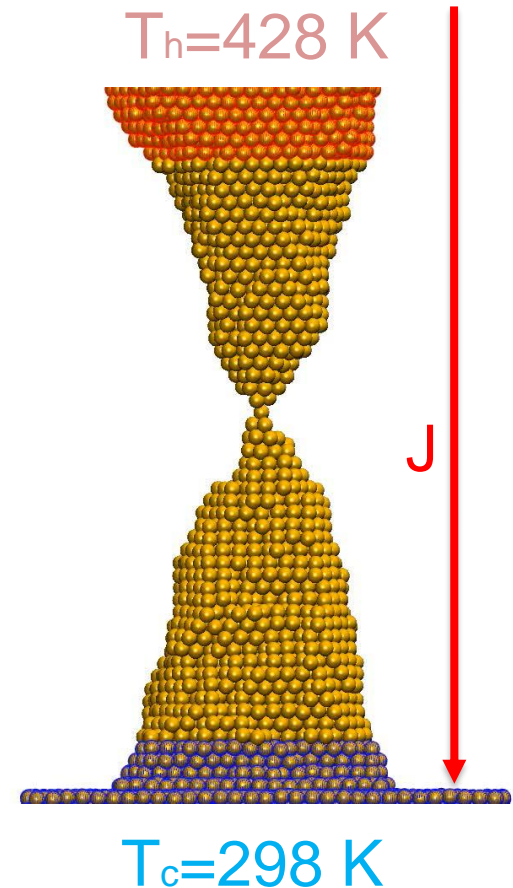
- All atoms included in the simulation.
- **Interaction:** classical force fields.
- **Movement:** Newton's Equations.
- **Temperature:** Thermal baths at different T



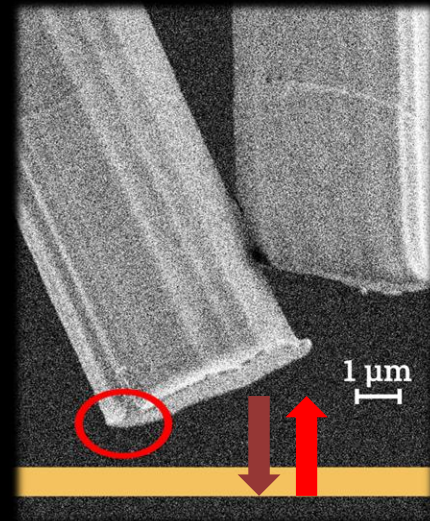
Methods: All-atom Molecular Dynamics simulations

- All atoms included in the simulation.
- **Interaction:** classical force fields.
- **Movement:** Newton's Equations.
- **Temperature:** Thermal baths at different T.

- **Conductance:**
$$K = \frac{J}{T_h - T_c}$$

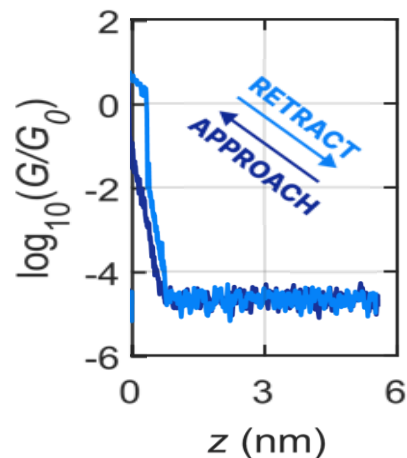
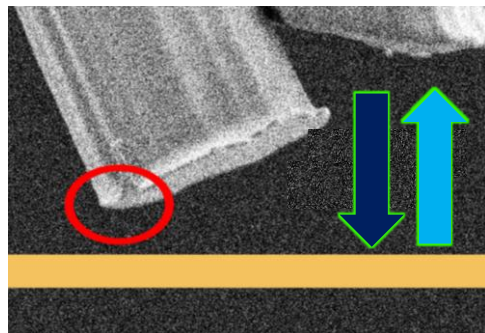


Experimental Results



Nature Communications, **16**, 7342 (2025)

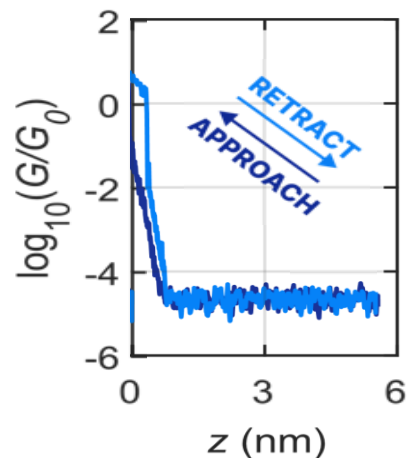
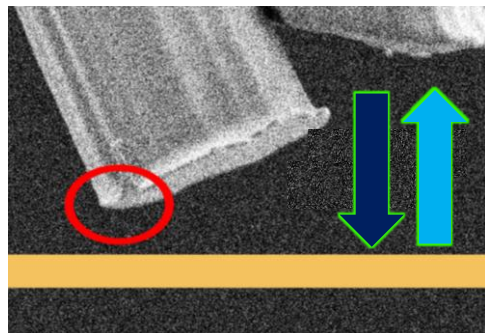
Experimental Results – Major features



Custom STM setup (High-Vacuum E-6 mbar)

➤ Electrical Conductance (**G**)

Experimental Results – Major features

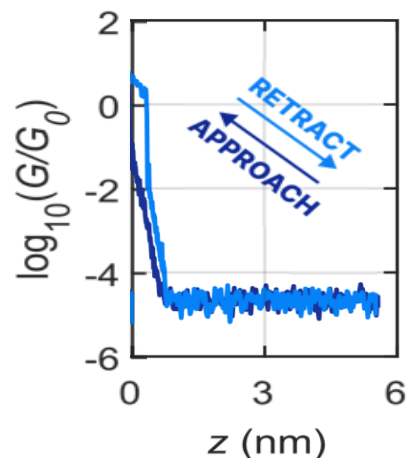
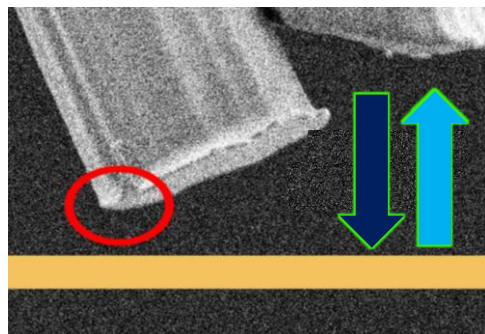


Custom STM setup (High-Vacuum E-6 mbar)

➤ Electrical Conductance (**G**)

➤ Order of magnitude (0.01 G_0)

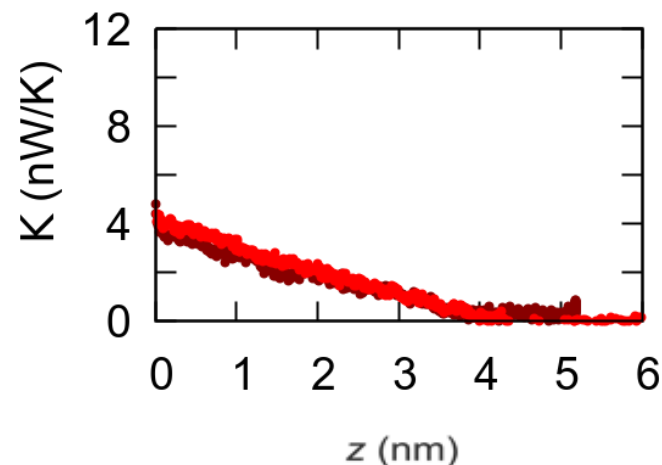
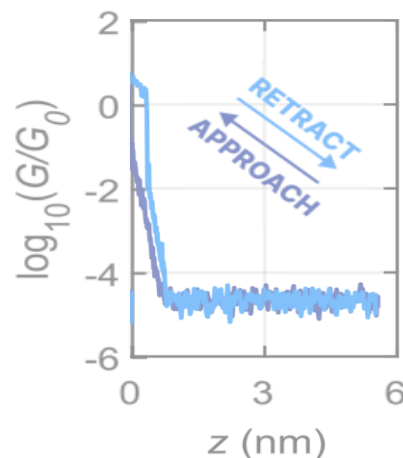
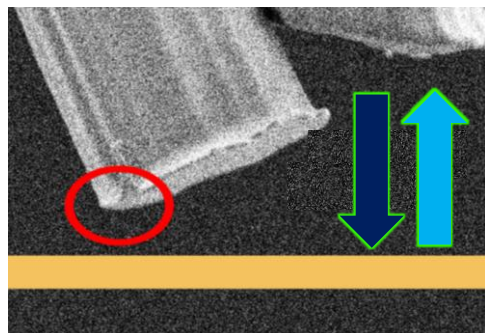
Experimental Results – Major features



Custom STM setup (High-Vacuum E-6 mbar)

- Electrical Conductance (**G**)
- Order of magnitude (0.01 G₀)
- Exponential decay with distance

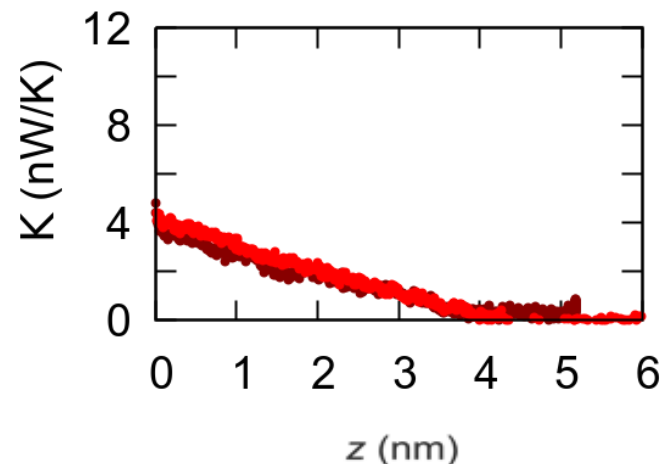
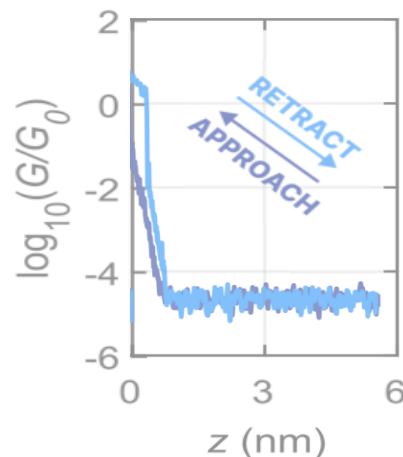
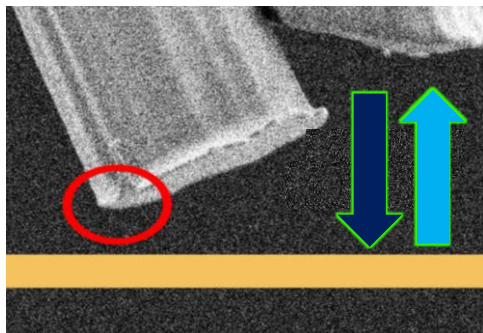
Experimental Results – Major features



Custom STM setup (High-Vacuum E-6 mbar)

- Electrical Conductance (**G**)
- Thermal conductance (**K**)
- Order of magnitude (0.01 G_0)
- Exponential decay with distance

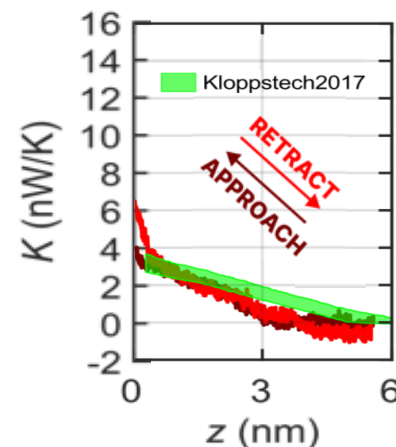
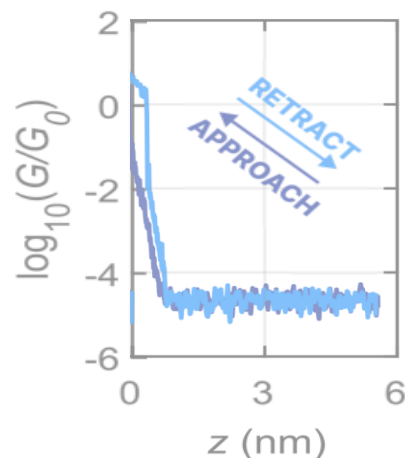
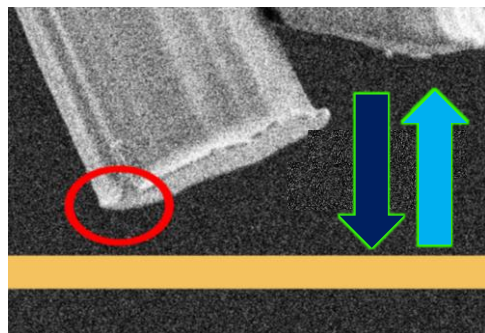
Experimental Results – Major features



Custom STM setup (High-Vacuum E-6 mbar)

- Electrical Conductance (**G**)
- Thermal conductance (**K**)
- Order of magnitude (0.01 G_0)
- Order of magnitude (nW/K)
- Exponential decay with distance

Experimental Results – Major features



Custom STM setup (High-Vacuum E-6 mbar)

➤ Electrical Conductance (**G**)

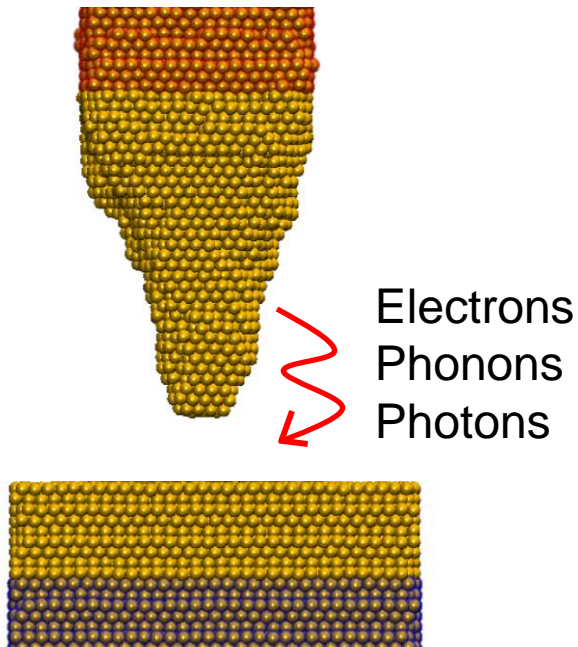
- Order of magnitude (0.01 G_0)
- Exponential decay with distance

➤ Thermal conductance (**K**)

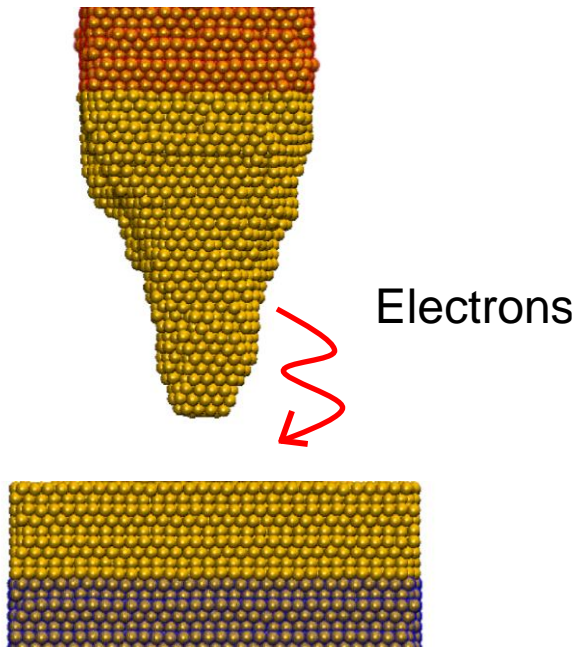
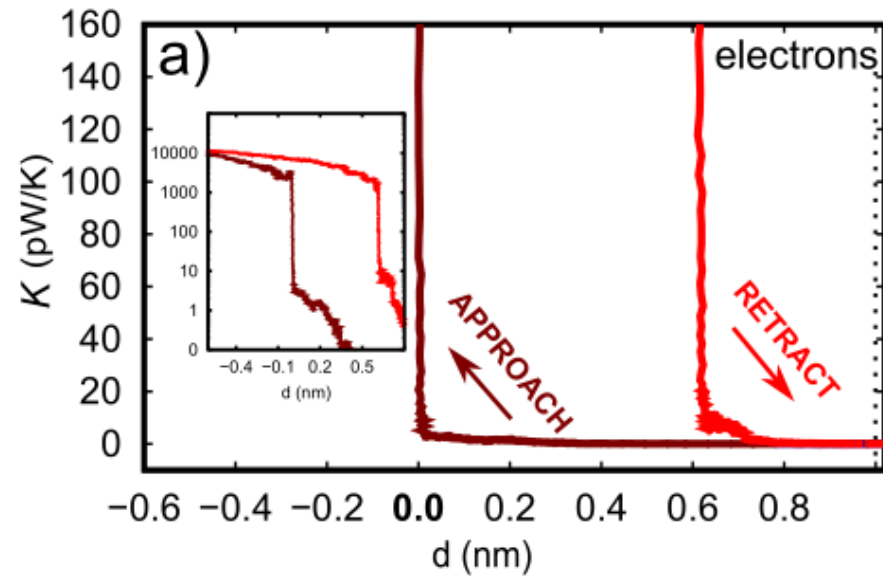
- Order of magnitude (nW/K)
- Linear decay with distance

Theoretical Results

Simulation Results – Conventional Heat-Carriers

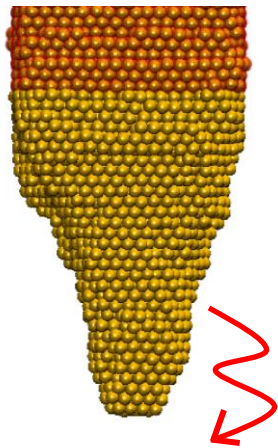
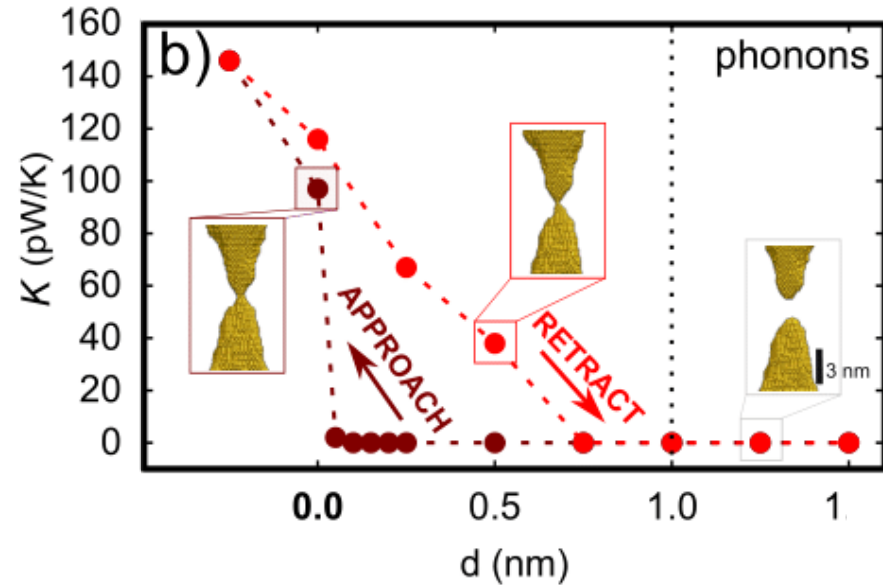
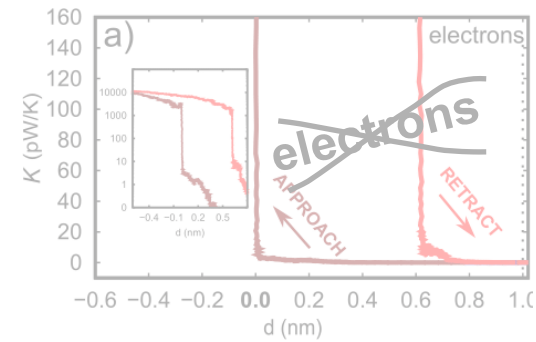


Simulation Results – Conventional Heat-Carriers: **Electrons**



➤ **Electrons:** too short in range

Simulation Results – Conventional Heat-Carriers: **Phonons**

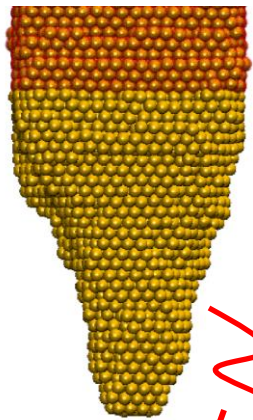
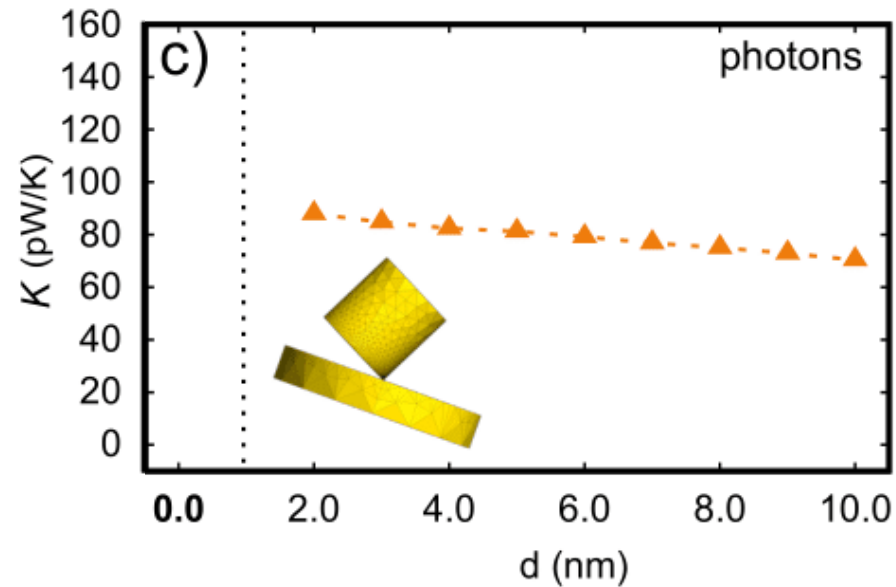
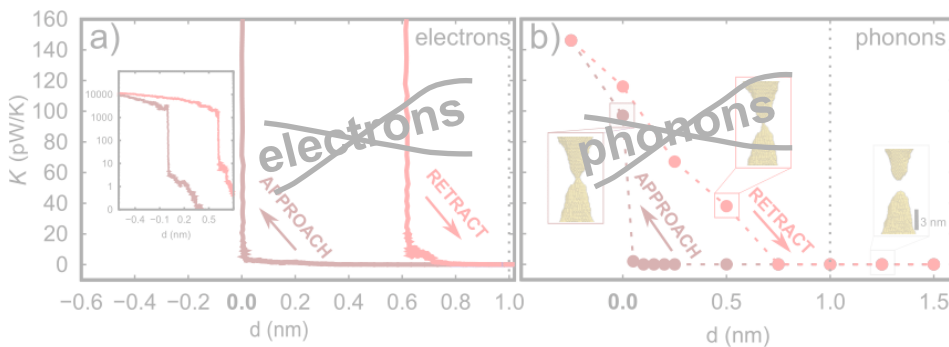


Electrons
Phonons

- **Electrons:** too short in range
- **Phonons:** weak carriers and short in range

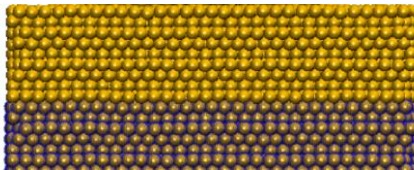


Simulation Results – Conventional Heat-Carriers: **Photons**

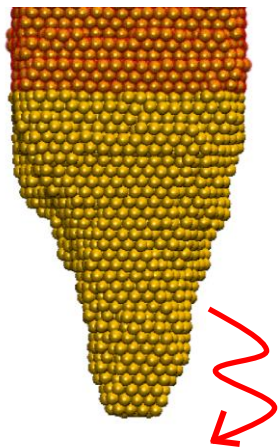
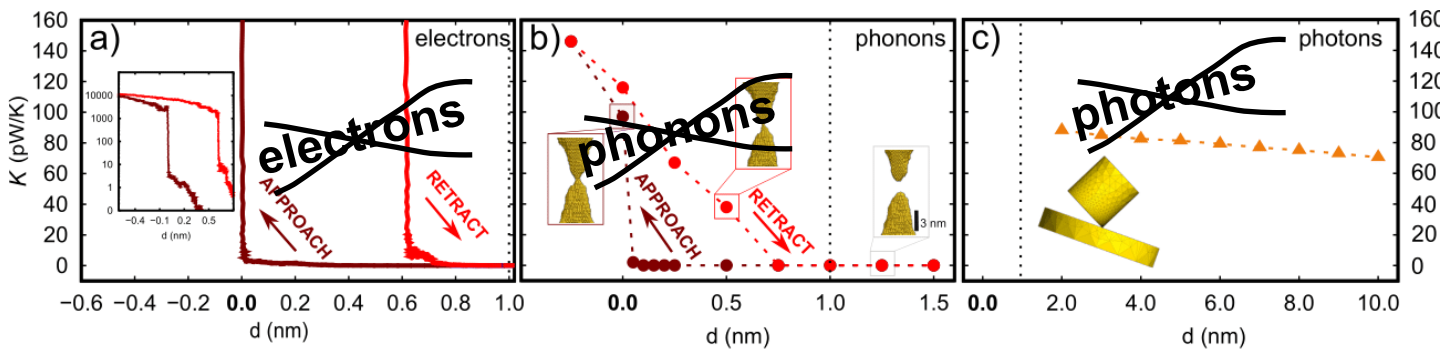


Electrons
Phonons
Photons

- **Electrons:** too short in range
- **Phonons:** weak carriers and short in range
- **Photons:** weak carriers



Simulation Results – Conventional Heat-Carriers **Failure**

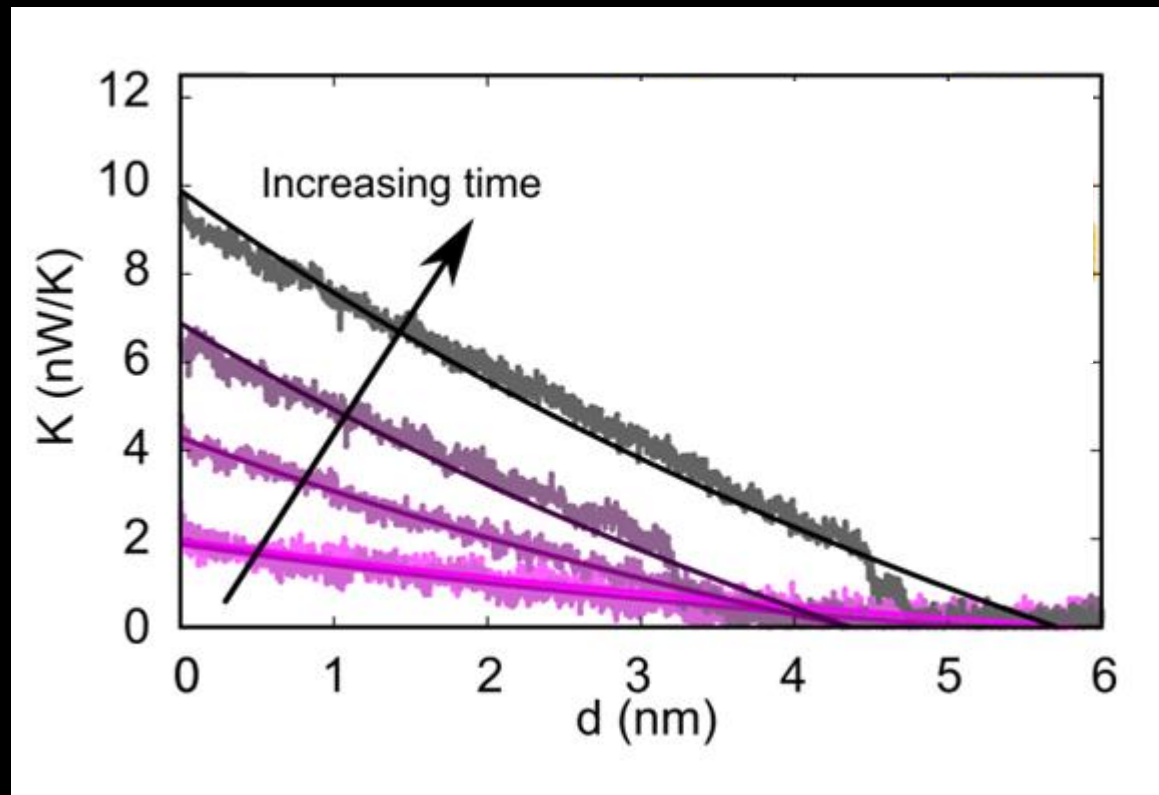


Electrons
Phonons
Photons

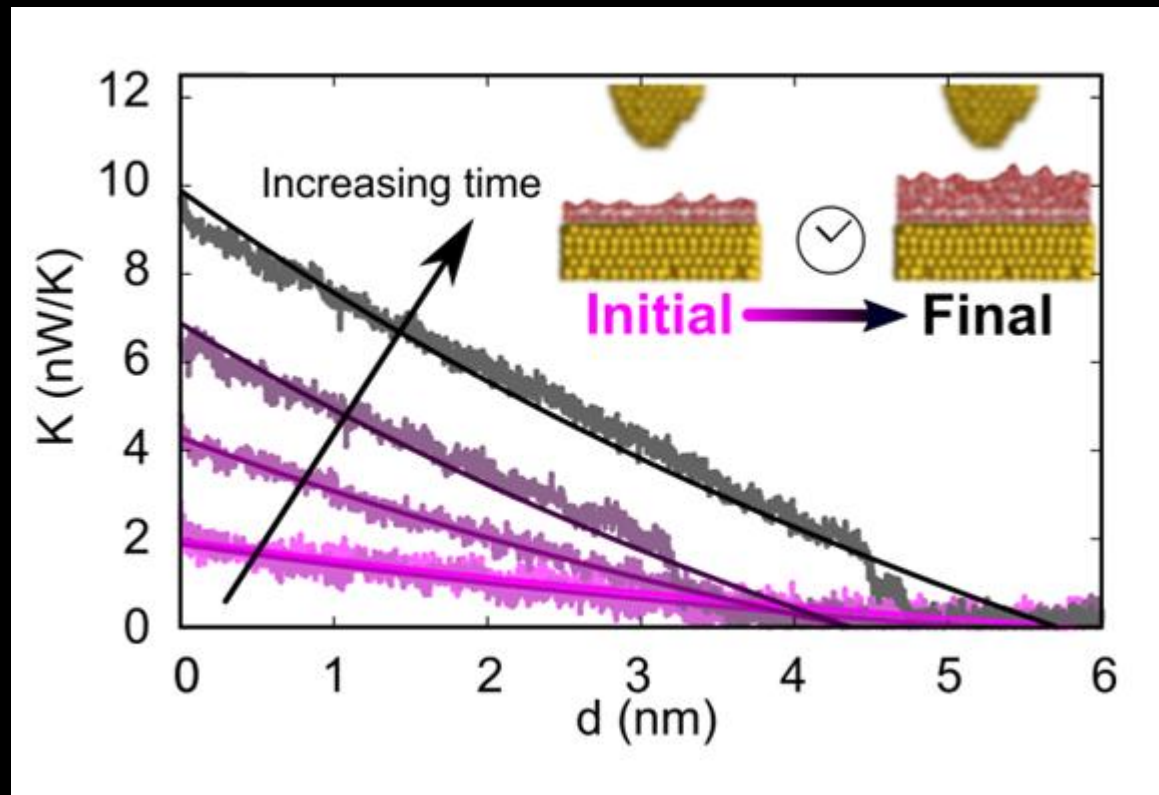
- **Electrons:** too short in range
- **Phonons:** weak carriers and short in range
- **Photons:** weak carriers

No conventional heat-carrier
explains the heat conductance measured

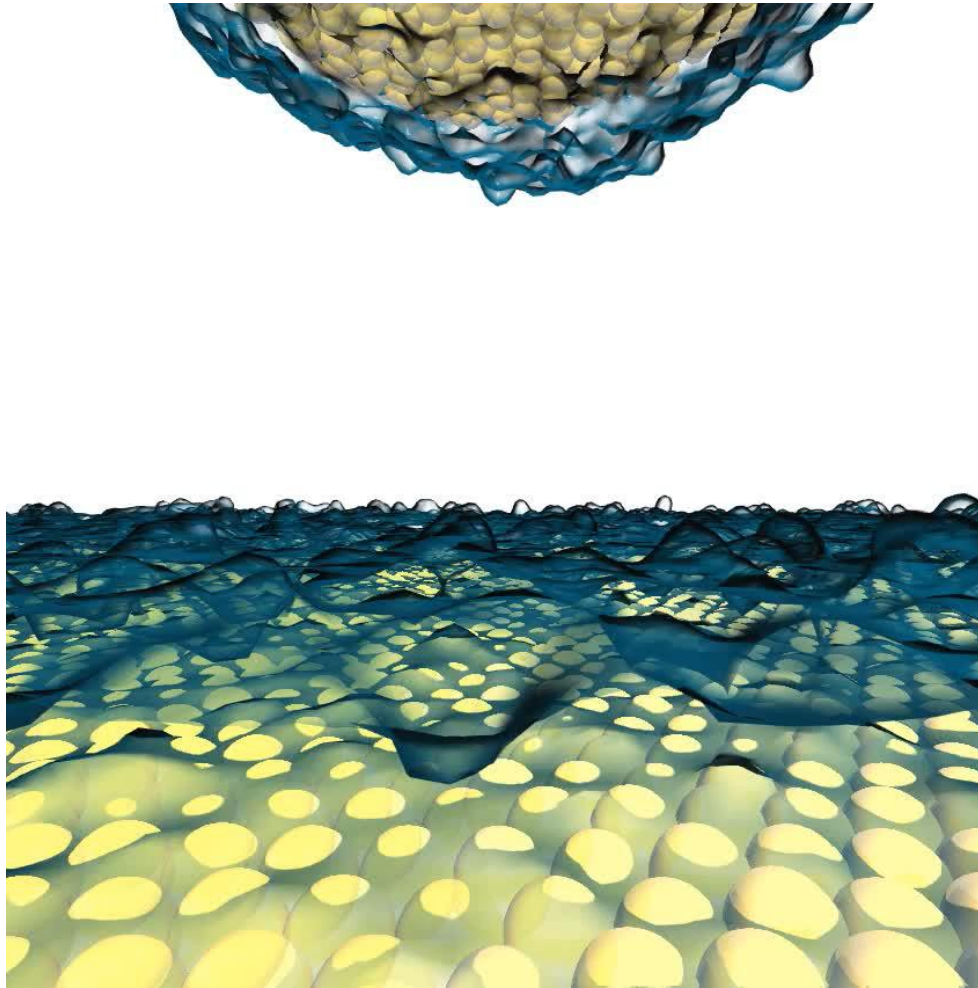
Time evolution



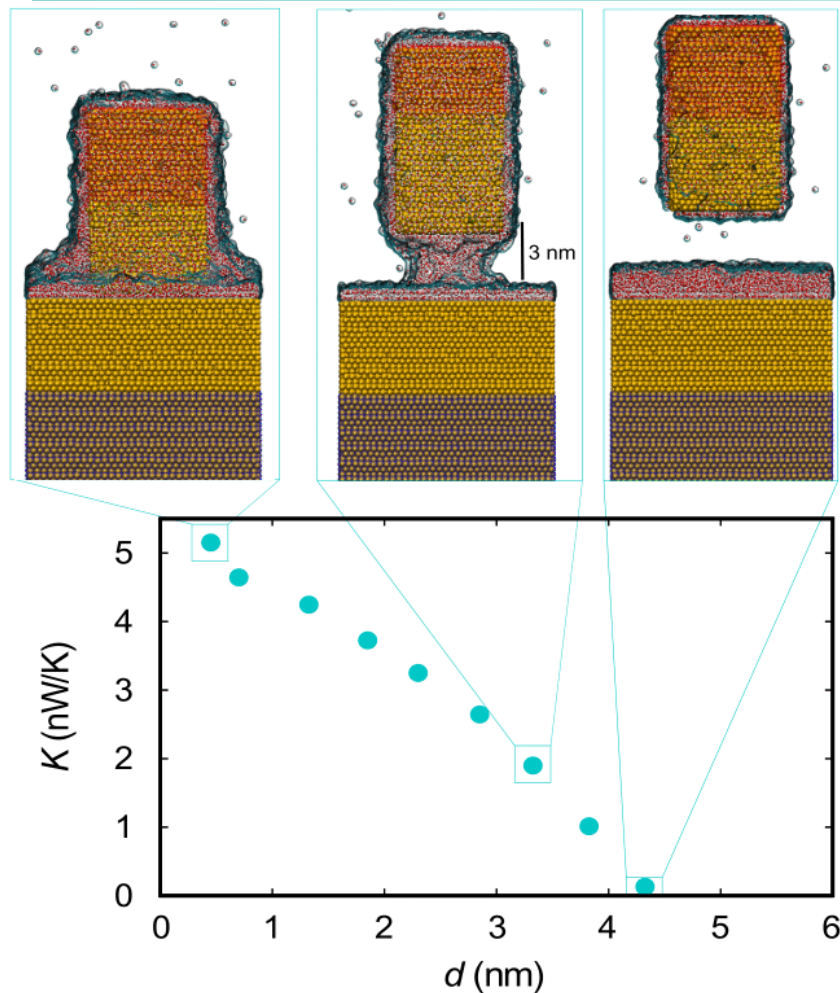
Time evolution



Simulation Results – Conventional Heat-Carriers **Failure**

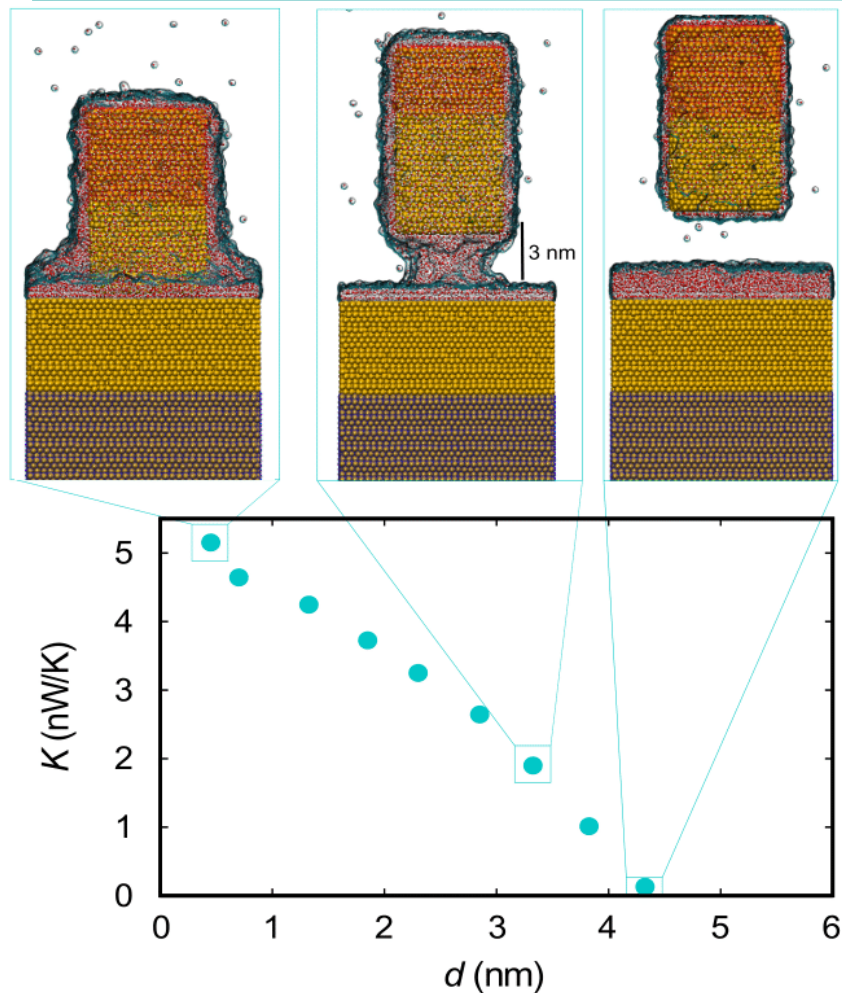


Simulation Results – Water meniscus

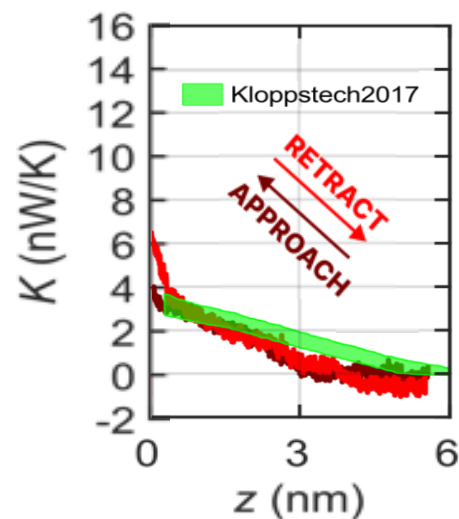


- Order of magnitude: nW/K
- Lineal dependence (4 nm)

Simulation Results – Water meniscus

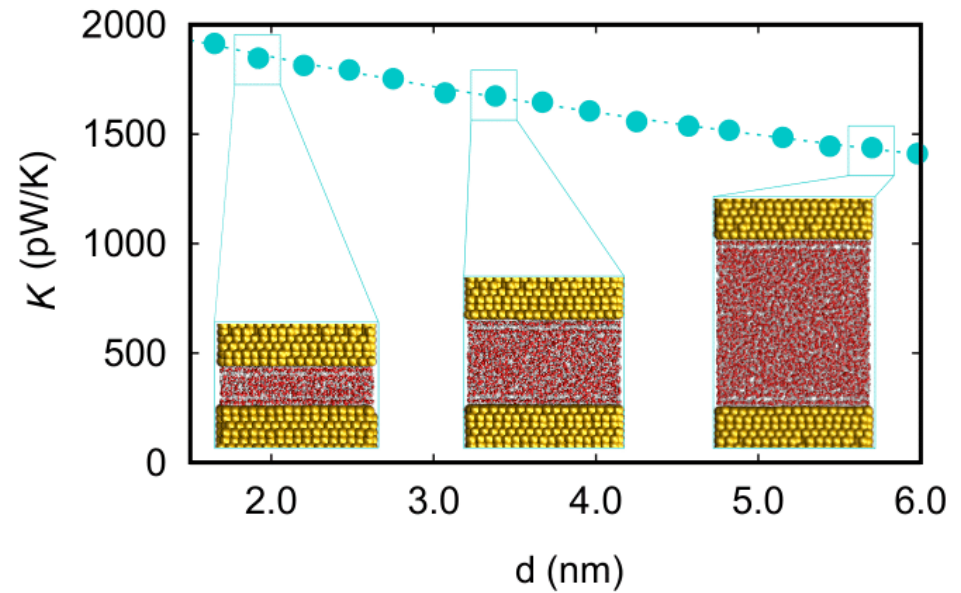
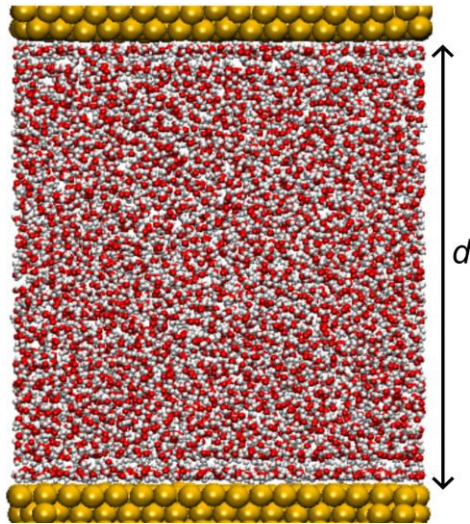


- Order of magnitude: nW/K
- Lineal dependence
- Experiment reproduced



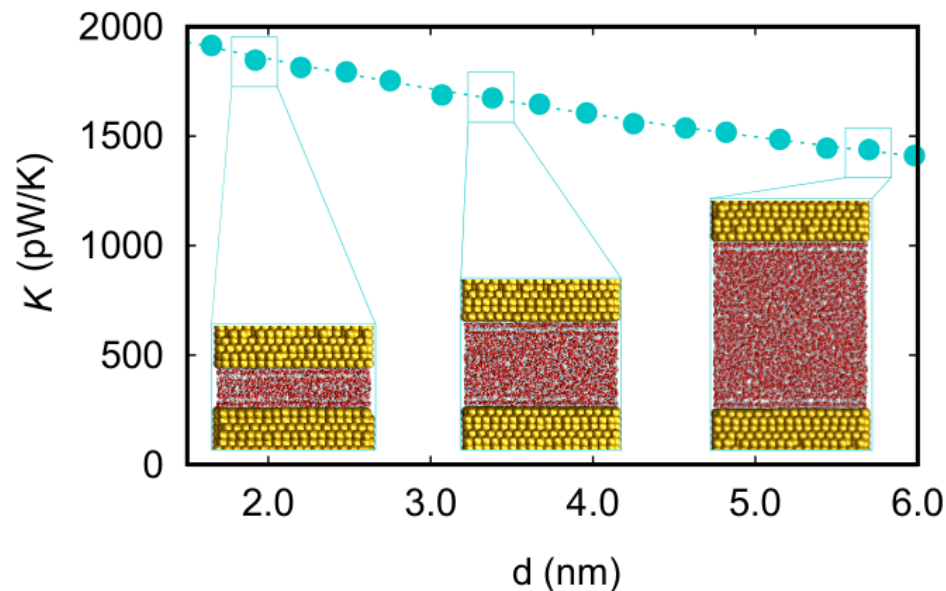
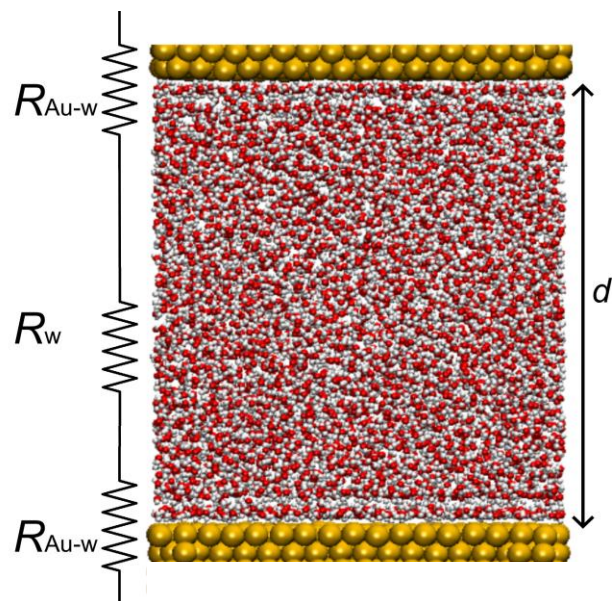
Order of magnitude

Simulation Results – Water meniscus: Magnitude



➤ Order of magnitude: nW/K

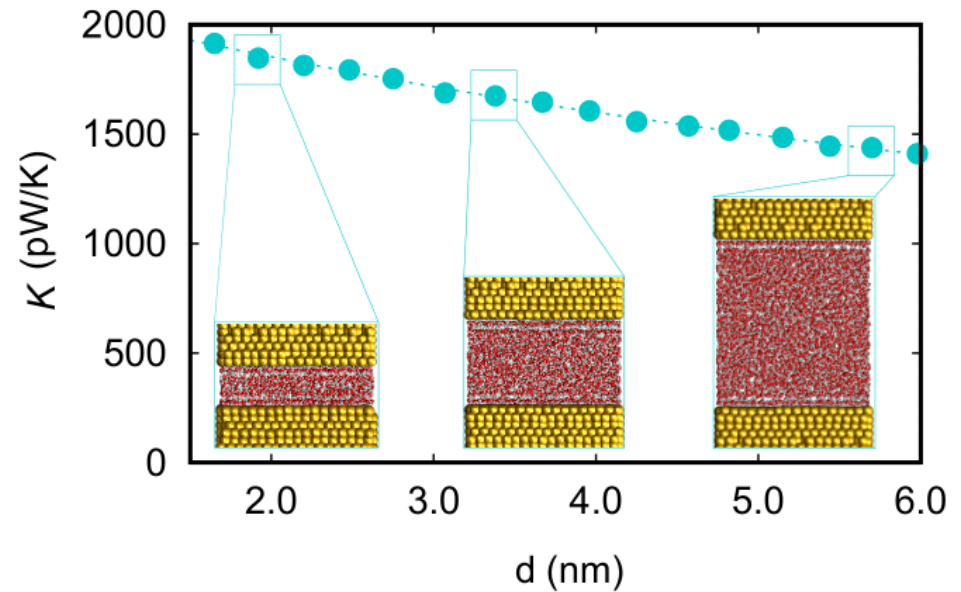
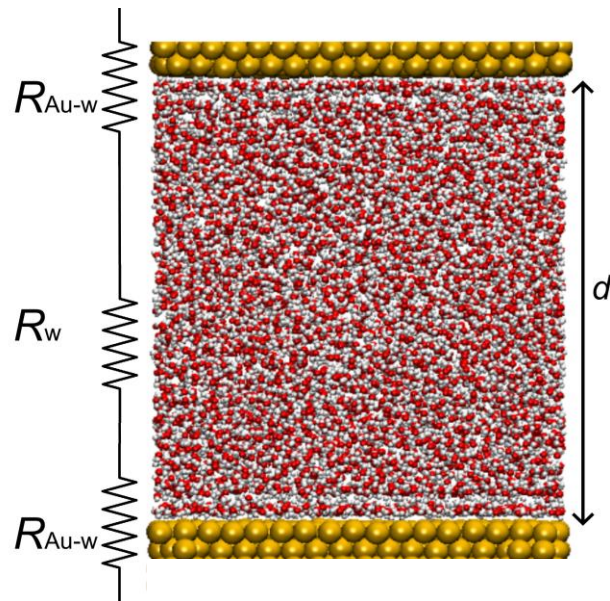
Simulation Results – Water meniscus: Magnitude



➤ Order of magnitude: nW/K

➤ Conductance modeled after 3 resistances:
$$K(d) = \frac{A}{2\sigma_{Au-w} + \sigma_w d}$$

Simulation Results – Water meniscus: Magnitude



➤ Order of magnitude: nW/K

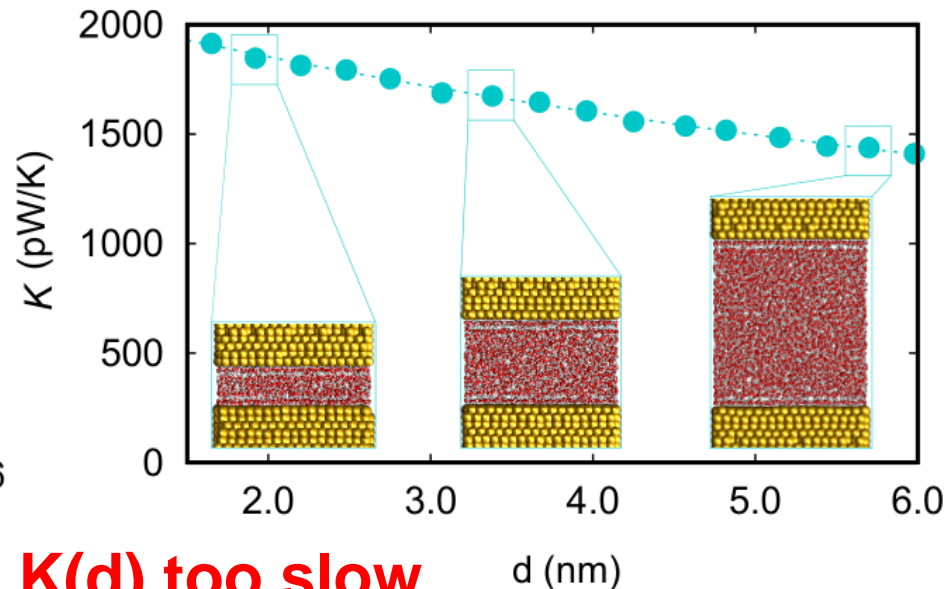
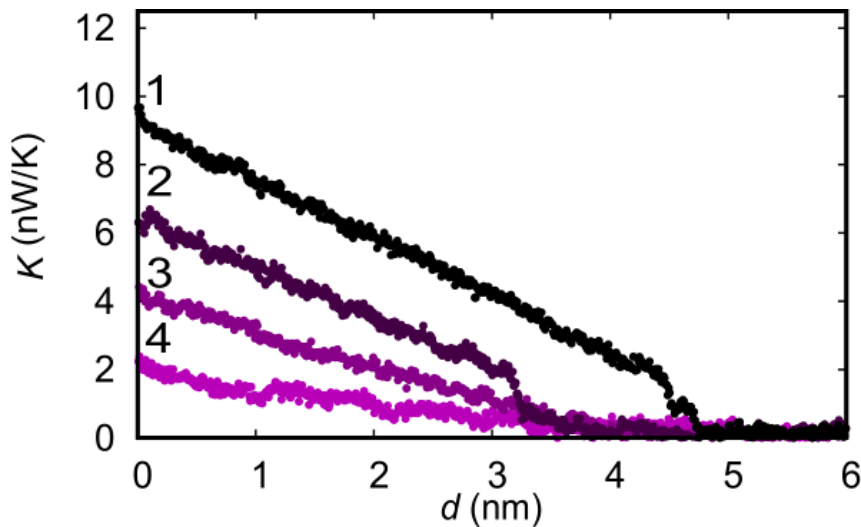
➤ Conductance modeled after 3 resistances: $K(d) = \frac{A}{2\sigma_{Au-w} + \sigma_w d}$

➤ Conductivity in line with literature $\kappa_{Au-w} = 0.12 \frac{nW}{Knm^2}$, $\kappa_w = 0.78 \frac{nW}{Knm^2}$

Touloukian *et al*, Purdue Research Foundation, TPRC Data Series Volume 3, pp. 120 (1970)

Olarte-Plata, Bresme, J. Chem. Phys, 156, 204701 (2022)

Simulation Results – Water meniscus: Magnitude



Decay of $K(d)$ too slow

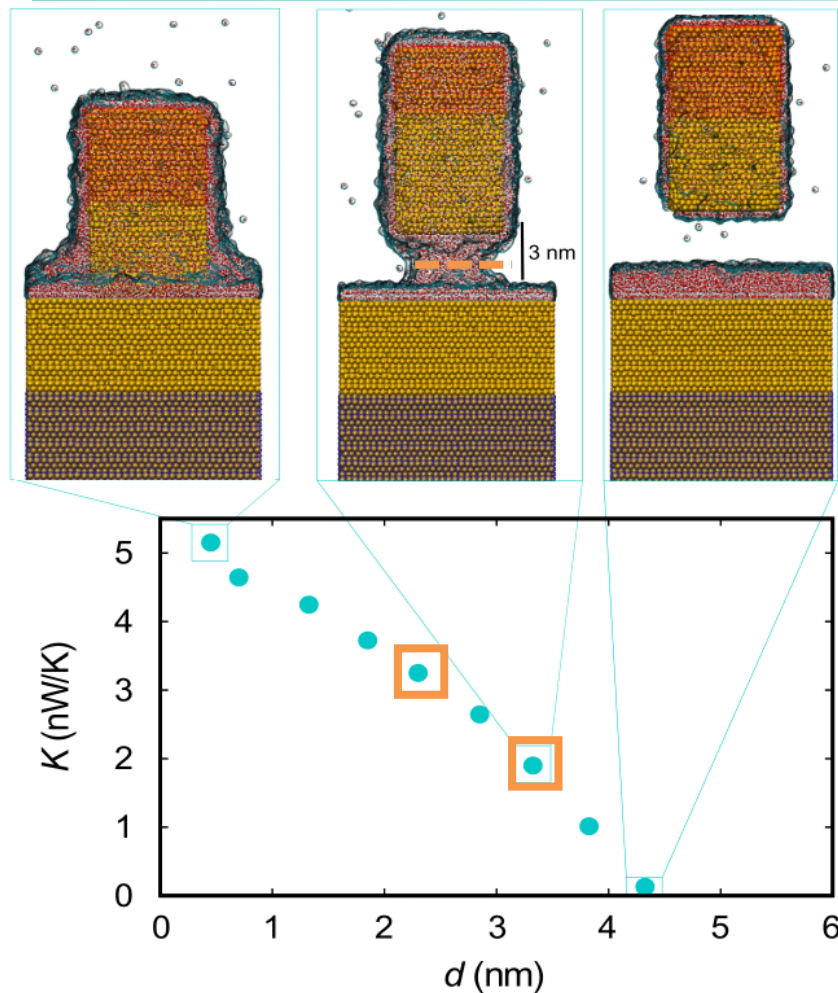
➤ Order of magnitude: nW/K

➤ Conductance modeled after 3 resistances: $K(d) = \frac{A}{2\sigma_{Au-w} + \sigma_w d}$

➤ Conductivity in line with literature: $\kappa_{Au-w} = 0.12 \frac{nW}{Knm^2}$, $\kappa_w = 0.78 \frac{nW}{Knm}$

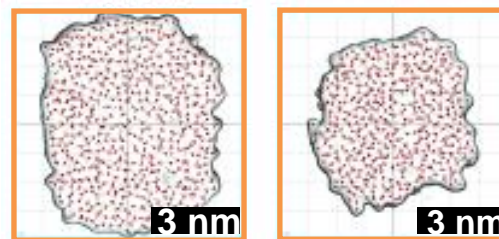
Lineal dependence

Simulation Results – Water meniscus

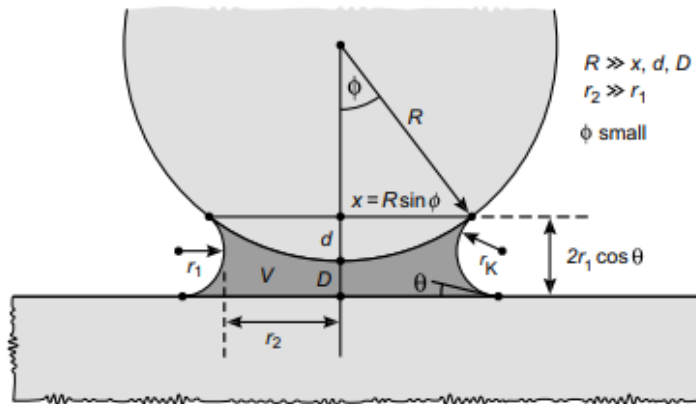


- Order of magnitude: nW/K
- Lineal dependence (4 nm)

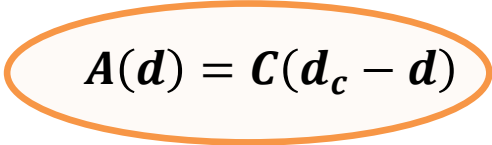
$$K(d) = \frac{A(d)}{2\sigma_{Au-w} + \sigma_w d}$$



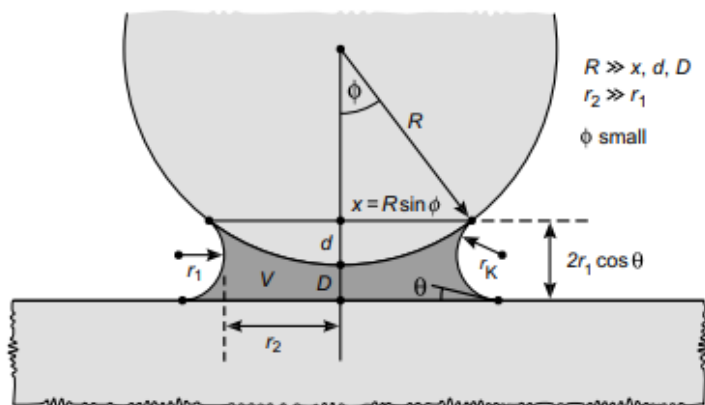
Simulation Results – Water meniscus: Dependence



J. N. Isrealachvili, *Intermolecular and surface forces*, 1992

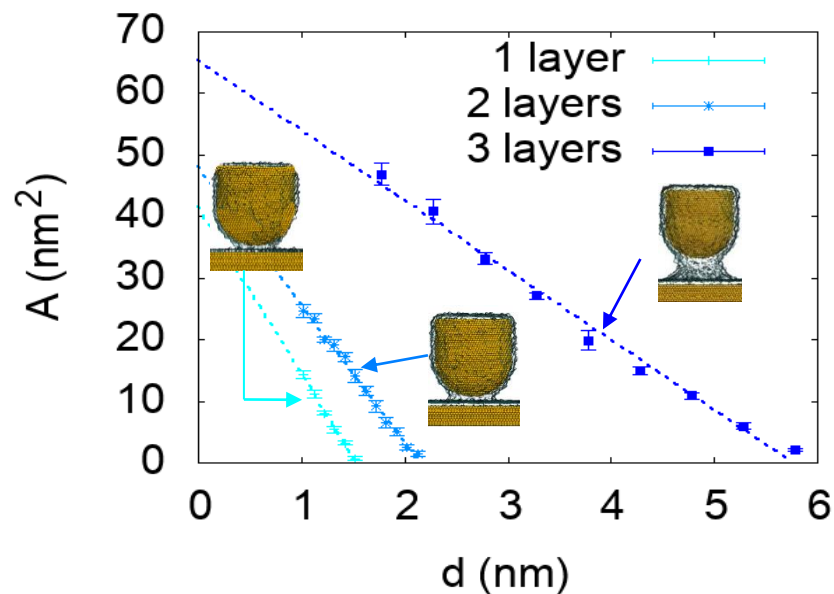
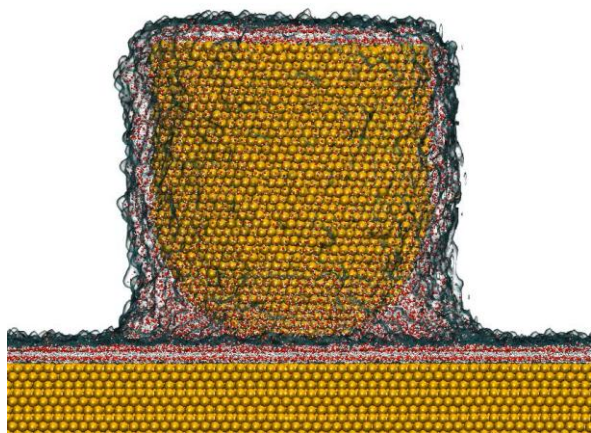


Simulation Results – Water meniscus: Dependence

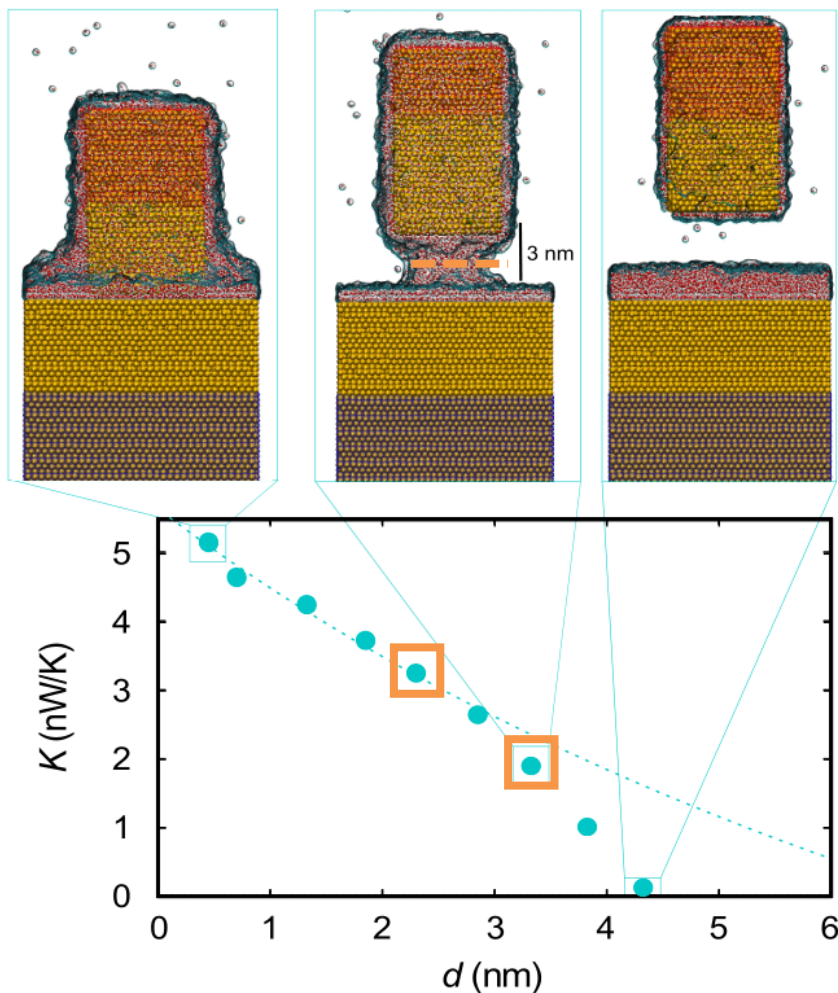


J. N. Isrealachvili, *Intermolecular and surface forces*, 1992

$$A(d) = C(d_c - d)$$



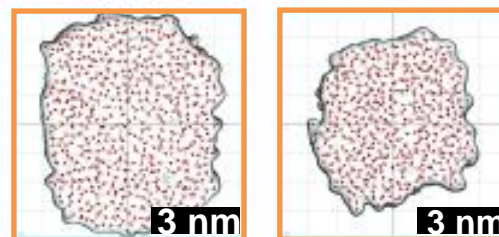
Simulation Results – Water meniscus



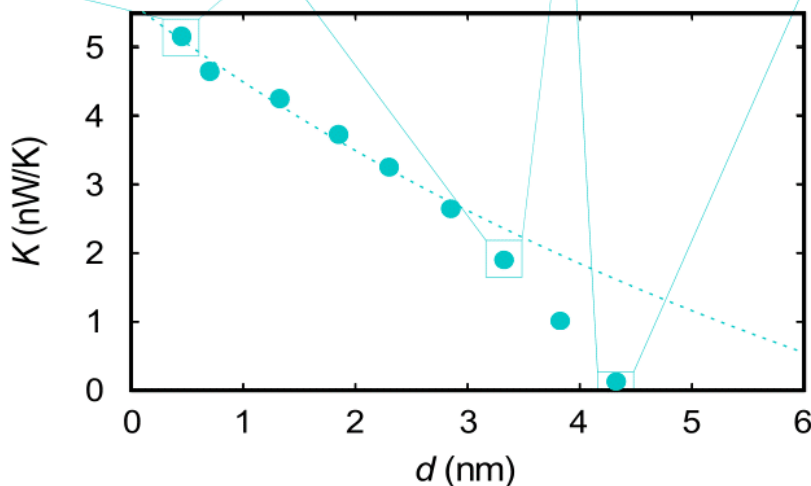
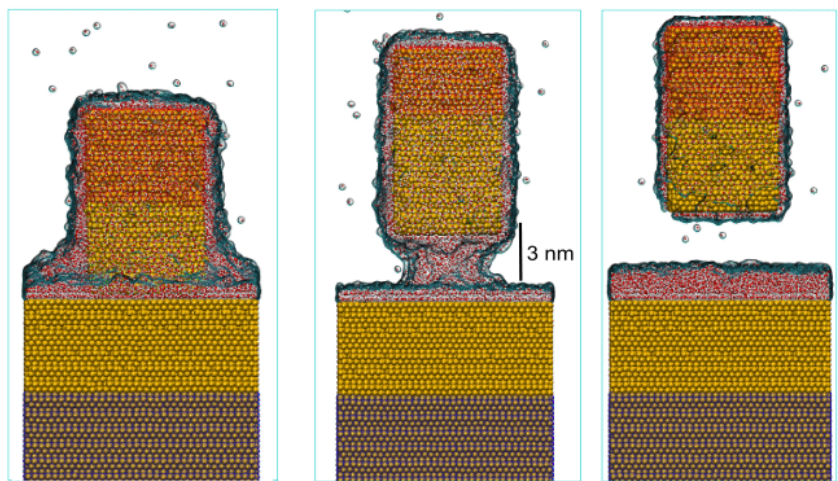
- Order of magnitude: nW/K
- Lineal dependence (4 nm)

$$K(d) = \frac{A(d)}{2\sigma_{Au-w} + \sigma_w d}$$

$$A(d) = C(d_c - d)$$



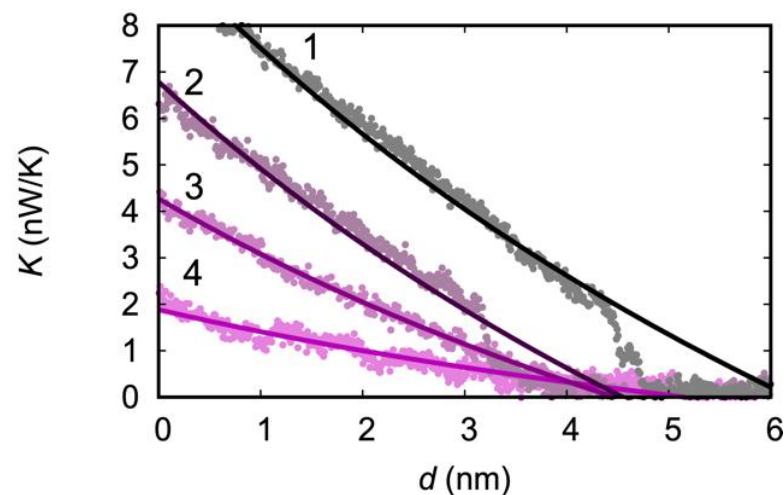
Simulation Results – Water meniscus



- Thermal conductance: nW/K
- Lineal dependence (4 nm)

$$K(d) = \frac{A(d)}{2\sigma_{Au-w} + \sigma_w d}$$

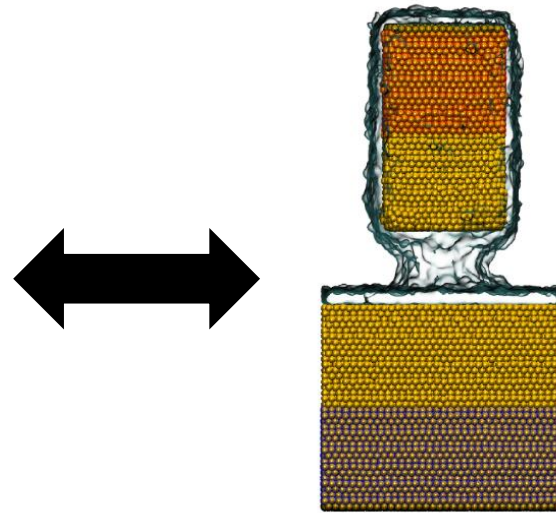
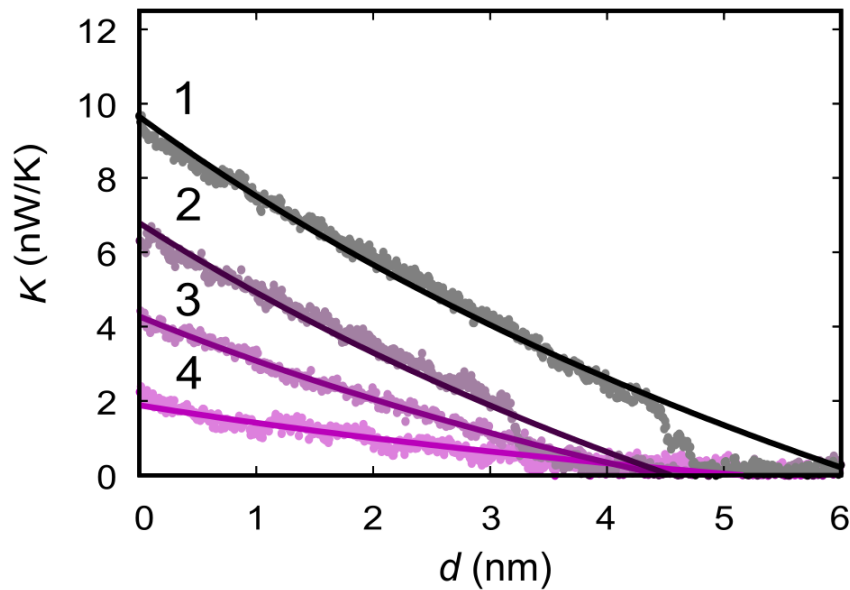
$$A(d) = C(d_c - d)$$



Conclusions

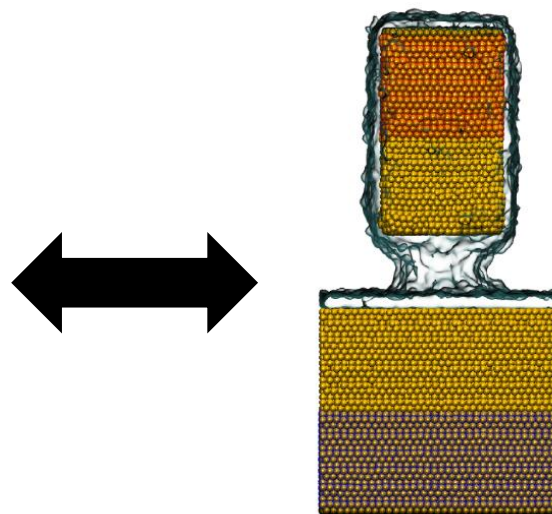
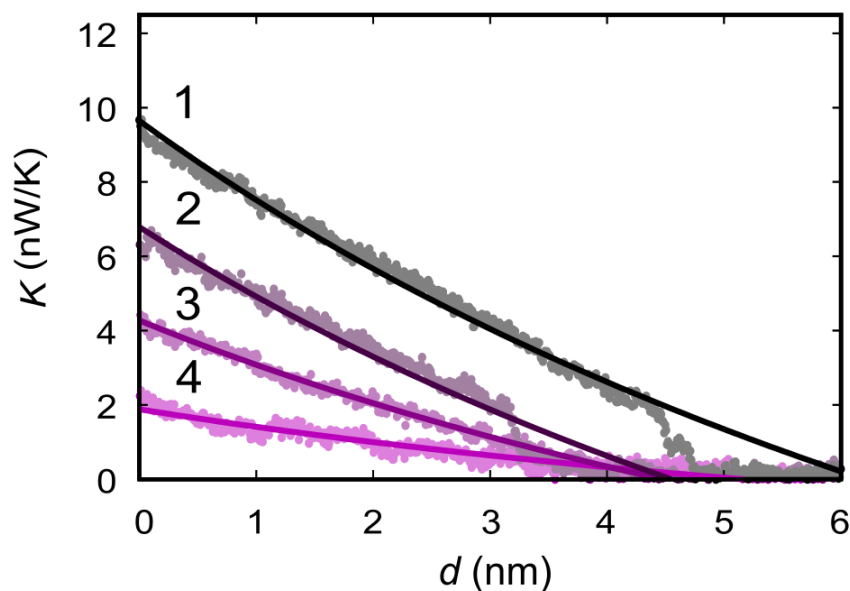
Summary

What happens in vacuum gaps?



Summary

What happens in vacuum gaps?



$$K(d) = \frac{C(d - d_c)}{2\sigma_{Au-w} + \sigma_w d}$$



Diffusive process
(~1nm)

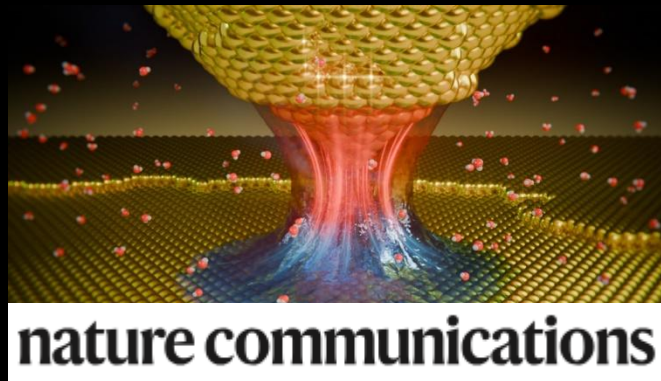
Acknowledgements



Collaborators:



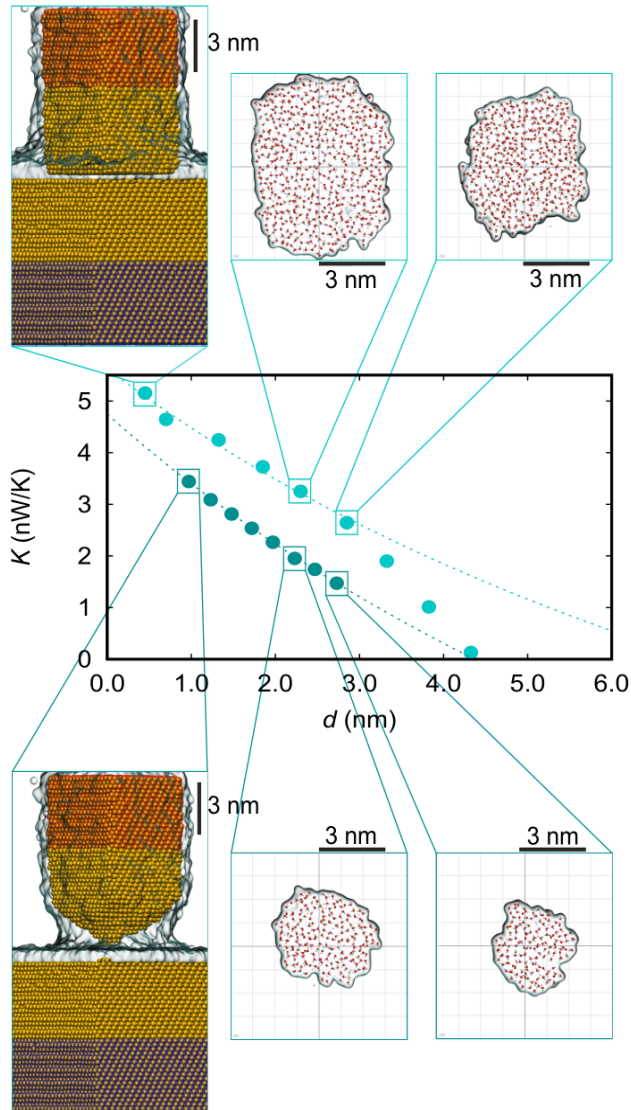
Thank you for your attention!!



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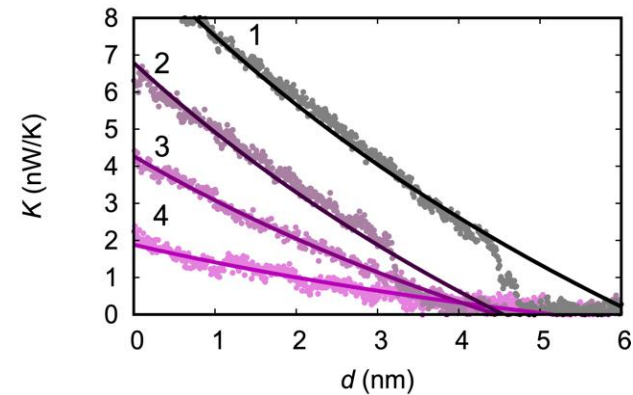
Simulation Results – Thermal conductance



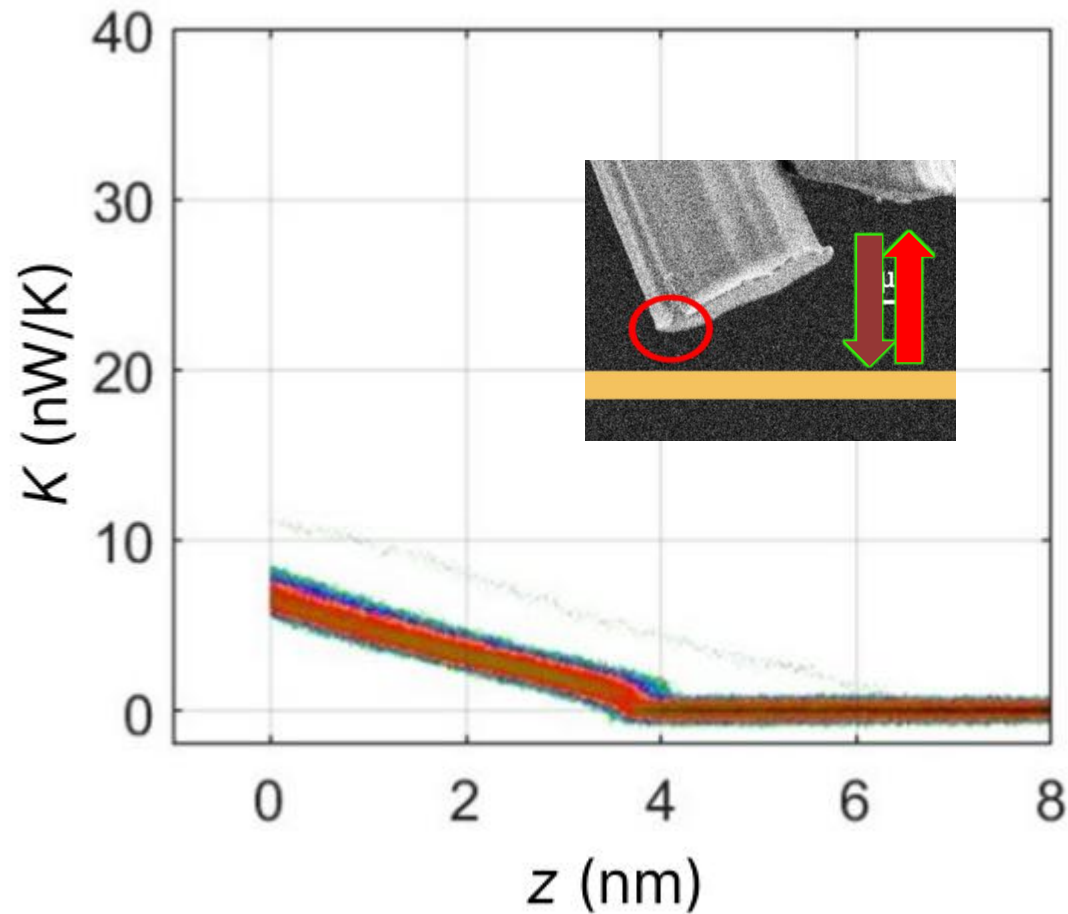
➤ Thermal conductance: nW/K

$$K(d) = \frac{A(d)}{2\sigma_{Au-w} + \sigma_w d}$$

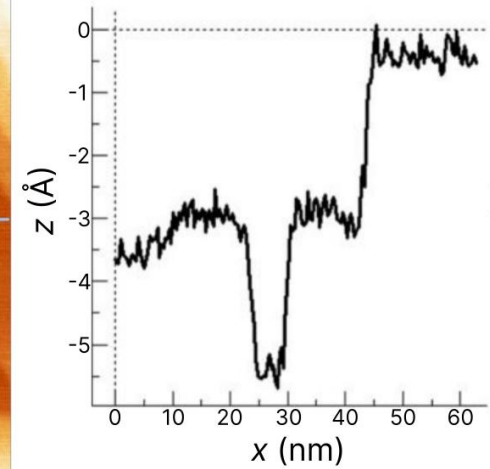
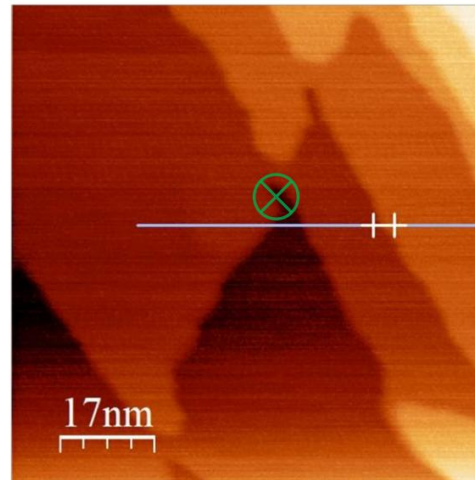
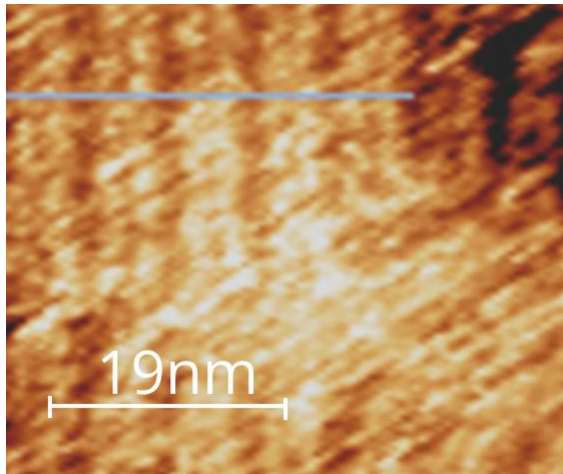
$$A(d) = C(d_c - d)$$



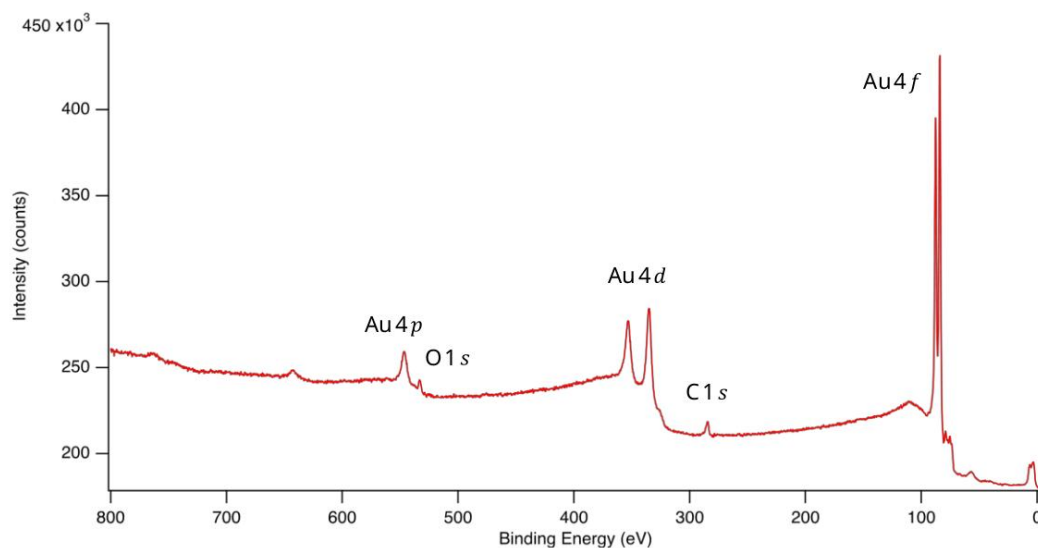
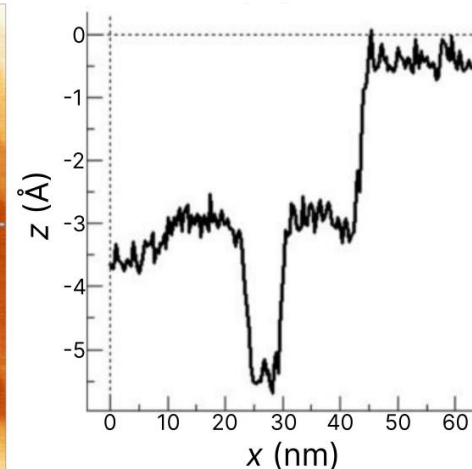
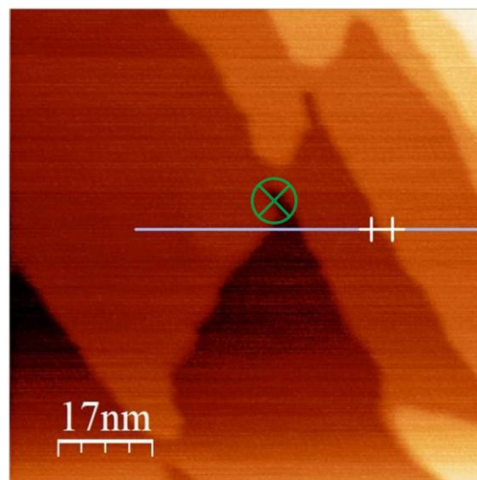
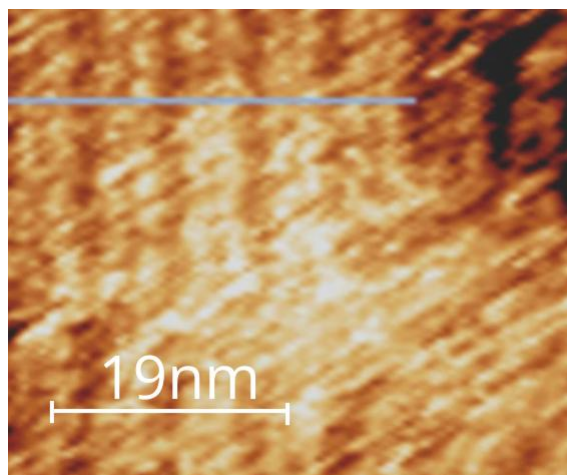
Experimental Results – Thermal conductance histogram



Experimental Results – Clean surfaces



Experimental Results – Clean surfaces



Methods: All-atom Molecular Dynamics simulations

- **Technique:** Non-Equilibrium Molecular Dynamics
- **Software:** Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- **Force field:**

Embedded Atom Method (EAM) parametrization for gold.

TIP4P model for water molecules

Lenard-Jones potential for gold-oxygen interactions

- **Timestep:** 1 fs
- **Simulation time:** 5 ns equilibration, 5 ns production results

