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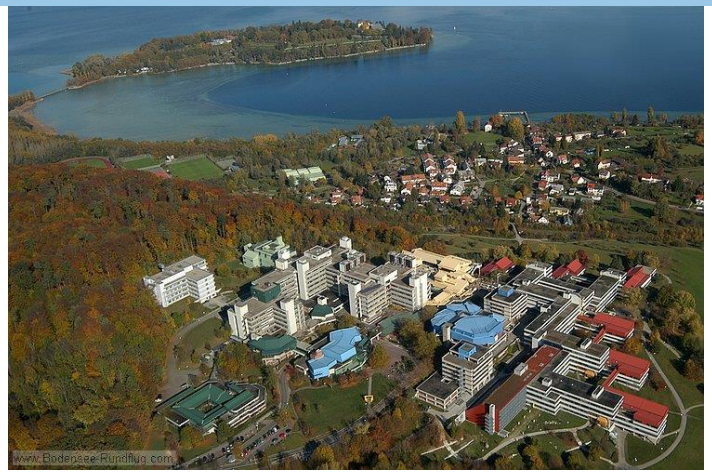
Heat dissipation and thermopower in atomic-scale junctions

Jun.-Prof. Fabian Pauly
Poznan, 27.09.2013

Theory of Nanostructures, Department of Physics, University of Konstanz



Outline

- **Introduction**
- **Heat dissipation and thermopower in atomic-scale junctions**
  - Motivation
  - Experimental approach
  - Theory
  - Tuning the heating
  - Conclusions
- **Influence of vibrations on electron transport**
  - Method
  - Gold junctions
  - Octane-based junctions
- **Miscellaneous**
  - Plasmon-induced conductance enhancement in single-molecule junctions
  - A current-driven single-atom memory

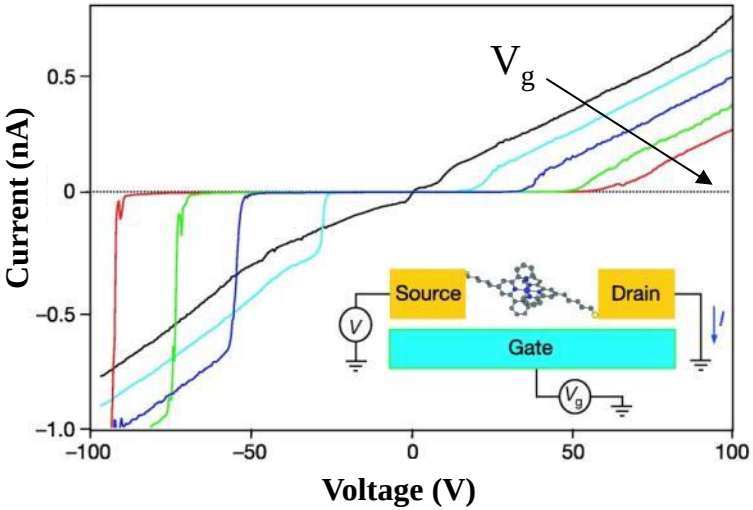
Introduction

Visions of molecular electronics

- Limits of miniaturization of electrical circuits
- Functional and possibly cheap devices at the smallest scale
- Understanding of interface-related or interface-dominated electronic behavior

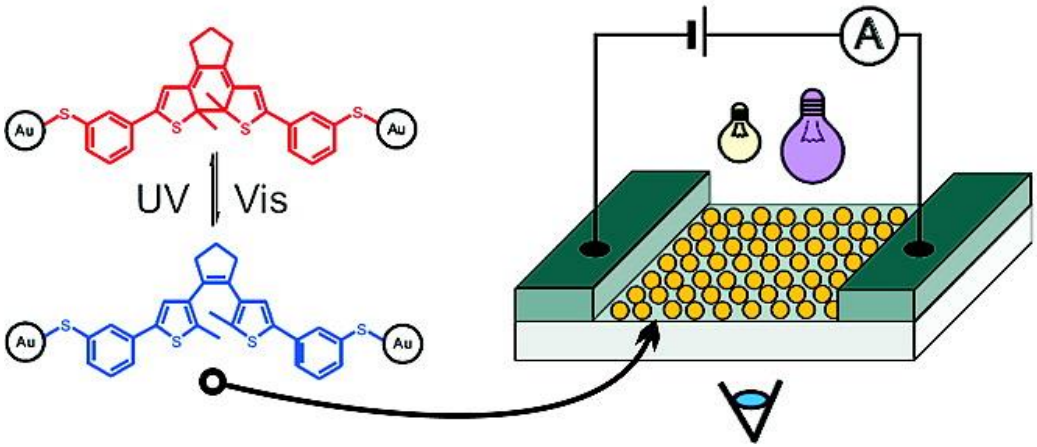
Single-molecule transistor

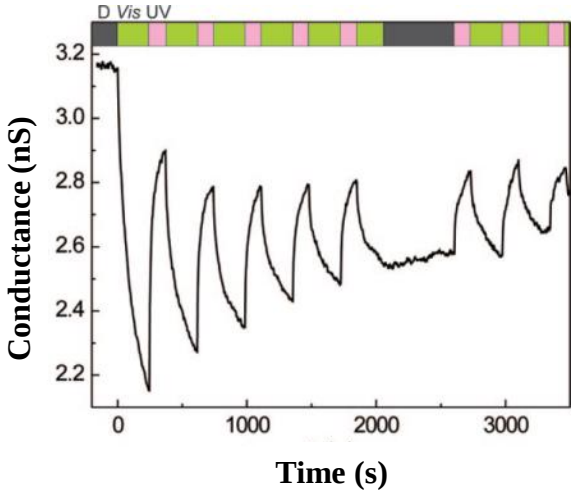
[J. Park *et al.*, Nature 2002]



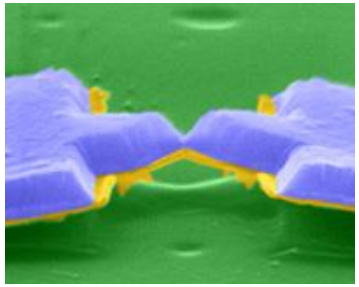
Molecule-gold nanoparticle array

[S. J. van der Molen *et al.*, Nano Lett. 2009]

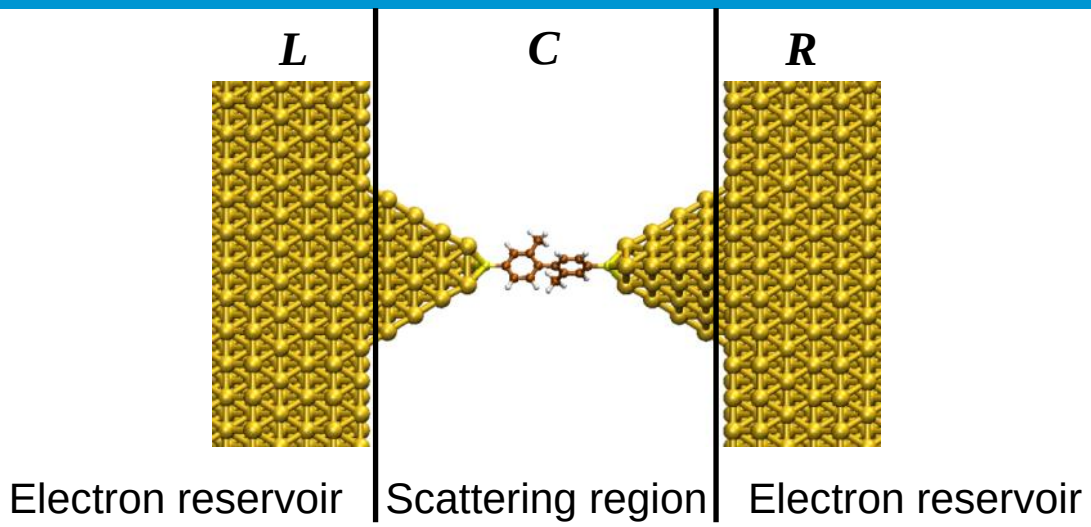




Atomistic modeling of charge transport



Real system



Goals

- Understand charge transport mechanisms at the molecular scale
- Quantitative description/prediction of charge transport properties

Challenges

- Material- and molecule-specific a*b-initio* description of the electronic structure; choice (large system size): DFT (**TURBOMOLE**)
- Determination of stable contact geometries (geometry optimization, **TURBOMOLE**)
- Consideration of electrodes and their coupling to the central scattering region → infinite, nonperiodic system
- Description of electric transport (Nonequilibrium due to finite bias/current, excitation of vibrations, …)

Landauer scattering theory and Green's functions

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Conductance

$$G = G_0 \tau(E_F) = G_0 \mathrm{Tr}[tt^\dagger] = G_0 \sum_i \tau_i$$

Transmission matrix

$$t(E) = \sqrt{\Gamma_L(E)} G^r_{CC}(E) \sqrt{\Gamma_R(E)}$$

Conductance quantum $G_0 = 2e^2 / h$

Green's function

$$G^r_{CC} = \left(ES_{CC} - H_{CC} - \Sigma^r_L - \Sigma^r_R \right)^{-1}$$

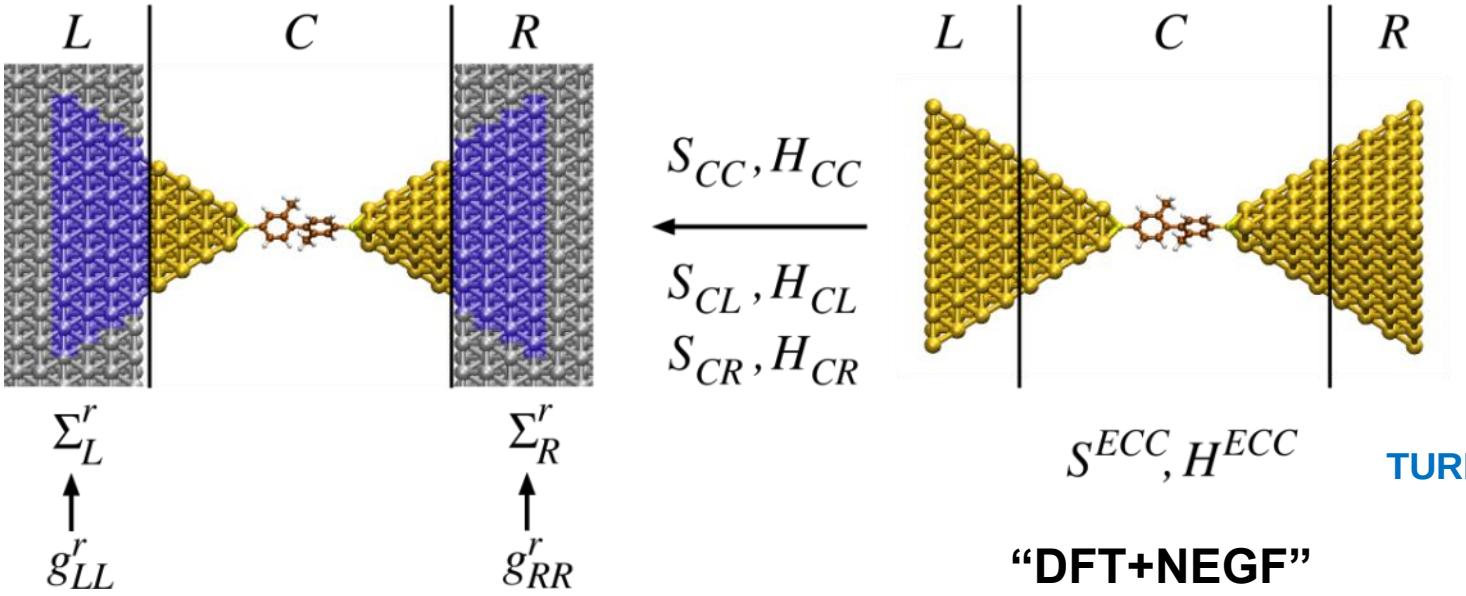
Self energies (X=L,R)

$$\Sigma^r_X = \left(H_{CX} - ES_{CX} \right) g^r_{XX} \left(H_{XC} - ES_{XC} \right)$$

Linewidth broadening matrix $\Gamma_X = -2\,\mathrm{Im}\left[\Sigma^r_X\right]$

Cluster-based ansatz

[F. Pauly *et al.*, New J. Phys. 10, 125019 (2008)]



TURBOMOLE@work

"DFT+NEGF"

Level alignment at metal-molecule contact

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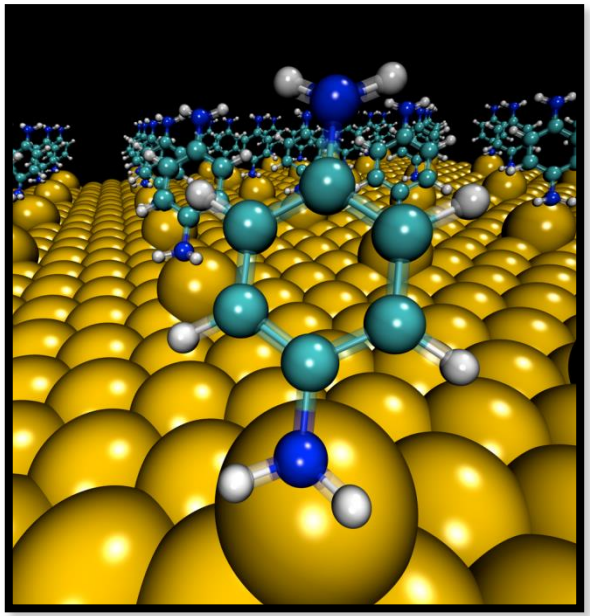
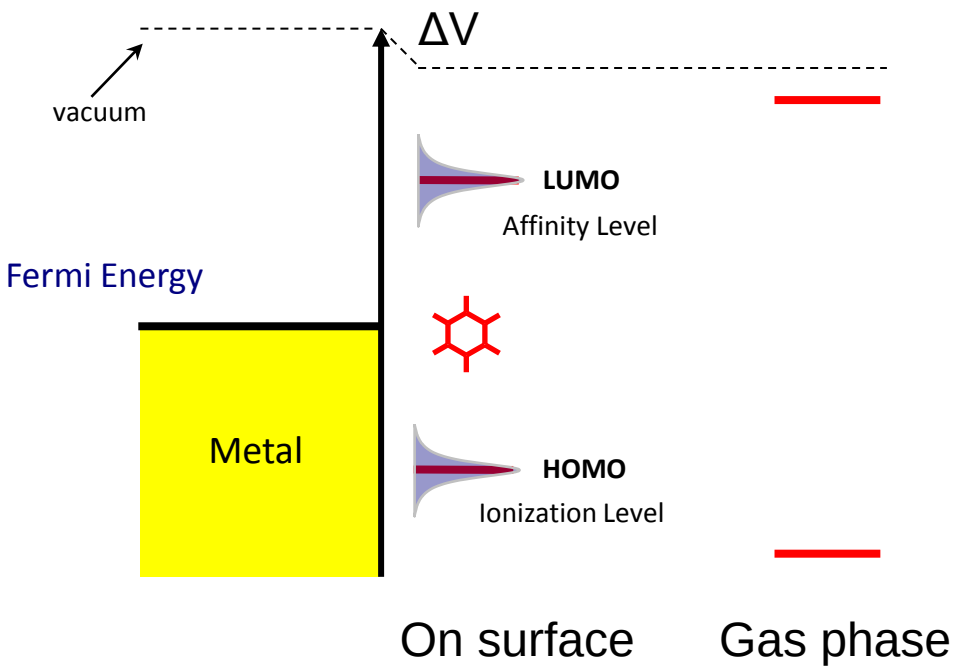
Metal-molecule contact



Energy level diagram



Physical effects influencing level alignment

- Interfacial charge rearrangement
- Quantum mechanical coupling
- Nonlocal surface polarization

Spectral adjustment: "DFT+Σ"

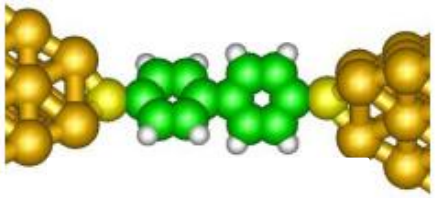
S. Y. Quek *et al.*, Nano Lett. 7, 3477 (2007)

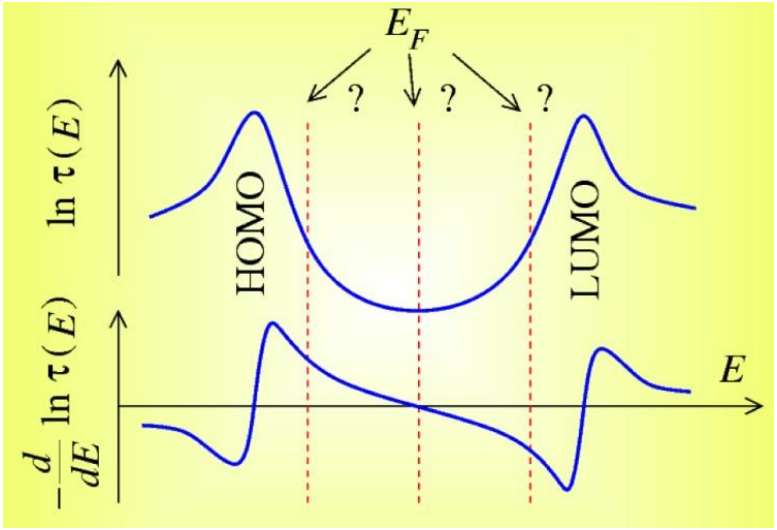
GW quasiparticle methods

M. Strange *et al.*, PRB 83, 115108 (2011).

Why thermopower?

Seebeck effect





M. Paulsson *et al.*, PRB 2003

Landauer-Büttiker formalism

Thermopower (electronic contribution):

$$S = -\left.\frac{\Delta V}{\Delta T}\right|_{I=0} \approx -\frac{\pi^2 k_B}{3e} k_B T \left.\frac{\partial \ln(\tau(E))}{\partial E}\right|_{E=E_F}$$

- Sign of *S* distinguishes "*electron* type" and „*hole* type" conduction; hint to position of E_F with respect to HOMO and LUMO

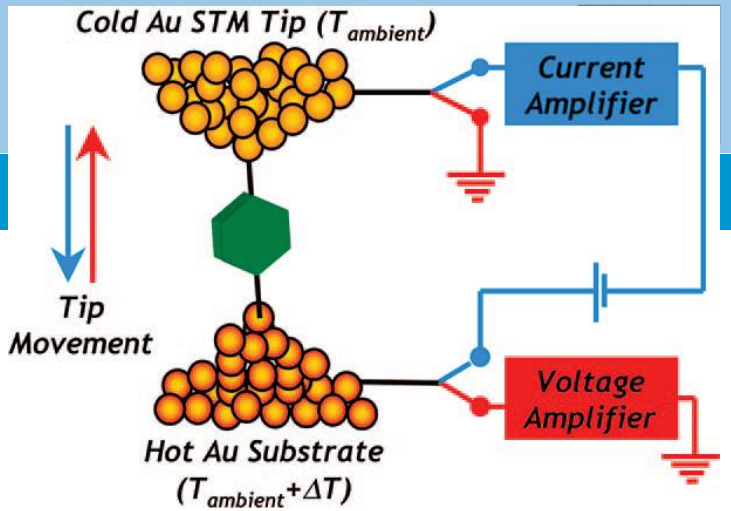
Experiments (Segalman/Majumdar, Berkeley)

- P. Reddy *et al.*, Science 315, 1568 (2007)
- J. A. Malen *et al.*, Nano Lett. 9, 1164 (2009)

Recently also other groups

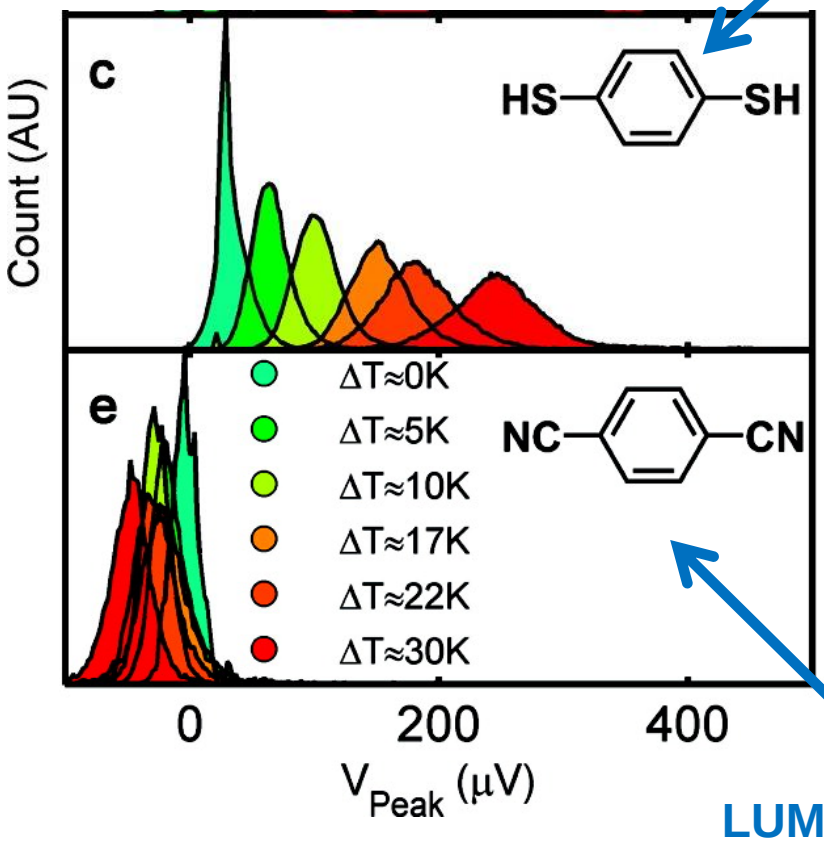
- J. R. Widawsky *et al.*, Nano Lett. 12, 354 (2012)
- C. Evangeli *et al.*, Nano Lett. 13, 2141 (2013)
- S. Guo *et al.*, Nano Lett. 13, 4326 (2013)

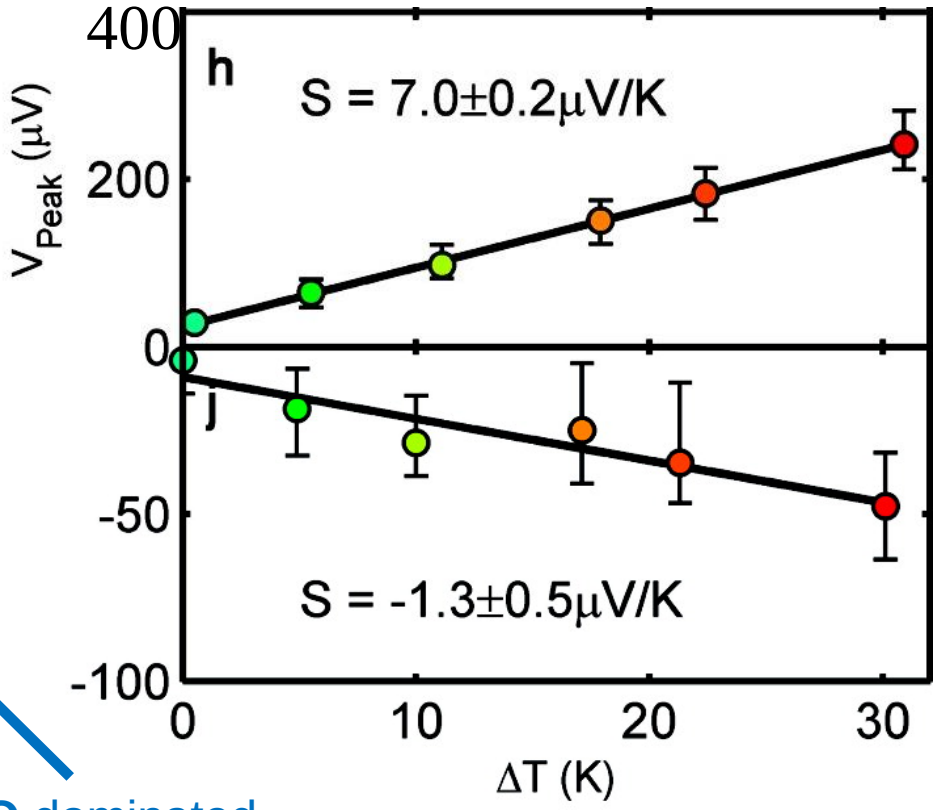
HOMO- vs. LUMO-Transport



HOMO dominated

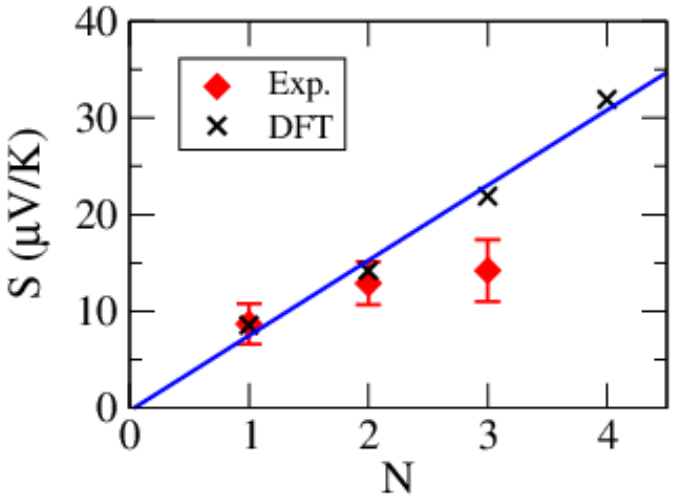
[K. Baheti *et al.*, Nano Lett. 2008]





LUMO dominated

Theoretical studies of the thermopower



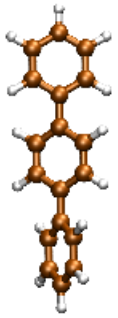
Length dependence

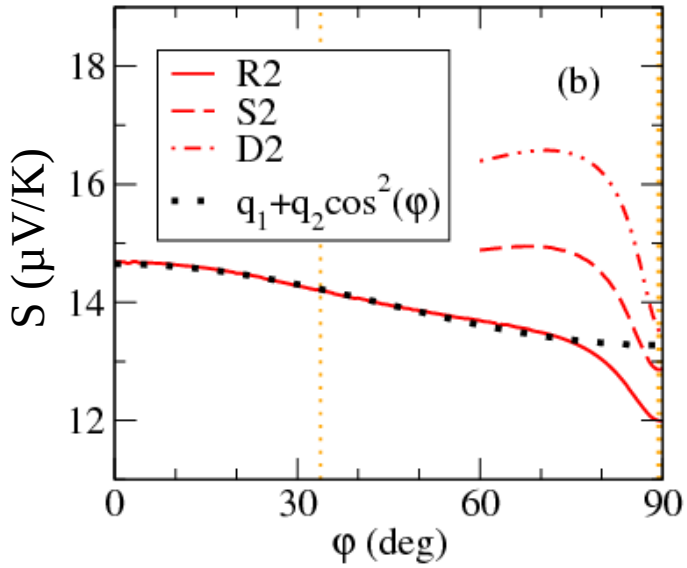
$$\tau(E) \approx \alpha(E)\exp(-\beta(E)N)$$

$$S = S^{(0)} + S^{(1)}N$$

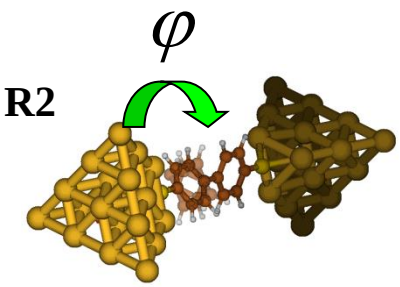
Exp.: P. Reddy *et al.*, Science 2007
Theory: F. Pauly *et al.*, PRB 2008

N=3





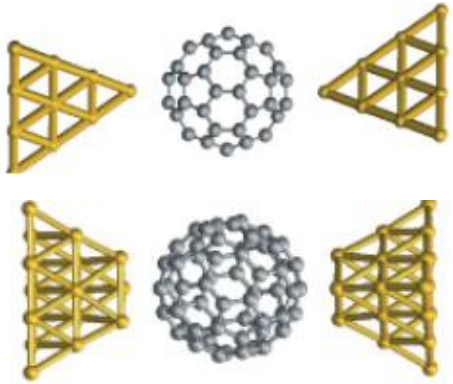
Influence of conjugation



F. Pauly *et al.*, PRB 2008
M. Bürkle *et al.*, PRB 2012

C_{60} junctions

S. Bilan et al., PRB 2012



Towards thermoelectrics

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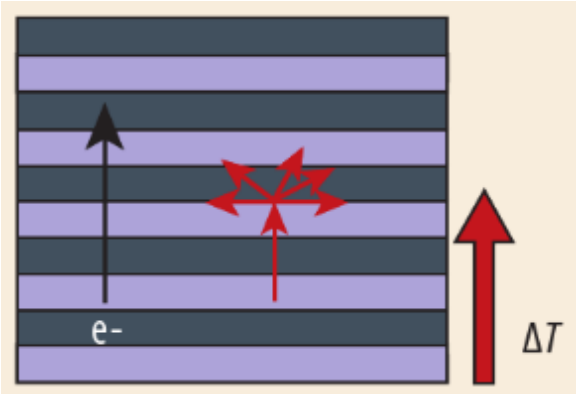
Thermoelectric elements

- Conversion of waste heat into electrical energy
- Nanorefrigerators

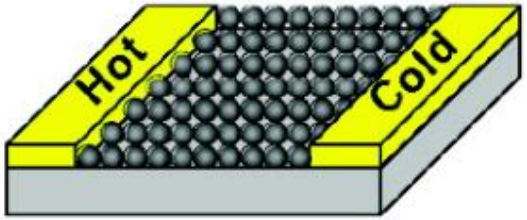


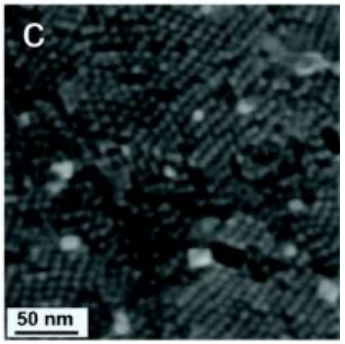
Phonon transport

Figure of merit: $ZT = S^2GT/\kappa$

Thermopower S
Temperature T
Electric conductance G
Thermal conductance κ

$$\kappa = \kappa_{el} + \kappa_{ph}$$



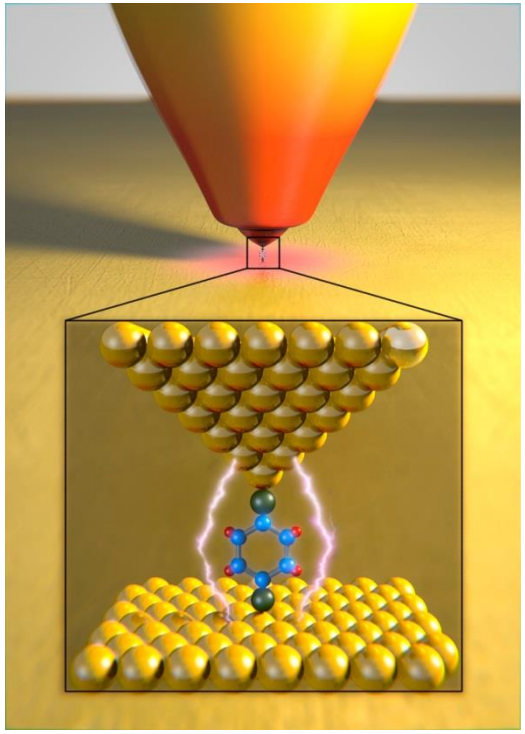


R. A. Segalman (UC Berkeley):
R.Y. Wang *et al.*, Nano Lett. 2008

Ultimate Goal: Enhancement of *ZT* through appropriate nanostructuring

Here: Study of *G* and *S*

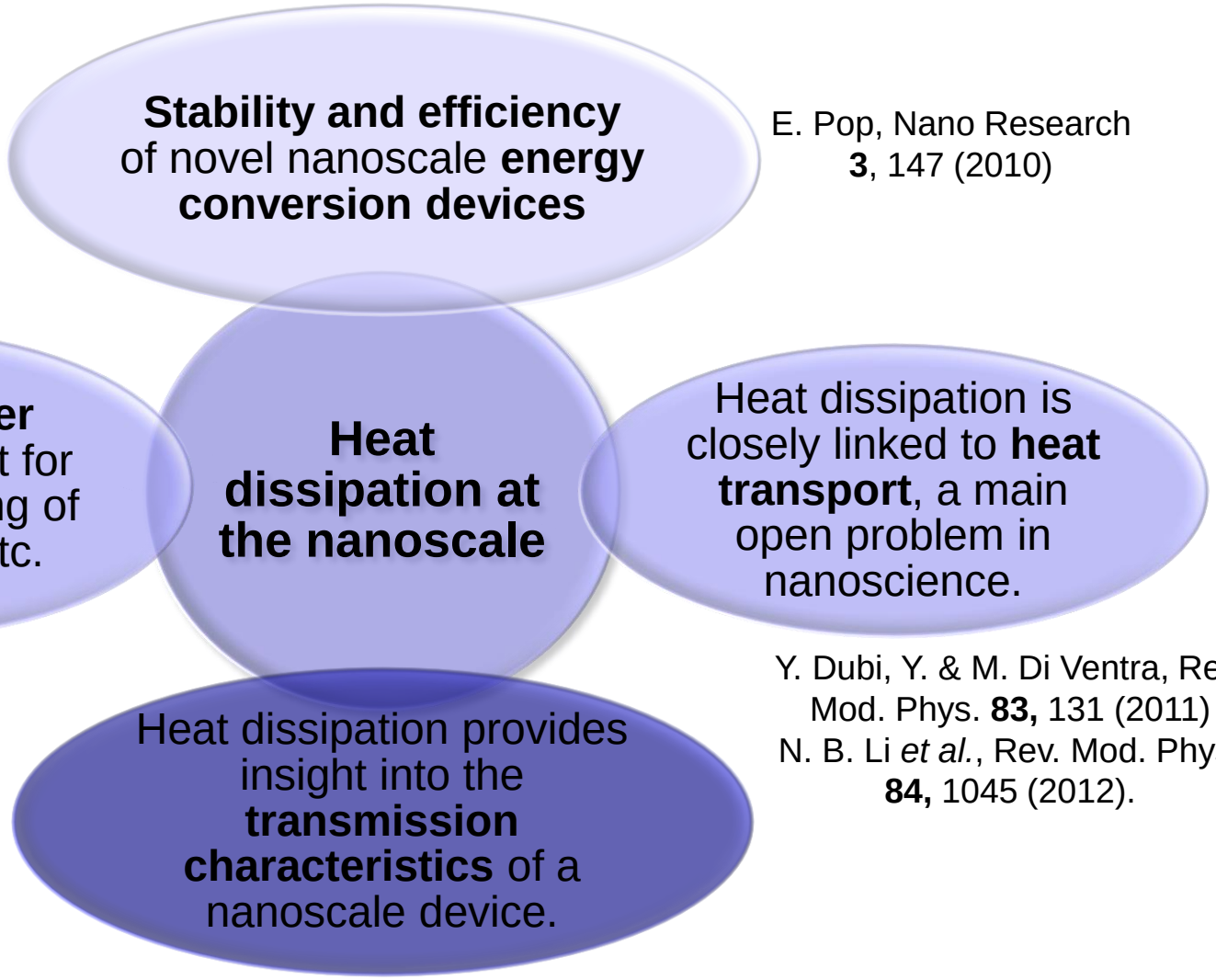
Heat dissipation and thermopower in atomic-scale junctions



W. Lee, K. Kim, W. Jeong, L. A. Zotti, F. Pauly, J. C. Cuevas, and P. Reddy, Nature 498, 209 (2013)

L. A. Zotti, M. Bürkle, F. Pauly, W. Lee, K. Kim, W. Jeong, Y. Asai, P. Reddy, J. C. Cuevas, arXiv:1307.8336

Why heat dissipation at the nanoscale?



E. Pop, Nano Research **3**, 147 (2010)

F. Giazotto *et al.*, Rev. Mod. Phys. **78**, 217 (2006)
J.T. Muhonen *et al.*, Rep. Prog. Phys. **75**, 046501 (2012)

Y. Dubi, Y. & M. Di Ventra, Rev. Mod. Phys. **83,** 131 (2011)
N. B. Li *et al.*, Rev. Mod. Phys. **84,** 1045 (2012).

This work.

Heat dissipation in atomic-scale junctions

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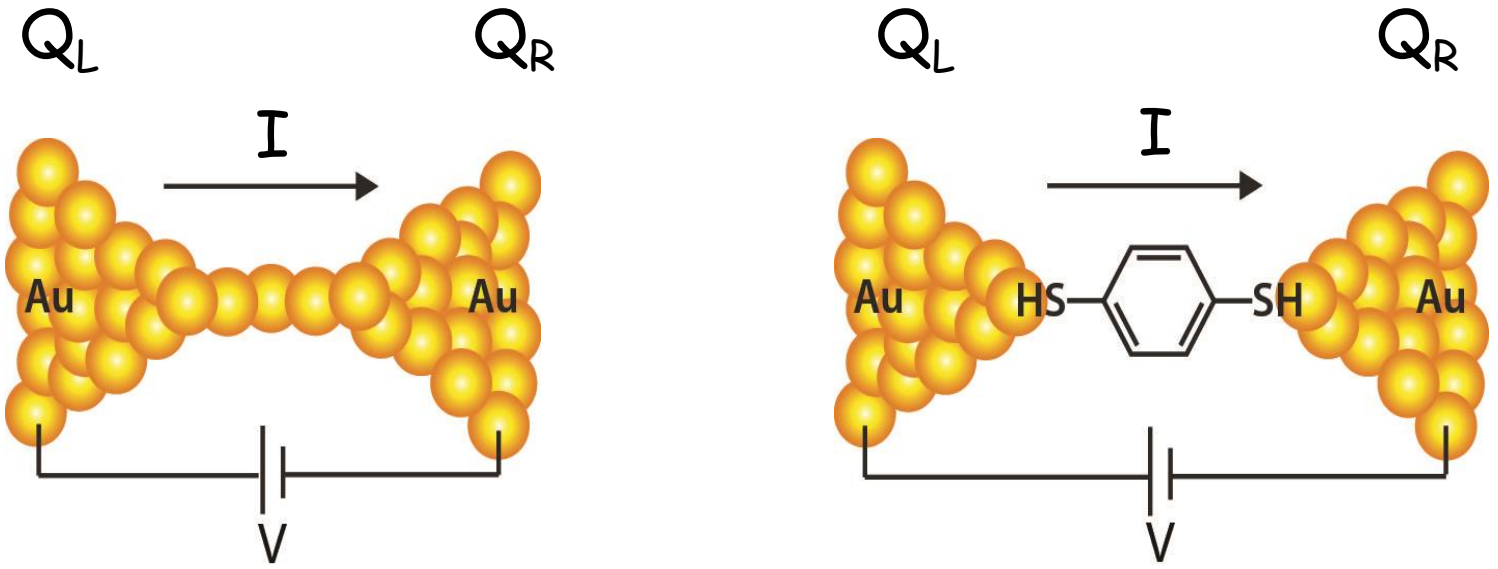
- Dimensions of the contact region in atomic-scale junctions are much smaller than the inelastic scattering length.

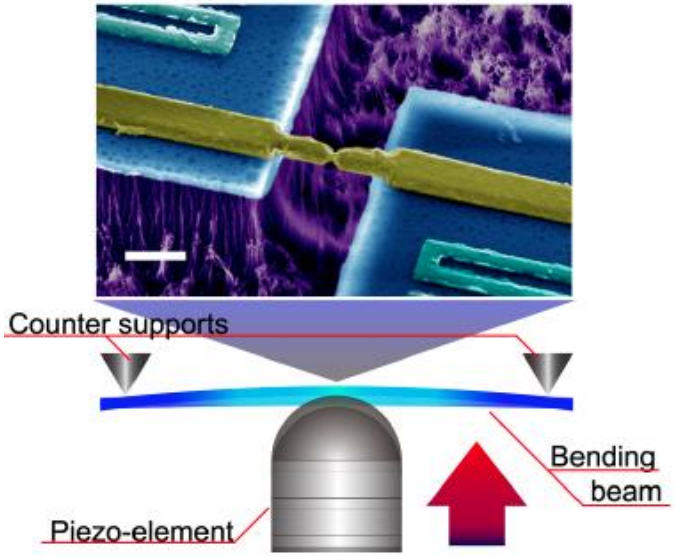
→ Transport is elastic and heat dissipation takes place inside the electrodes.

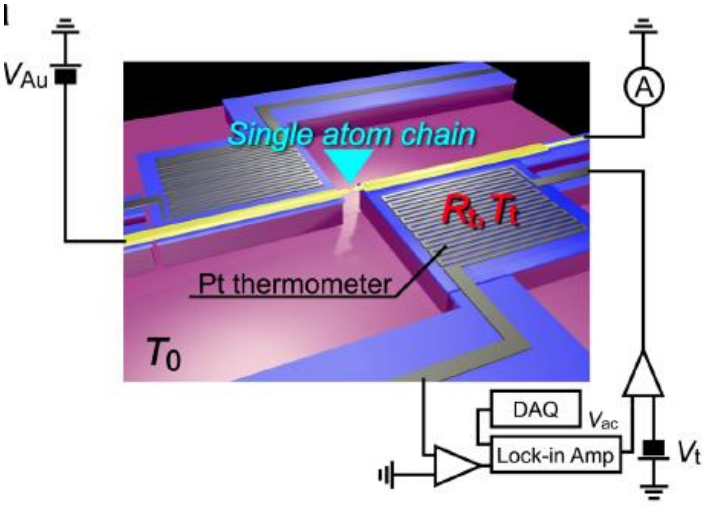


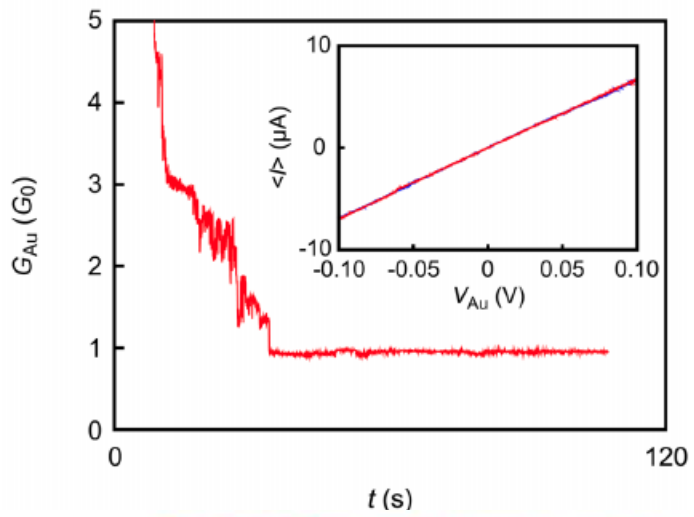
Where is the heat dissipated?
Is it equally dissipated in both electrodes?
What is the relation between the dissipated heat and the electronic structure of the atomic-scale contact?

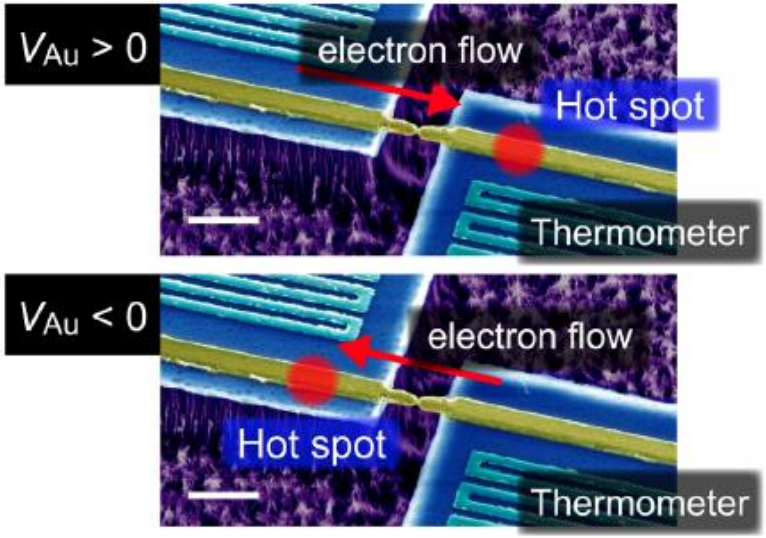
Recent experimental efforts: Au atomic chains

M. Tsutsui, T. Kawai, and M. Taniguchi, *Sci. Rep.* **2**, 217 (2012)









Asymmetric heating: Hot electrons create hotspots downstream of electron flow?

Heat dissipation and thermopower in atomic-scale junctions

Motivation

Experimental approach

Theory

Tuning the heating

Conclusions

Scanning probes with integrated thermocouple

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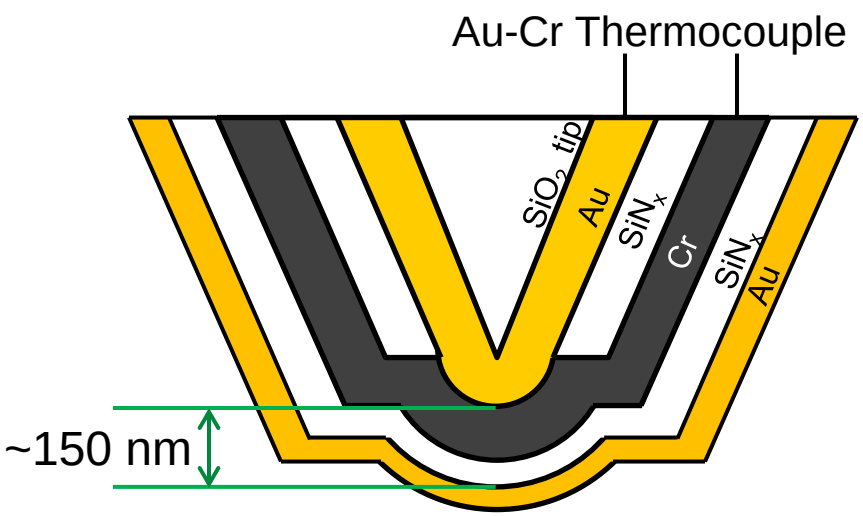
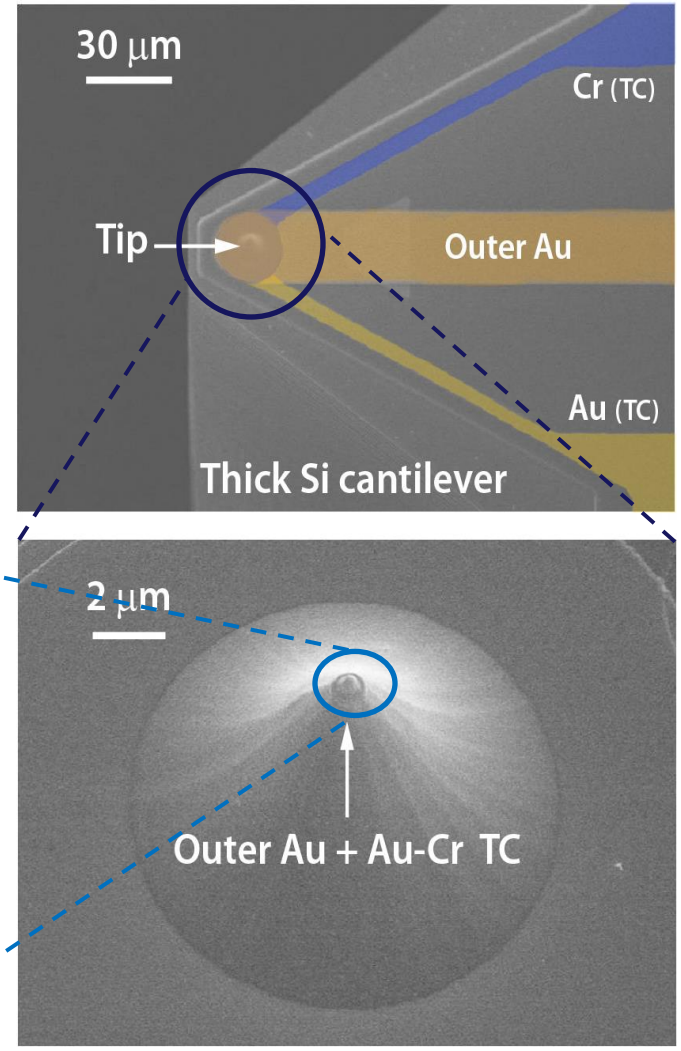
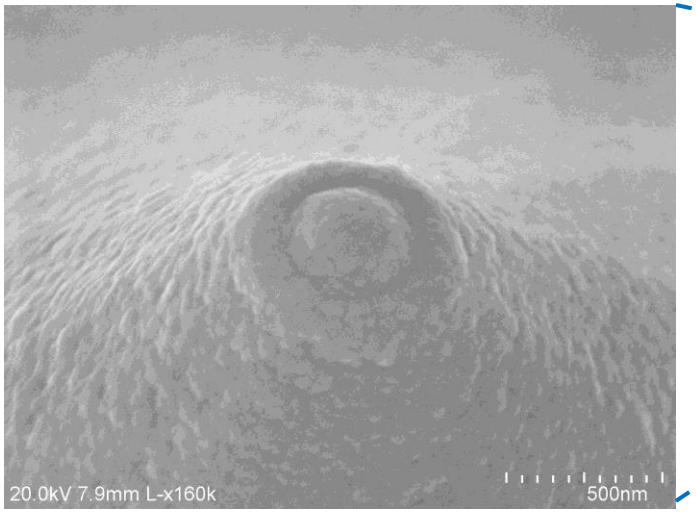
Schematic

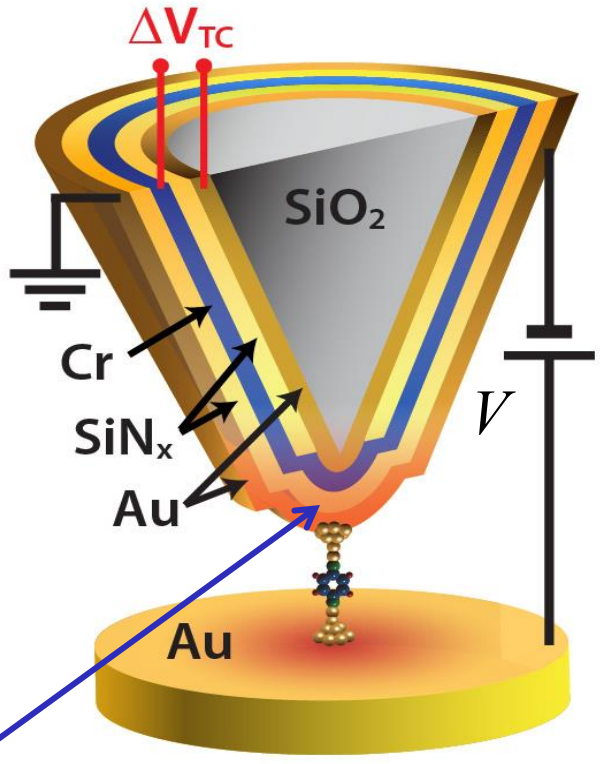


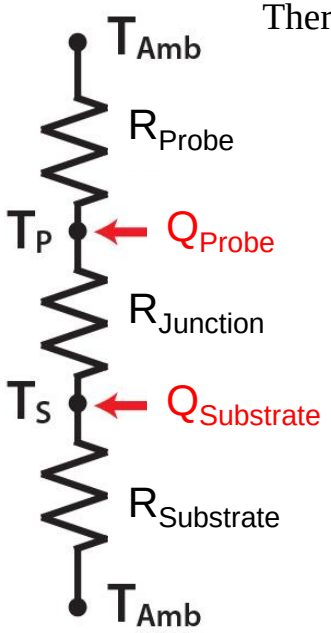
Fabricated probe





Strategy for probing heat dissipation





$$\Delta V_{TC} = -S_{TC} \times \Delta T_{TC}$$

Thermovoltage — Thermopower — Temperature rise

$R_{Junction}$: Thermal resistance of the junction

$R_{Junction} \gg R_{Probe}, R_{Substrate}$

$$Q_{Probe}(V) = \Delta T_{TC} / R_{Probe}$$

R_{Probe} : Thermal resistance of probe

Power dissipation:

$$Q_{Probe}(V) + Q_{Substrate}(V) = Q_{Total}(V) = I \times V$$

$$R_{\mathrm{Probe}} = 72800 \pm 500 \ \mathrm{K/W} \quad \text{and} \quad S_{TC} = 16.3 \pm 0.2 \ \mu\mathrm{V/K}$$

Key experimental details

- The fabricated probes ***are much stiffer than traditional scanning thermal microscopy probes*** so as to enable stable formation of atomic and molecular junctions.

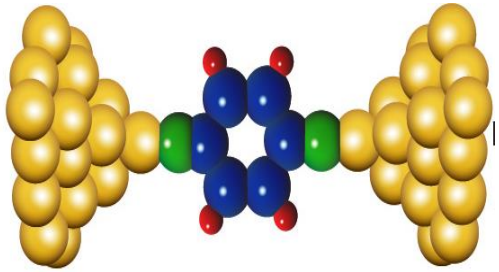
  K. Kim, W.H. Jeong, W.C. Lee & P. Reddy, ACS Nano **6**, 4248 (2012).

- The expected temperature changes in the thermocouple for the studied AMJs (< 100 mK) are smaller than the electrically-induced temperature noise (~ 200 mK). For this reason, ***a modulation scheme is used to reduce the bandwidth and the electrical noise*** (see next slides).

- A small thermal time constant (~ 10 μs) of the thermocouple enables high fidelity tracking of temperature changes.

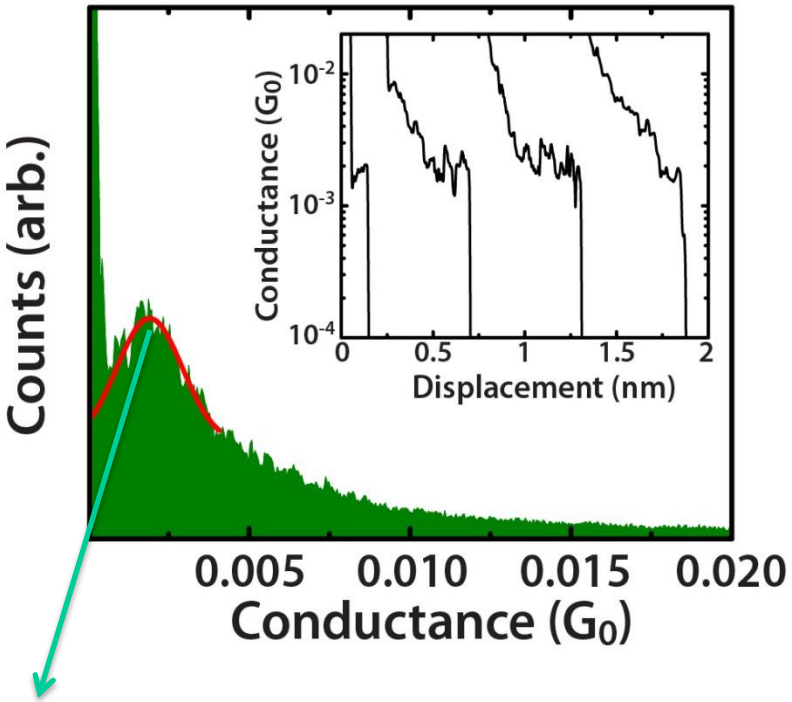
- With the modulation scheme ***the noise equivalent temperature is well below 1 mK*** for all the cases studied in our work.

BDNC single-molecule junctions

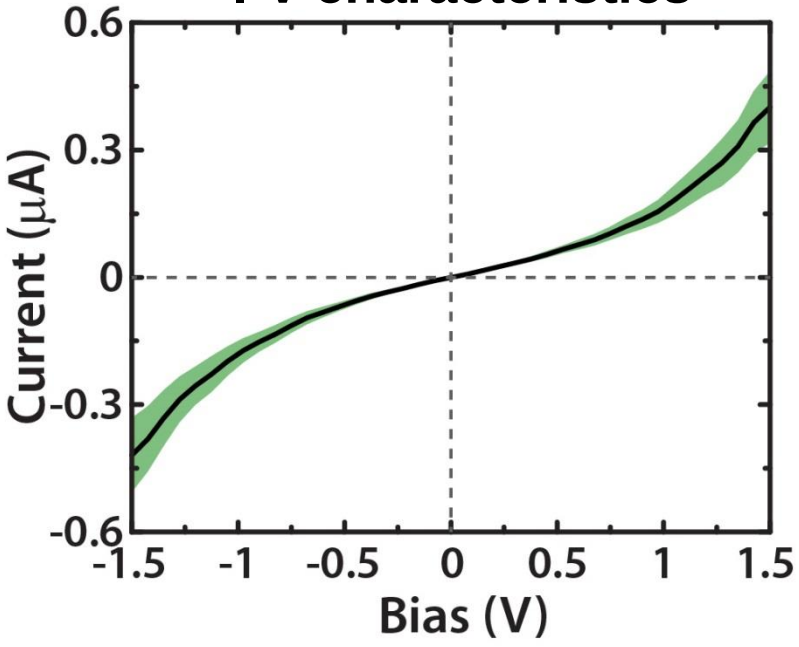


1,4-benzenediisonitrile

Conductance traces and histogram



I-V characteristics



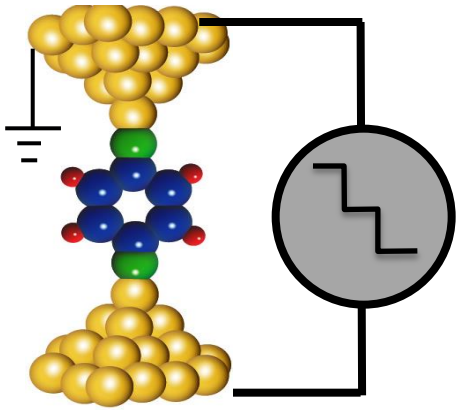
Conductance peak at $0.002G_0$ compatible with M. Kiguchi *et al.*, APL 89, 213104 (2006).

BDNC junctions: Representative raw data and modulation scheme

Here, a positive (negative) bias corresponds to a scenario where the probe is grounded, while the substrate is at a higher (lower) potential.

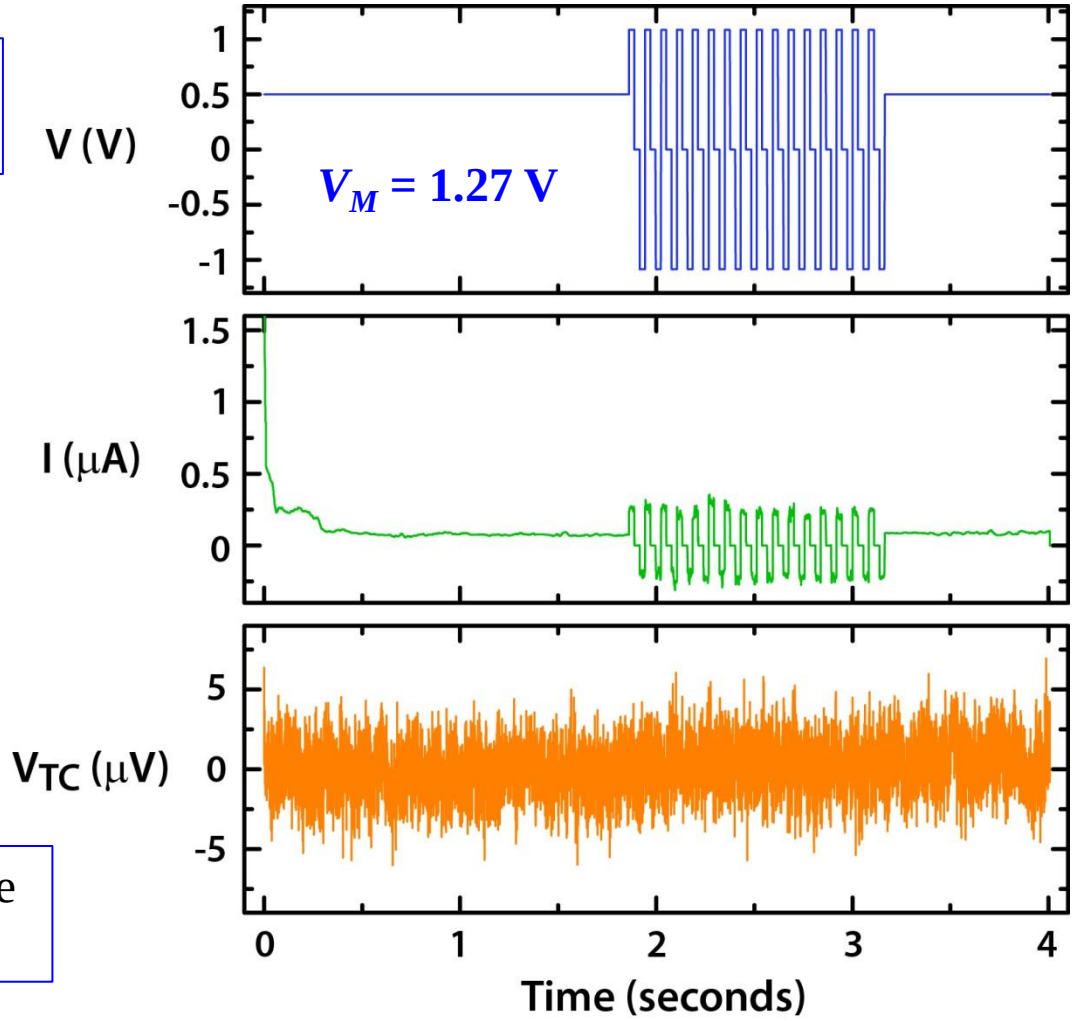
V_M = amplitude of the modulation voltage.

Probe



Substrate

T_P = 80 ms period of the voltage pulses.



BDNC junctions: Representative raw data and modulation scheme

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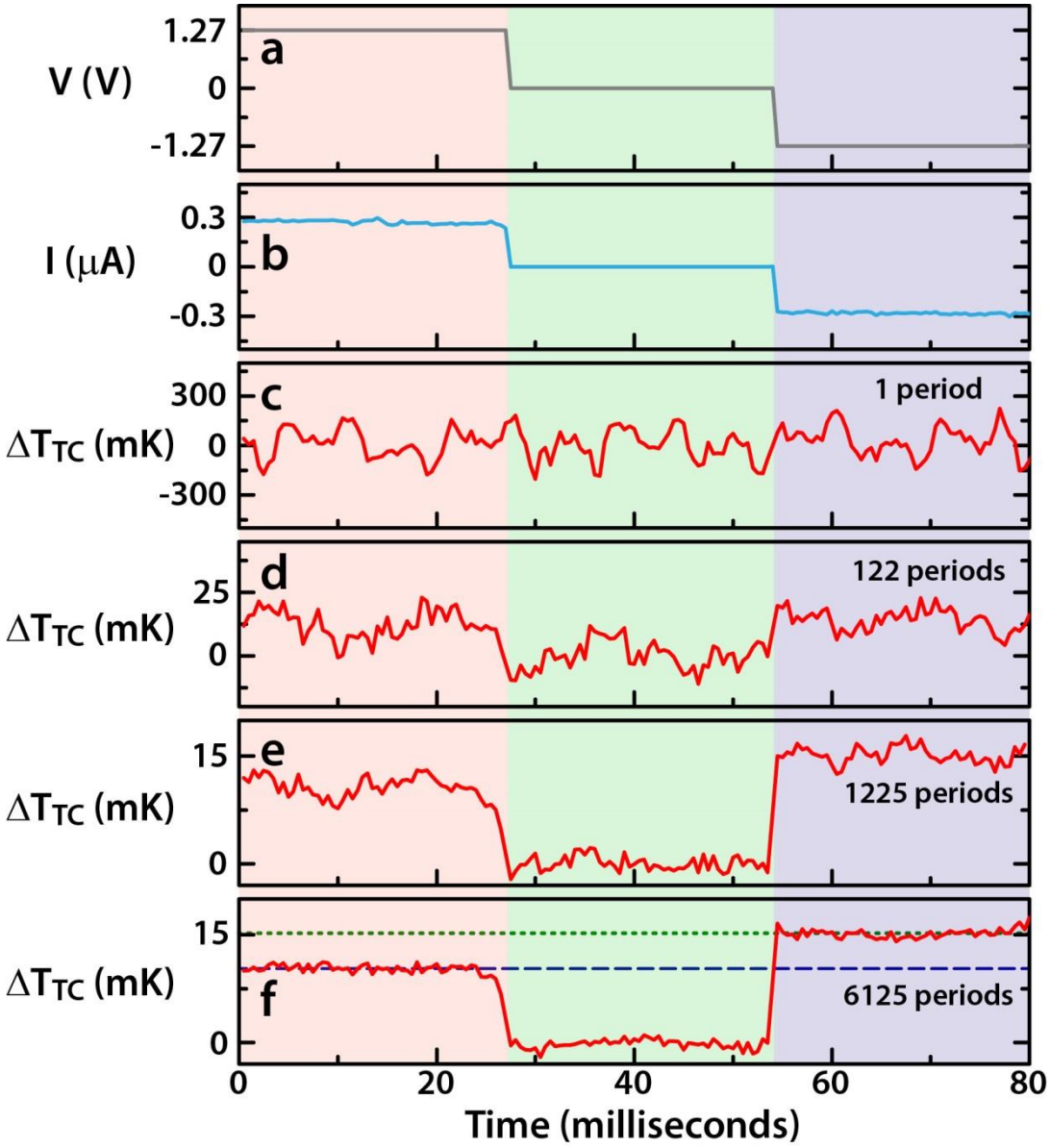
$V_M = 1.27$ V

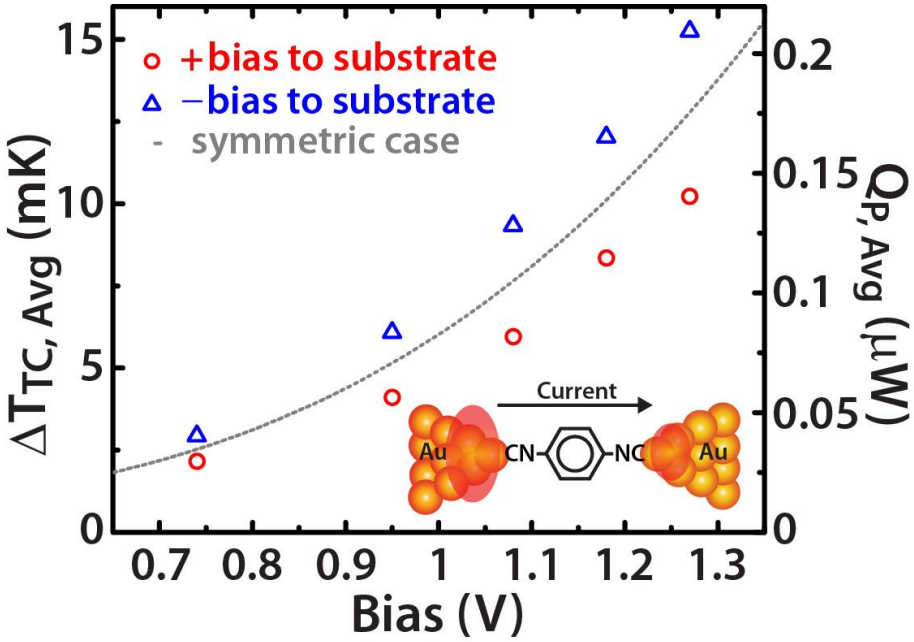
$Q_{Total} = 0.35$ mW

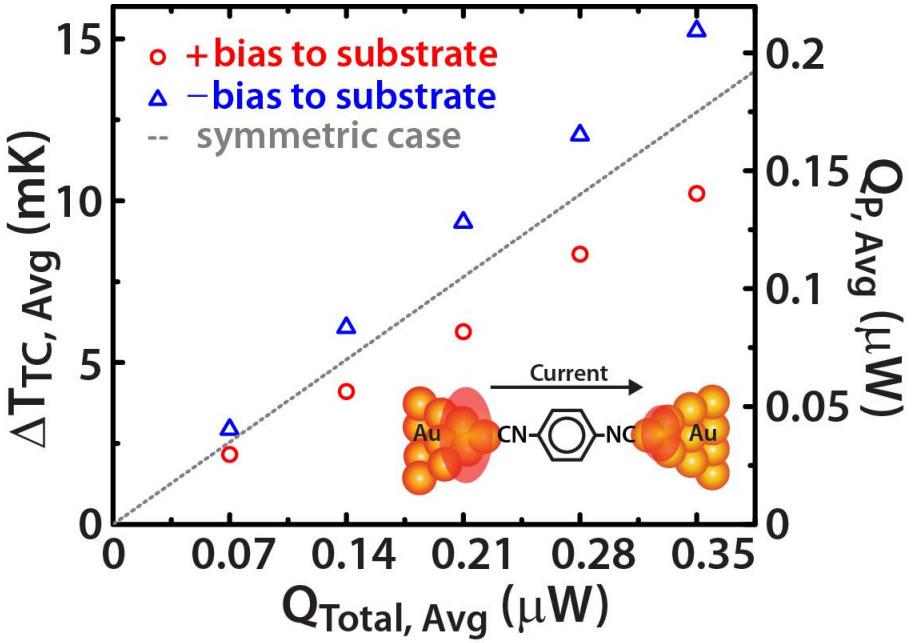
1 period = 80 ms



BDNC single-molecule junctions

A positive (negative) bias corresponds to a scenario where the probe is grounded, while the substrate is at a higher (lower) potential.





- Heat dissipation in the electrodes of Au-BDNC-Au junctions is bias-polarity-dependent and unequal.
- Why is the heat dissipation in the electrodes unequal in spite of the symmetric geometry of the molecular junctions?

Heat dissipation and thermopower in atomic-scale junctions

Motivation
Experimental approach
Theory
Tuning the heating
Conclusions

Landauer theory of heat dissipation

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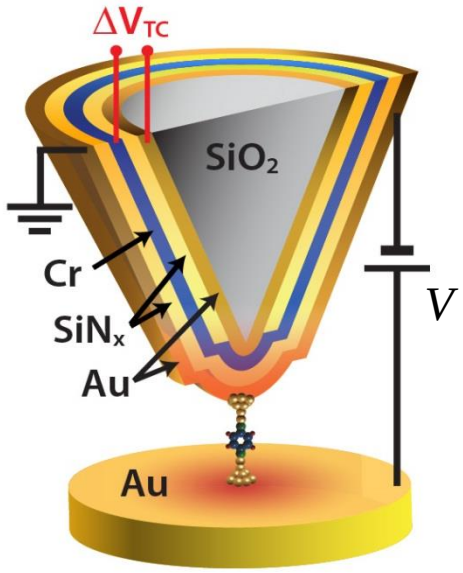
Heat current from a reservoir with potential μ

$$I_Q = I_E - \frac{\mu}{e} I_e$$

Heat current Energy current Charge current



Charge and energy currents

$$I_e(V) = \frac{2e}{h} \int_{-\infty}^{\infty} \tau(E,V)[f_P(E,\mu_P) - f_S(E,\mu_S)]dE$$

$$I_E(V) = \frac{2}{h} \int_{-\infty}^{\infty} E\tau(E,V)[f_P(E,\mu_P) - f_S(E,\mu_S)]dE$$

Power dissipated in the electrodes

$$Q_P(V) = \frac{2}{h} \int_{-\infty}^{\infty} (\mu_P - E)\tau(E,V)[f_P(E,\mu_P) - f_S(E,\mu_S)]dE$$

$$Q_S(V) = \frac{2}{h} \int_{-\infty}^{\infty} (E - \mu_S)\tau(E,V)[f_P(E,\mu_P) - f_S(E,\mu_S)]dE$$

$$Q_P(V) + Q_S(V) = IV = Q_{Total}(V)$$ [energy conservation]

General conclusions

- **Is the heat equally dissipated in both electrodes?**

$$Q_P(V) = Q_S(V) \quad \text{if} \quad \tau(E,V) = \tau(-E,V)$$

[electron-hole symmetry implies equal dissipation]

- **Does the power dissipation depend on the bias polarity?**

$$Q_P(V) = Q_P(-V) \quad \text{if} \quad \tau(E,V) = \tau(-E,-V)$$

[in general, the power dissipated in the probe depends on bias polarity]

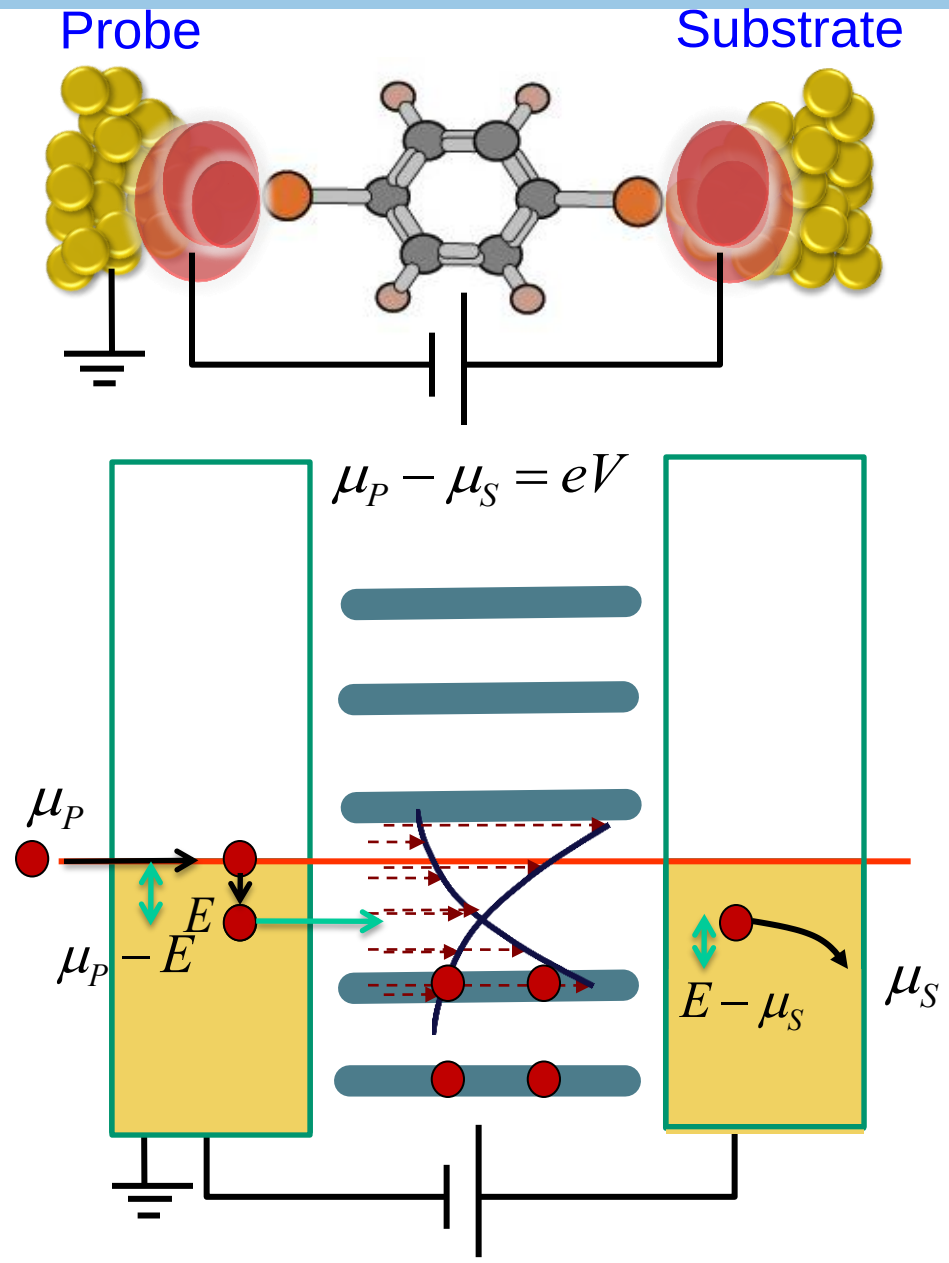
General conclusion: the heat dissipation in the electrodes of an atomic-scale contact is, in general, asymmetric and it depends on both the bias polarity and the nature of the majority carriers (electrons vs. holes).

- **Low-bias expansions to illustrate the statements above**

$$Q_P(V) - Q_P(-V) = 2TGSV + O(V^3)$$
$$Q_P(V) - Q_S(V) = 2TGSV + O(V^2)$$

$T =$ temperature
$G =$ linear conductance
$S =$ thermopower

Asymmetric heat dissipation: a simple argument



- A electron flows elastically through the contact with energy *E* leaving behind a hole.
- The electron thermalizes and dissipates an energy (E-μ_S) in the substrate.
- The hole left in the probe is filled by an electron releasing an energy (μ_P-E) in the probe.
- Power balance

$$Q_P(V) = \frac{2}{h}\int_{-\infty}^{\infty}(\mu_P - E)\tau(E,V)[f_P - f_S]dE$$

$$Q_S(V) = \frac{2}{h}\int_{-\infty}^{\infty}(E - \mu_S)\tau(E,V)[f_P - f_S]dE$$

$$Q_P(V) + Q_S(V) = IV$$

→ **An energy-dependent transmission leads to asymmetric heating.**

Lessons from a toy model

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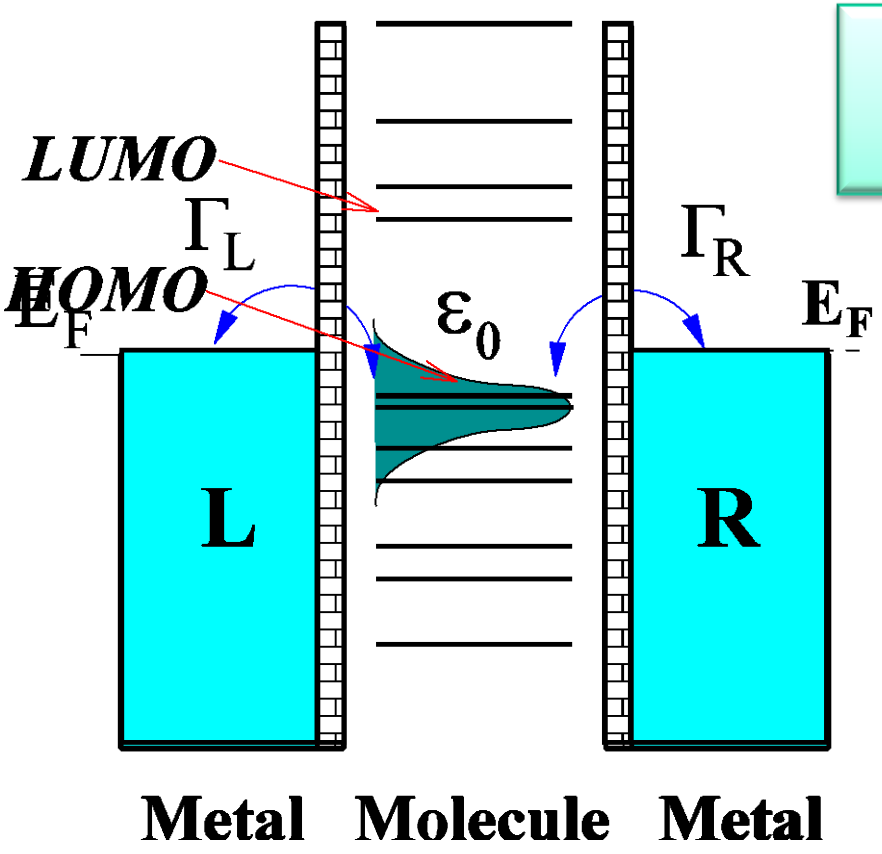
Often the transport through a molecular junction is dominated by a single molecular orbital. Those situations can be described within the **single-level model**.



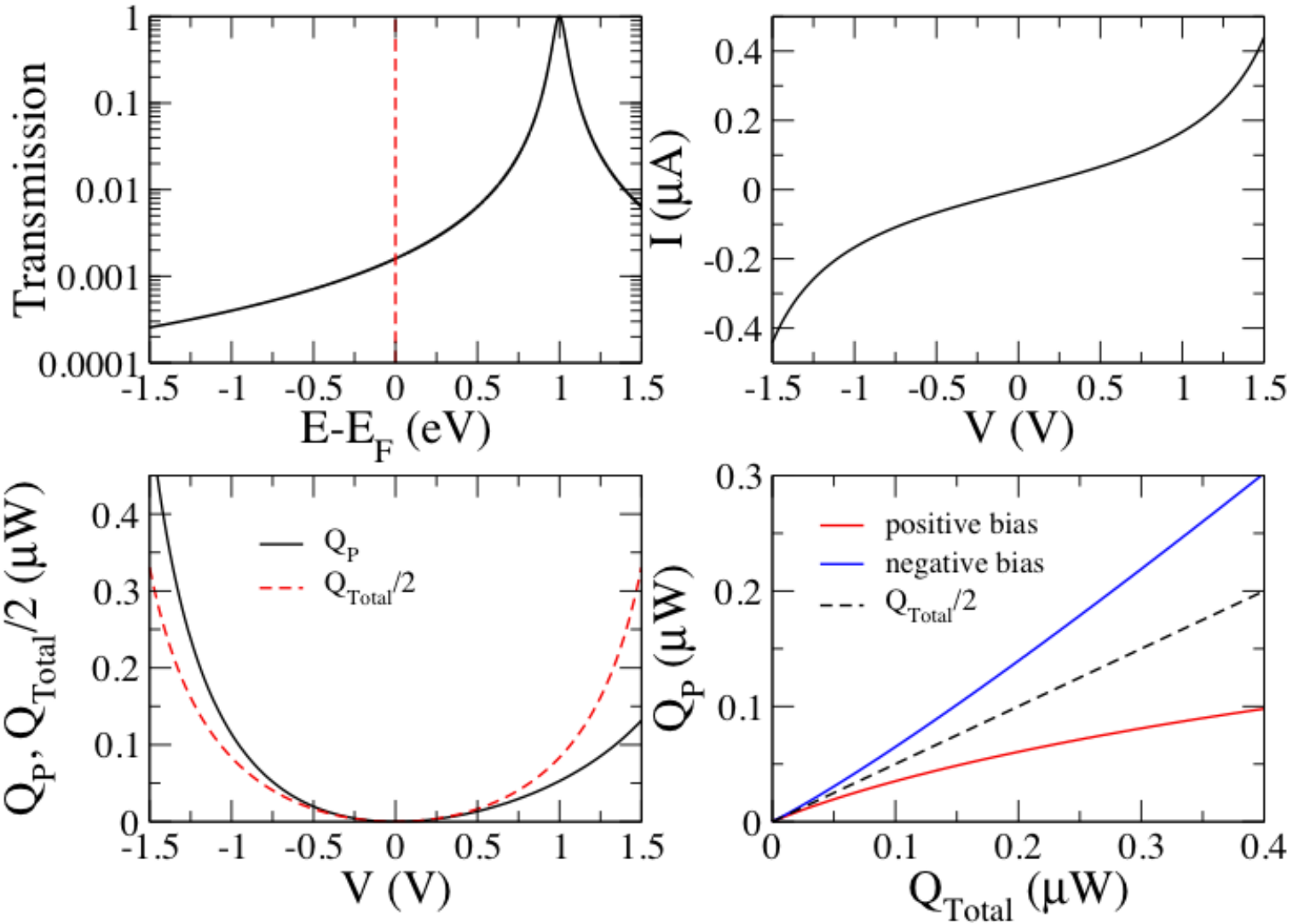
$$\tau(E,V) = \frac{\Gamma_L \Gamma_R}{[E - \varepsilon_0(V)]^2 + [\Gamma_L + \Gamma_R]^2 / 4}$$

Breit-Wigner formula

$$\begin{cases} \varepsilon_0 = \text{level position} \\ \Gamma_L + \Gamma_R = \text{level width} \end{cases}$$

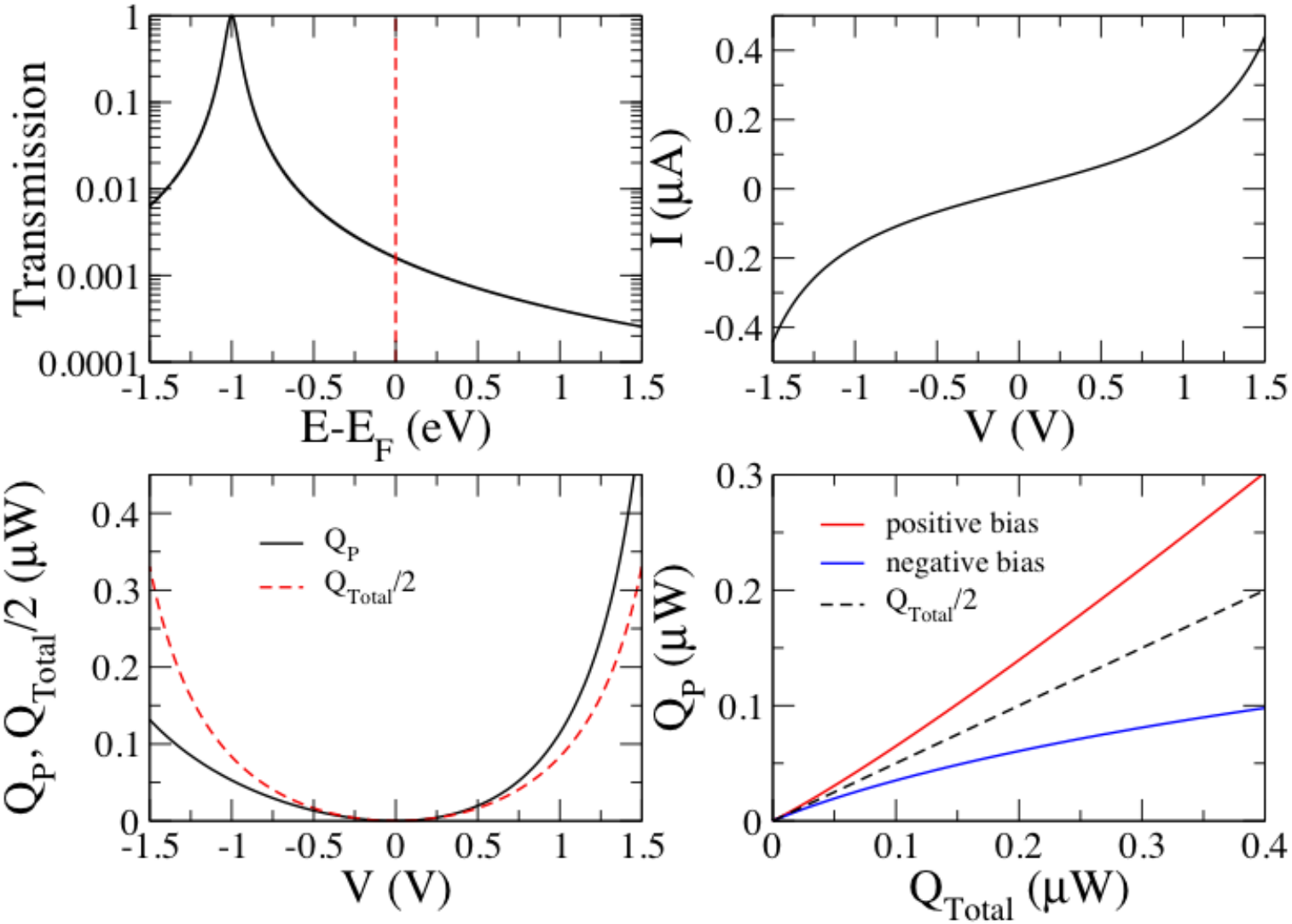
Single-level model: LUMO-dominated transport

$\varepsilon_0 = +1$ eV; $T = 300$ K; $\Gamma_L = \Gamma_R = \Gamma = 40$ meV (symmetric contact)



Single-level model: HOMO-dominated transport

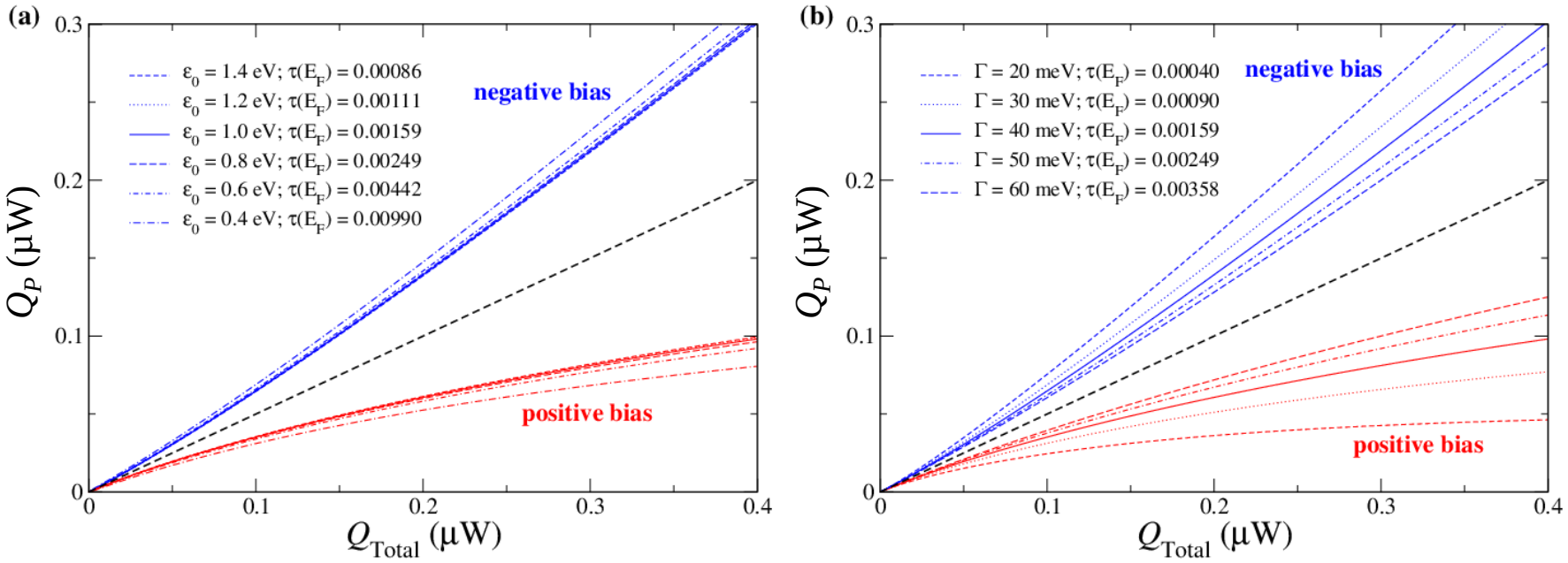
$\varepsilon_0 = -1$ eV; $T = 300$ K; $\Gamma_L = \Gamma_R = \Gamma = 40$ meV (symmetric contact)



Single-level model

In off-resonant situations, the relation between Q_P and Q_{Total} is not very sensitive to the level alignment.

$T = 300$ K



Low-power expansion in the off-resonant situation ($|\varepsilon_0| >> \Gamma$ and $T = 0$ K)

$$Q_P(Q_{Total}) \approx \begin{cases} \frac{1}{2}Q_{Total} + \text{sgn}(\varepsilon_0)\frac{e}{6G_0^{1/2}}\frac{1}{\Gamma}Q_{Total}^{3/2} & \text{(for negative bias)} \\ \frac{1}{2}Q_{Total} - \text{sgn}(\varepsilon_0)\frac{e}{6G_0^{1/2}}\frac{1}{\Gamma}Q_{Total}^{3/2} & \text{(for positive bias)} \end{cases}$$

BDNC single-molecule junctions: Comparison between theory & experiment

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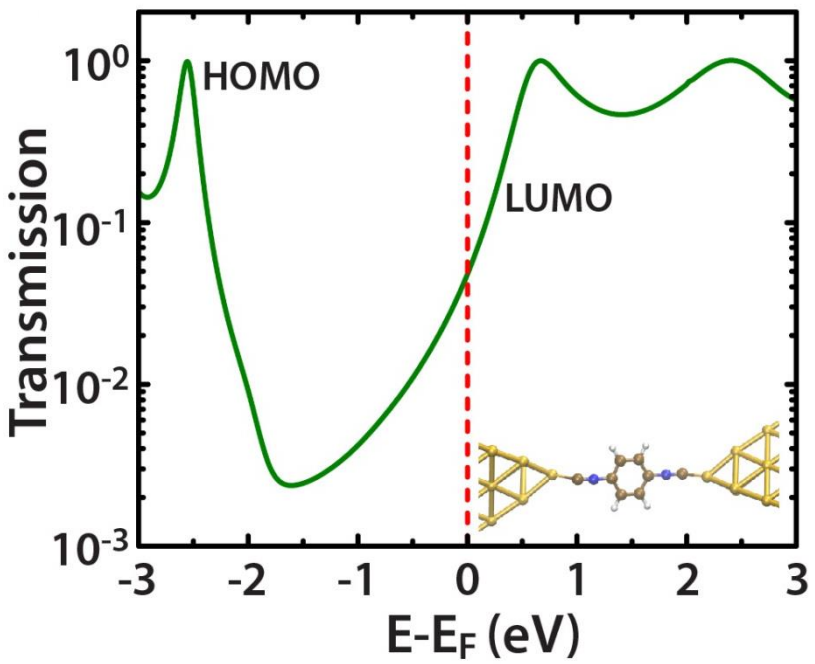
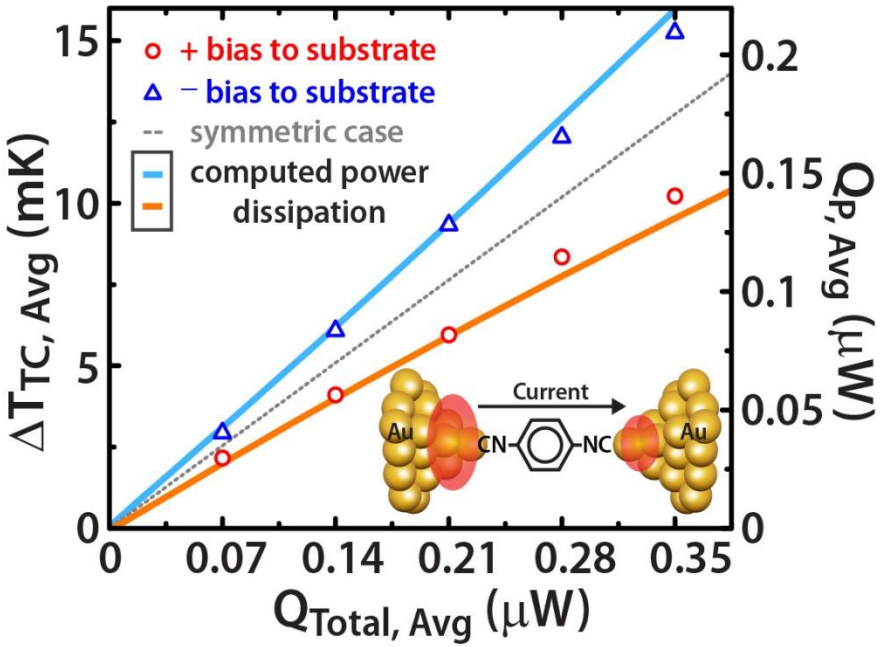
DFT + NEGF



Power Dissipation



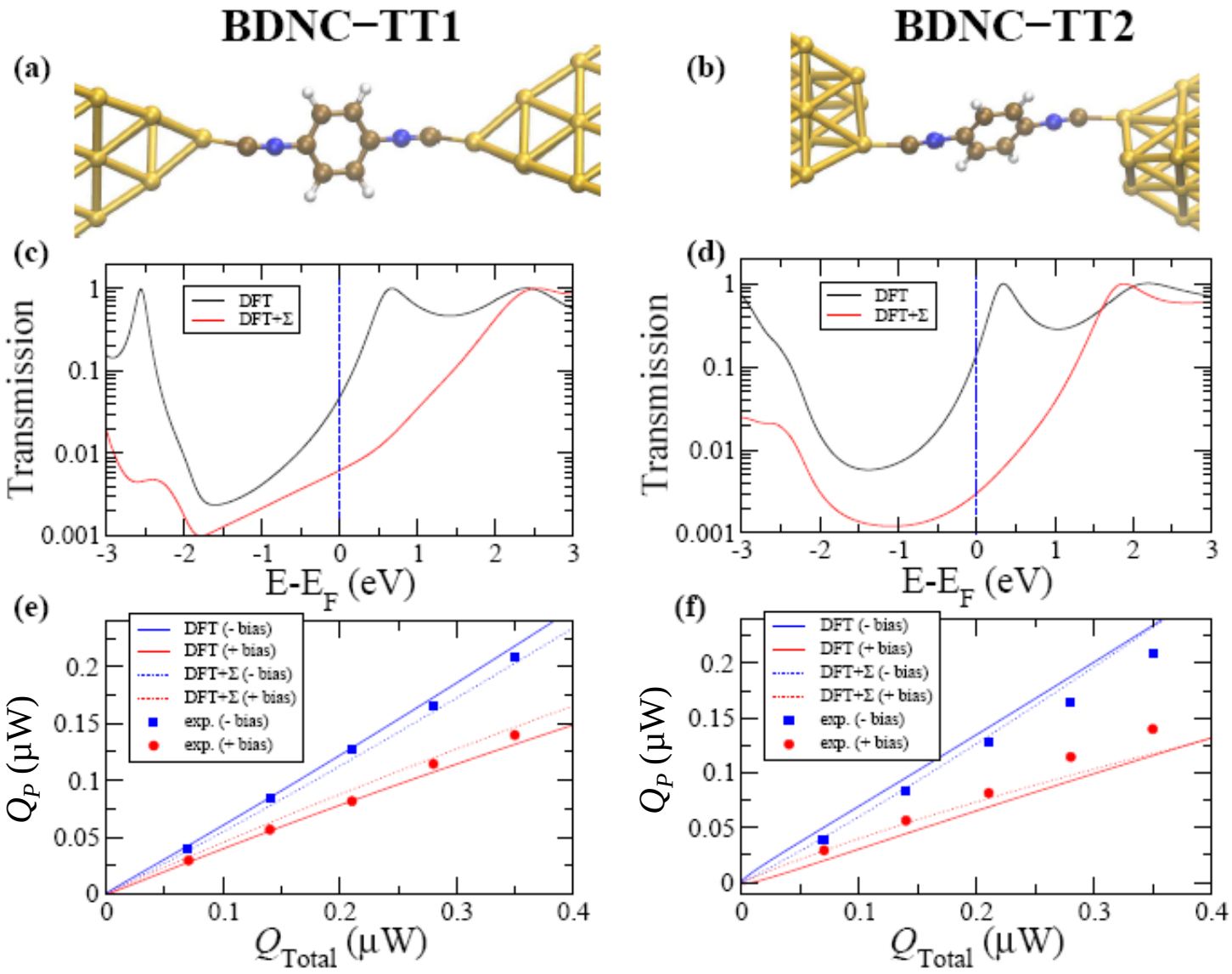
Approximation: Use zero-bias transmission

$$I(V) = \frac{2e}{h}\int_{-\infty}^{\infty} \tau(E, V=0)[\,f_P - f_S\,]dE \Rightarrow Q_{Total}(V) = I(V)\times V$$

$$Q_P(V) = \frac{2}{h}\int_{-\infty}^{\infty} (\mu_P - E)\tau(E, V=0)[\,f_P - f_S\,]dE$$

BDNC single-molecule junctions: Comparison between theory & experiment

Universität Konstanz



Heat dissipation and thermopower in atomic-scale junctions

Motivation
Experimental approach
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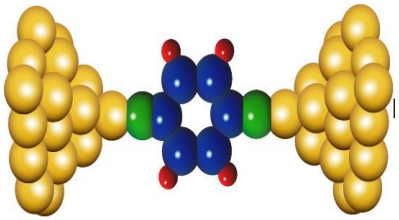
Tuning the heating
Conclusions

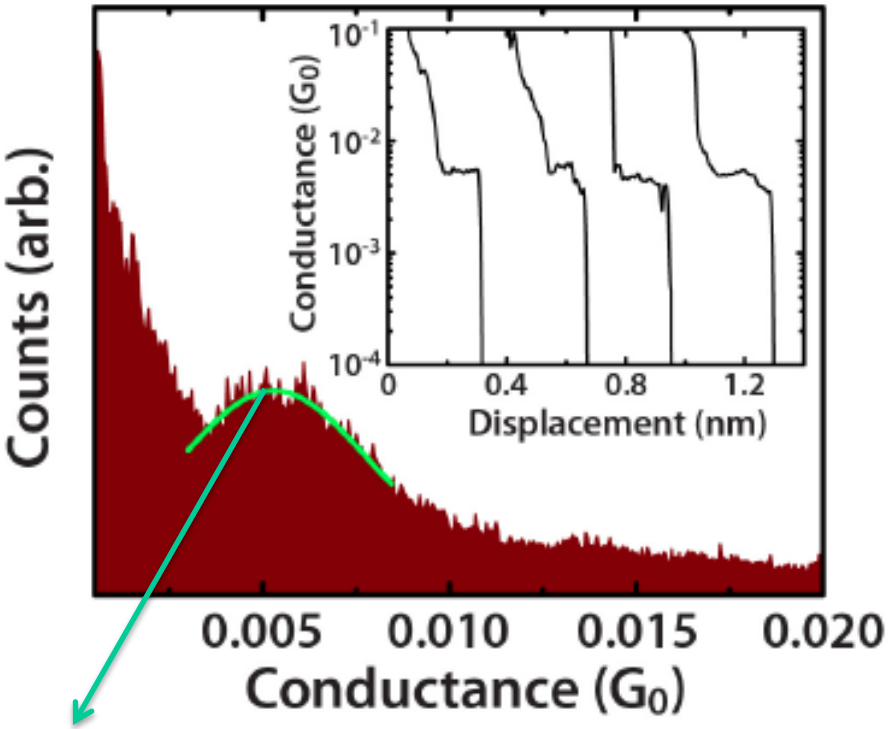
BDA single-molecule junctions



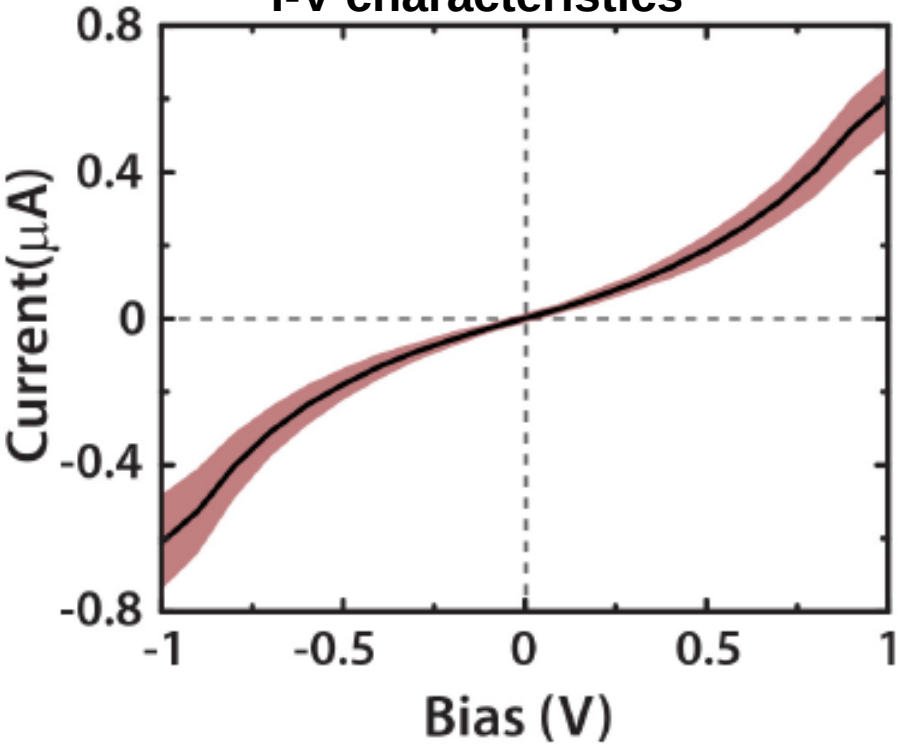
BDA

1,4-benzenediamine

Conductance traces and histogram

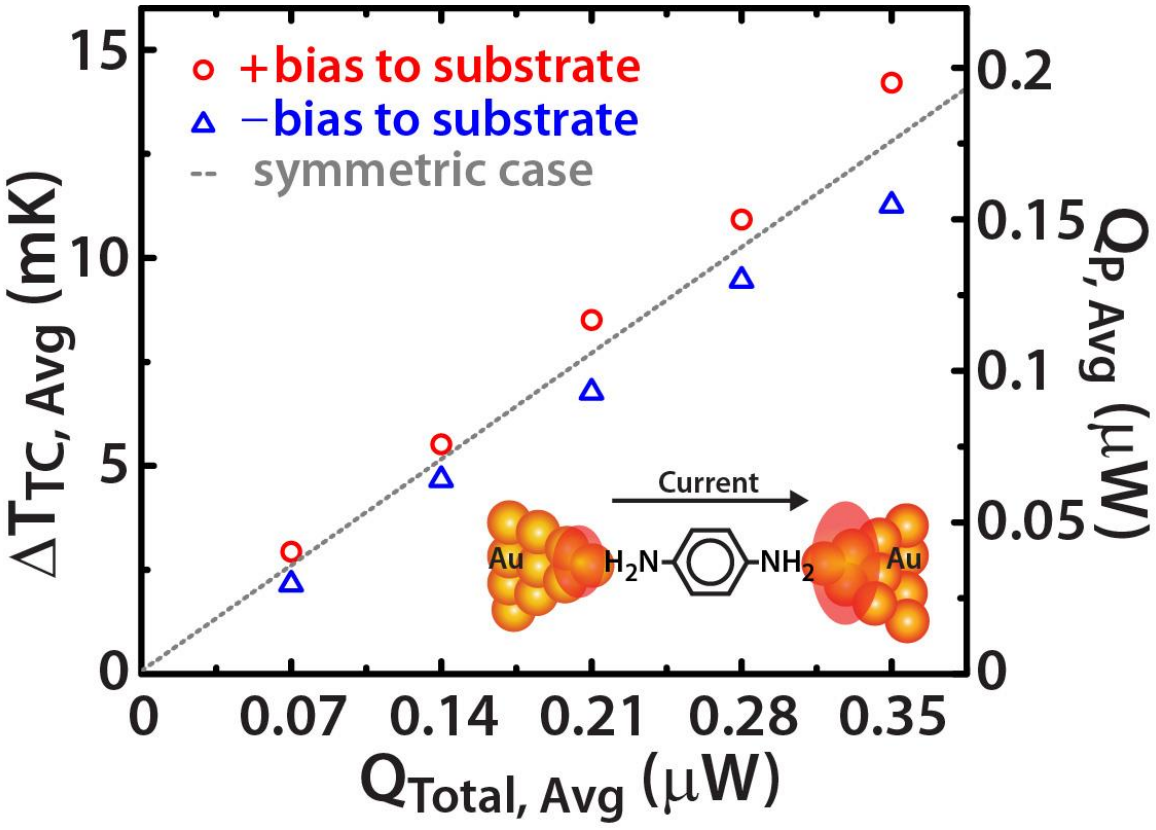


I-V characteristics



Conductance peak at $0.005G_0$ compatible with L. Venkataraman *et al.,* Nano Lett. 6, 458 (2006).

BDA single-molecule junctions



The BDA junctions show larger power dissipation in the probe for a positive bias than for a negative one in contrast to the observations in BDNC junctions.

BDA single-molecule junctions: Comparison between theory and experiment

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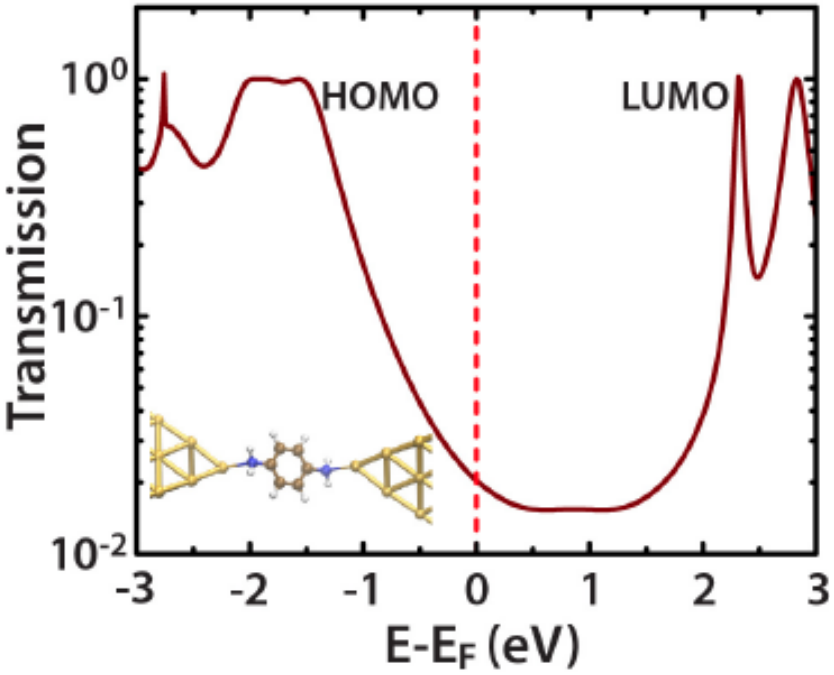
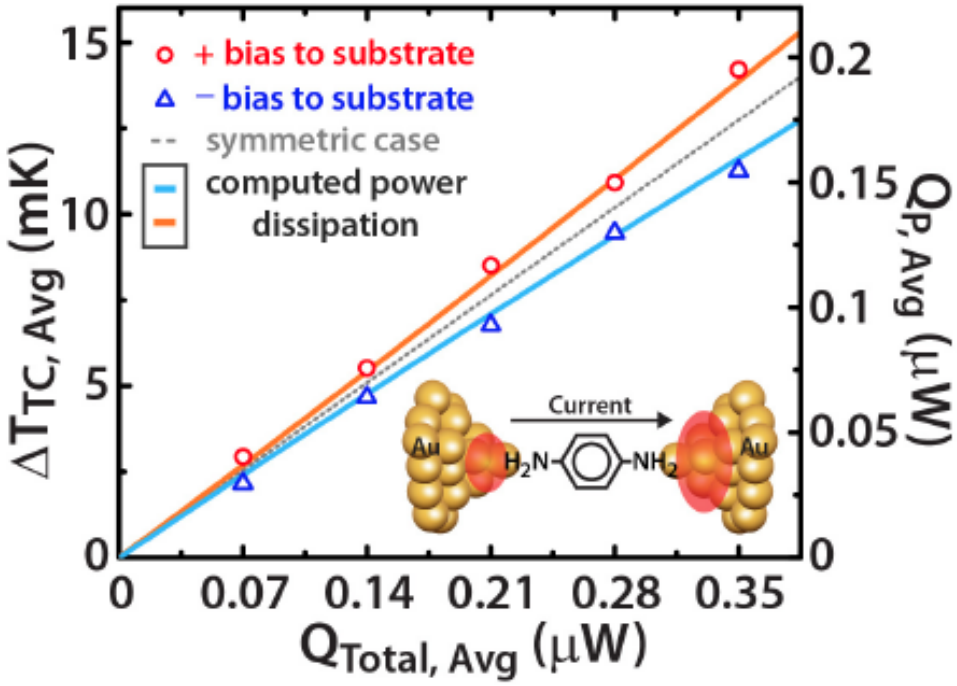
DFT + NEGF

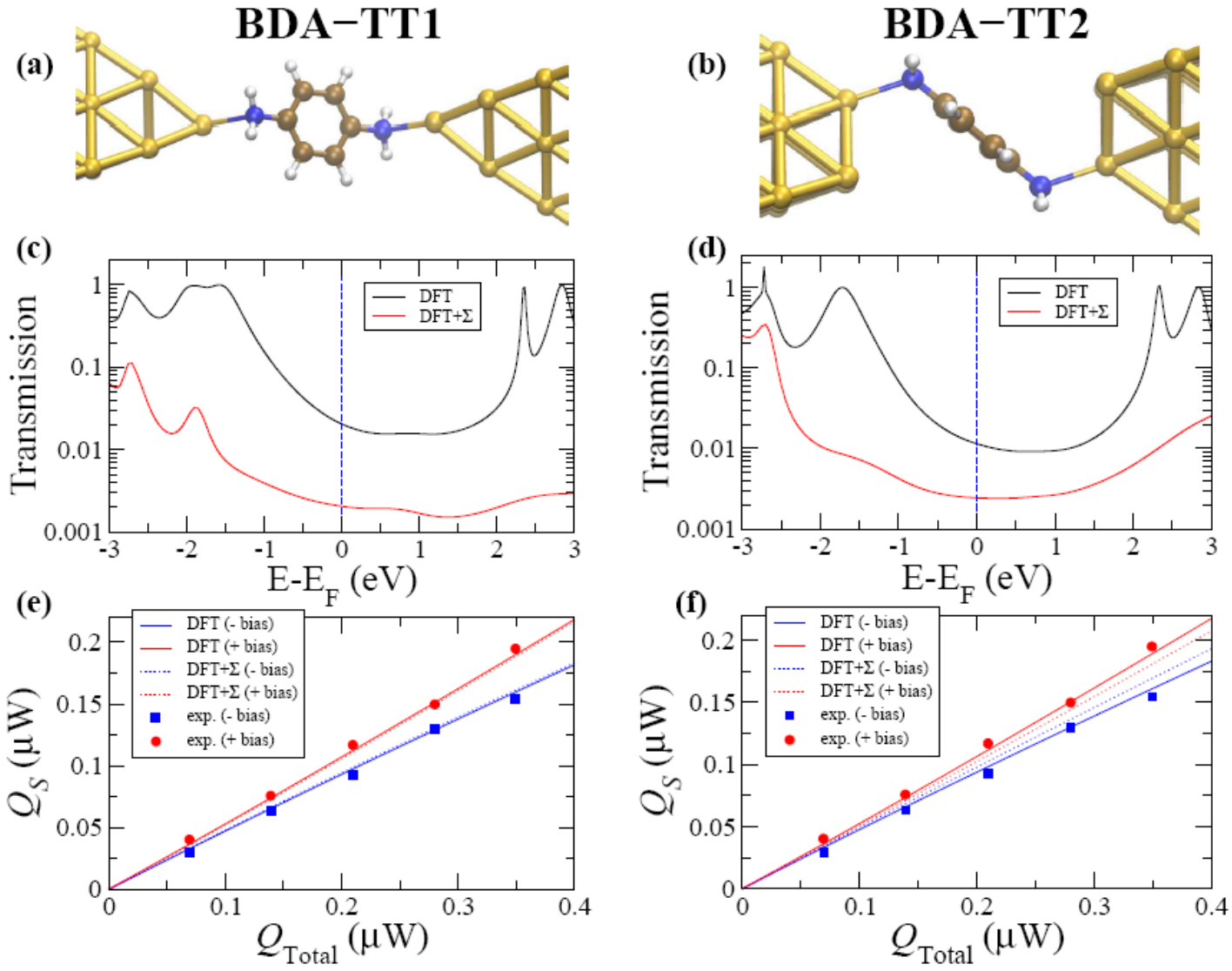


Power Dissipation

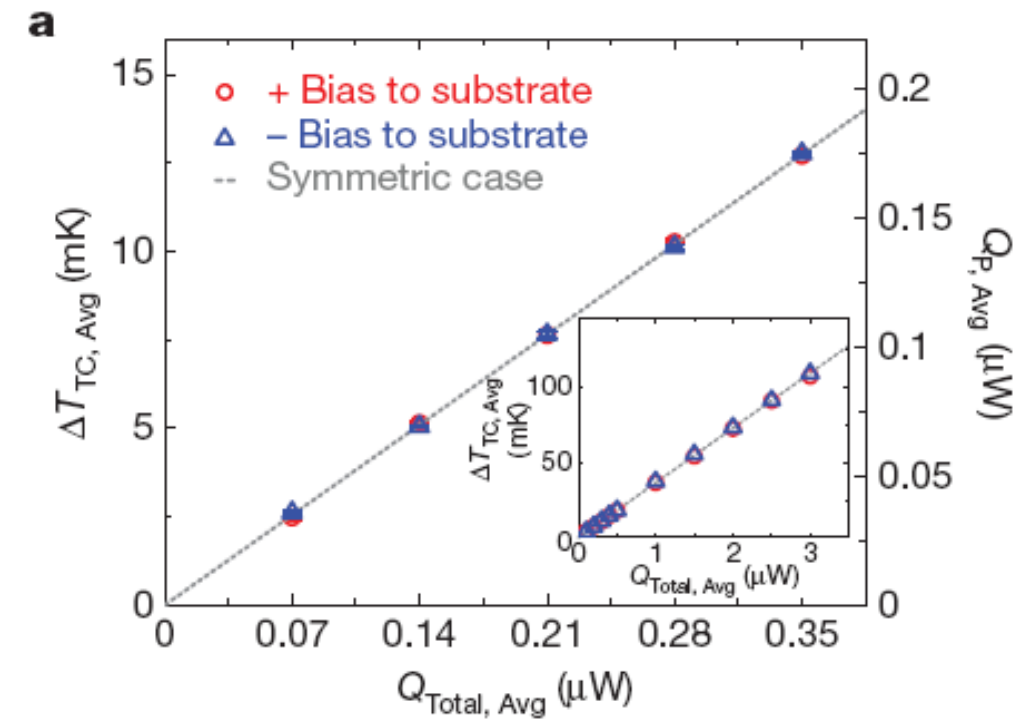


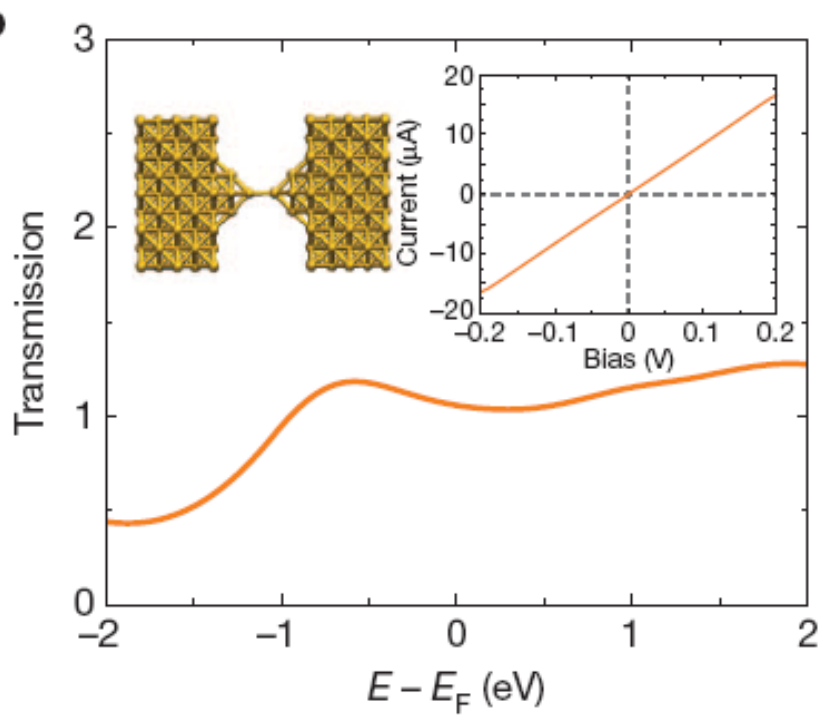
The BDA junctions show larger power dissipation in the probe for a positive bias because the transport is dominated by the HOMO, which leads to positive Seebeck coefficient.

BDA single-molecule junctions: Comparison between theory and experiment



Gold single-atom contacts





In Au atomic junctions the heat is equally dissipated in both electrodes irrespective of the magnitude or polarity of the bias voltage. This is due to the weak energy dependence of the transmission around the Fermi energy.

Heat dissipation and thermopower in atomic-scale junctions

Motivation
Experimental approach
Theory
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Conclusions

Conclusions

- Novel scanning tunnelling probes with integrated thermocouples allow to probe heat dissipation in the electrodes of atomic and molecular junctions.
- The good agreement between measured and computed asymmetries in the heat dissipation confirms that heat dissipation is intimately related to the transmission characteristics of the junctions, as predicted by the Landauer theory.
- Our results contradict recent claims of asymmetric heat dissipation in Au atomic junctions, which are not in agreement with theoretical predictions.
- The insights obtained here regarding heat dissipation should hold for any mesoscopic system where charge transport is predominantly elastic. Such systems include semiconductor nanowires, two-dimensional electron gases, semiconductor heterostructures, carbon nanotubes, graphene, etc.

Perspectives

- Peltier cooling & heat transport in atomic-scale junctions may be explored by extension of the developed techniques.

W. Lee, K. Kim, W. Jeong, L. A. Zotti, F. Pauly, J. C. Cuevas, and P. Reddy, Nature 498, 209 (2013)

L. A. Zotti, M. Bürkle, F. Pauly, W. Lee, K. Kim, W. Jeong, Y. Asai, P. Reddy, J. C. Cuevas, arXiv:1307.8336

Influence of vibrations on electron transport

Method

Gold junctions

Octane-based junctions

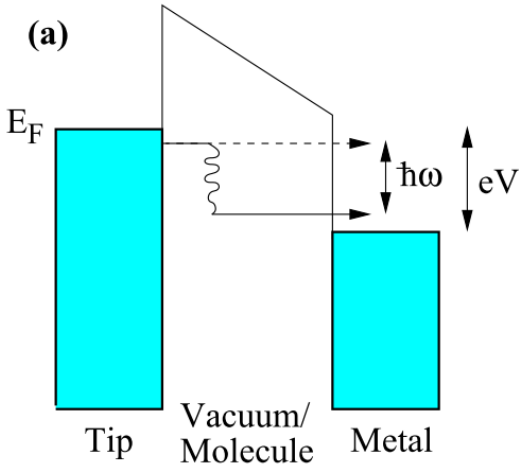
Inelastic electron tunneling spectra (IETS)

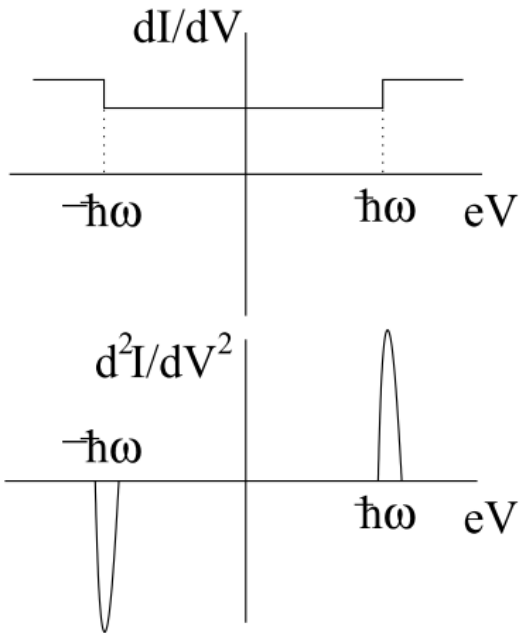
Energy of vibrational mode: $\hbar\omega$

Conductance changes if the voltage is $eV \approx \hbar\omega$.

Second derivative of the current shows changes clearly

Goal:
Determine vibrational modes and e-vib couplings from first principles (DFT)





See for instance:

J. K. Viljas *et al.*, Phys. Rev. B 72, 245415 (2005)

J. C. Cuevas and E. Scheer, *Molecular Electronics*, World Scientific Pub. Co. (2010)

Inelastic transport method

$$H = H_e + H_{vib} + H_{e-vib} \qquad H_e = \sum_{i,j} d_i^\dagger H_{ij} d_j \qquad H_{vib} = \sum_\alpha \hbar\omega_\alpha b_\alpha^\dagger b_\alpha \qquad H_e = \sum_{i,j}\sum_\alpha d_i^\dagger \lambda_{ij}^\alpha d_j \left(b_\alpha^\dagger + b_\alpha\right)$$

$$\lambda_{ij}^\alpha = \sqrt{\frac{\hbar}{2\omega_\alpha}} \sum_{k,\mu} \left\langle i \left| \nabla_{k\mu} H_e \right|_{\vec{Q}=0} \right| j \right\rangle A_{k\mu,\alpha}$$

→ Implementation in TURBOMOLE by M. Bürkle using density functional perturbation theory (DFPT)
→ “analytical” derivatives
→ available in TURBOMOLE 6.6

Lowest-order expansion of current in electron-vibration coupling

$$I = I_{el} + \delta I_{el} + I_{inel}$$

$$I_{el} = \frac{2e}{h} \int \mathrm{d}E \mathrm{Tr}[\boldsymbol{G}^r \boldsymbol{\Gamma}_R \boldsymbol{G}^a \boldsymbol{\Gamma}_L](f_L - f_R)$$

$$\delta I_{el} = \frac{4e}{h} \int \mathrm{d}E \mathrm{ReTr}[\boldsymbol{\Gamma}_L \boldsymbol{G}^r \boldsymbol{\Sigma}_{e\text{-vib}}^r \boldsymbol{G}^r \boldsymbol{\Gamma}_R \boldsymbol{G}^a](f_L - f_R)$$

$$I_{inel} = -\mathrm{i}\frac{2e}{h} \int \mathrm{d}E \mathrm{Tr}\left[\boldsymbol{G}^a \boldsymbol{\Gamma}_L \boldsymbol{G}^r \left\{(f_L - 1)\Sigma_{e-vib}^< - f_L \Sigma_{e-vib}^>\right\}\right]$$

Transport theory: J. K. Viljas, J. C. Cuevas, F. Pauly, and M. Häfner, Phys. Rev. B 72, 245415 (2005)

M. Bürkle, J. K. Viljas, T. J. Hellmuth, E. Scheer, F. Weigend, G. Schön, F. Pauly, arXiv:1309.4552

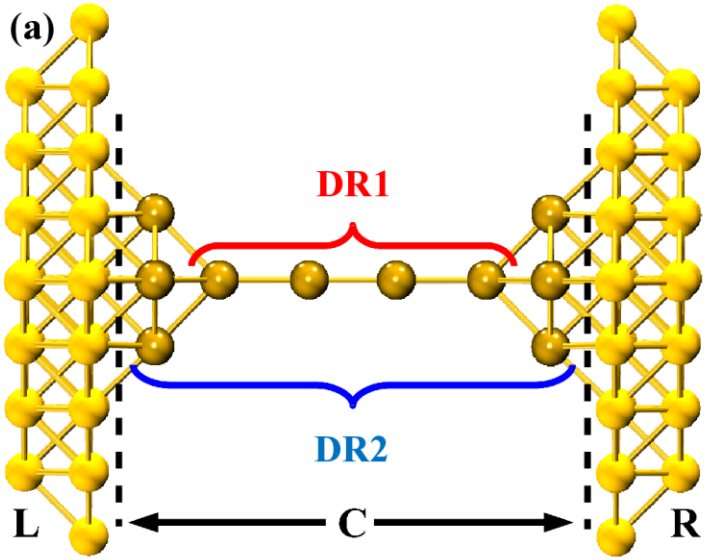
Influence of vibrations on electron transport

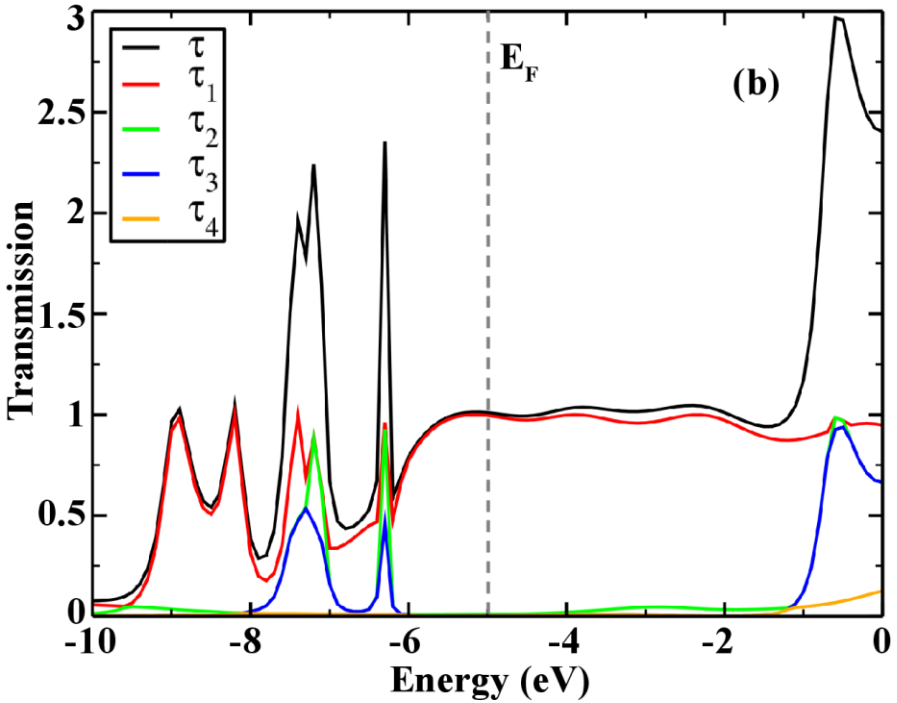
Method

Gold junctions

Octane-based junctions

Elastic transport in gold junctions

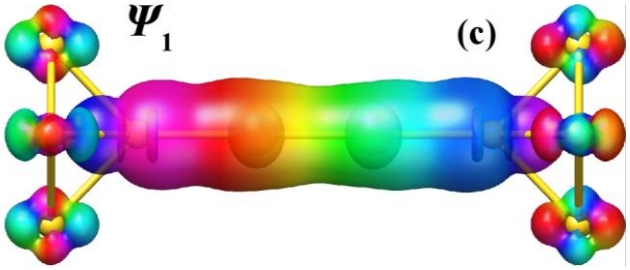


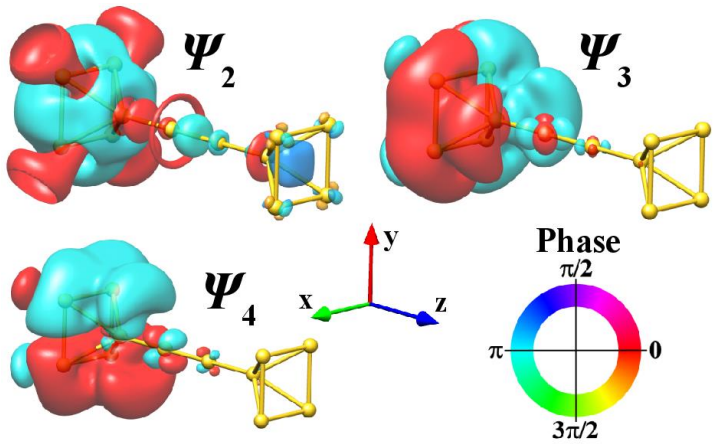


$\tau_1 = 0.996$

$\tau_2 = 0.009$

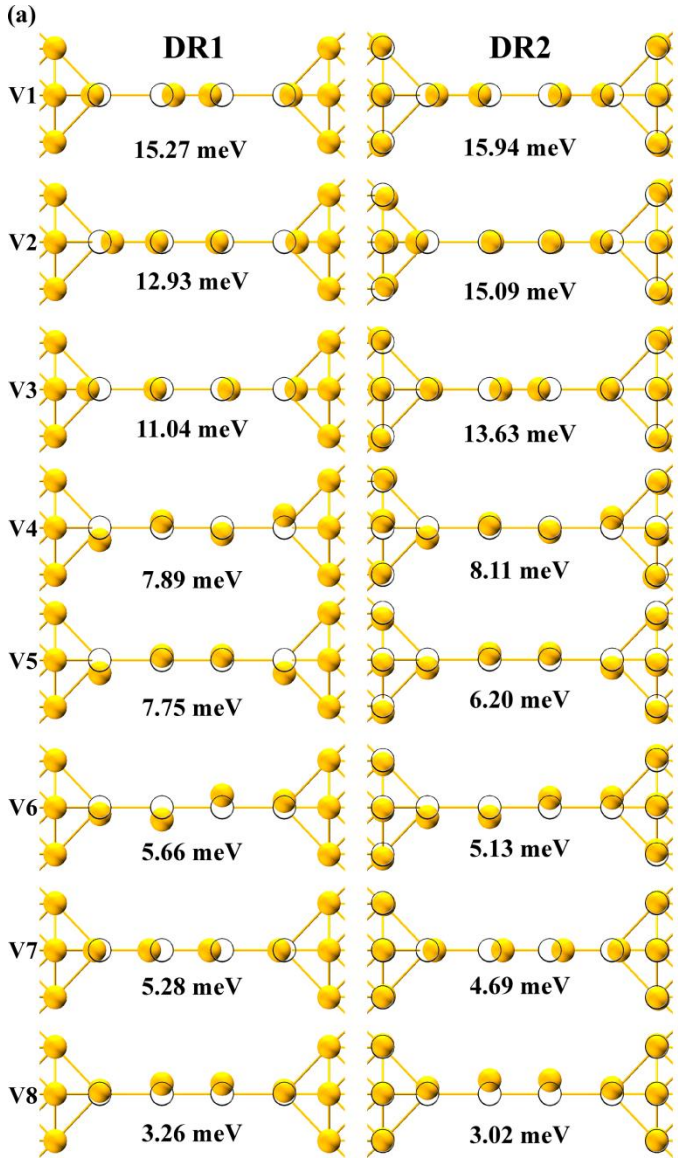
$\tau_3 = \tau_4 = 0.003$

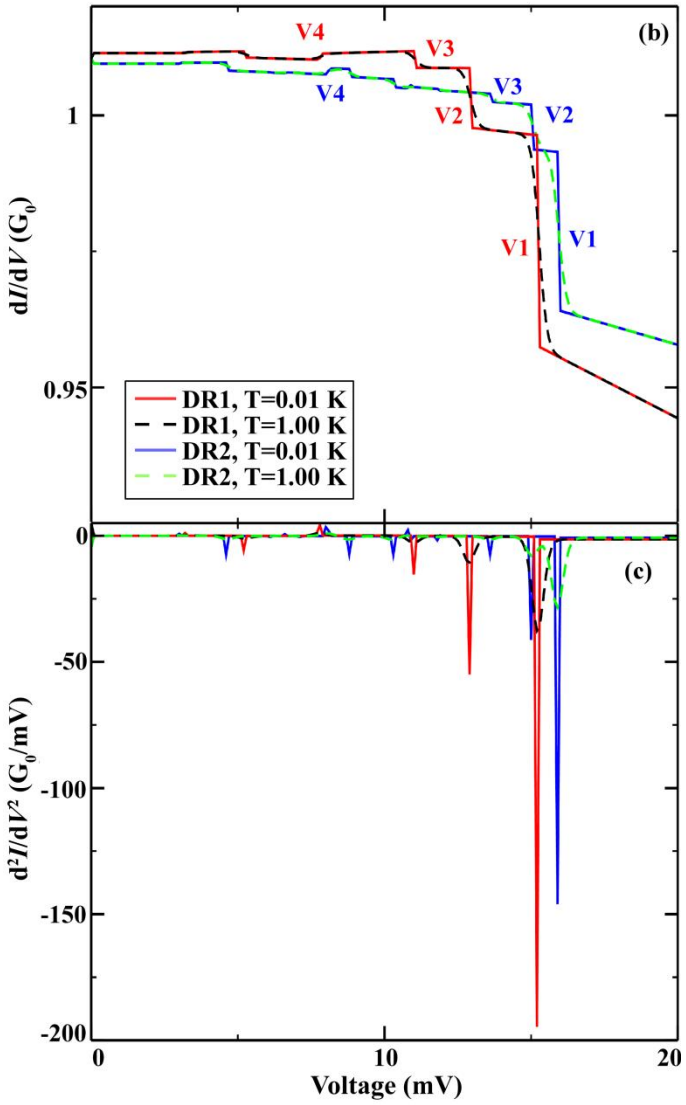




M. Bürkle et al., Phys. Rev. B 85, 075417 (2012)
M. Bürkle et al., arXiv:1309.4552

Inelastic transport in gold junctions





M. Bürkle *et al.*, arXiv:1309.4552

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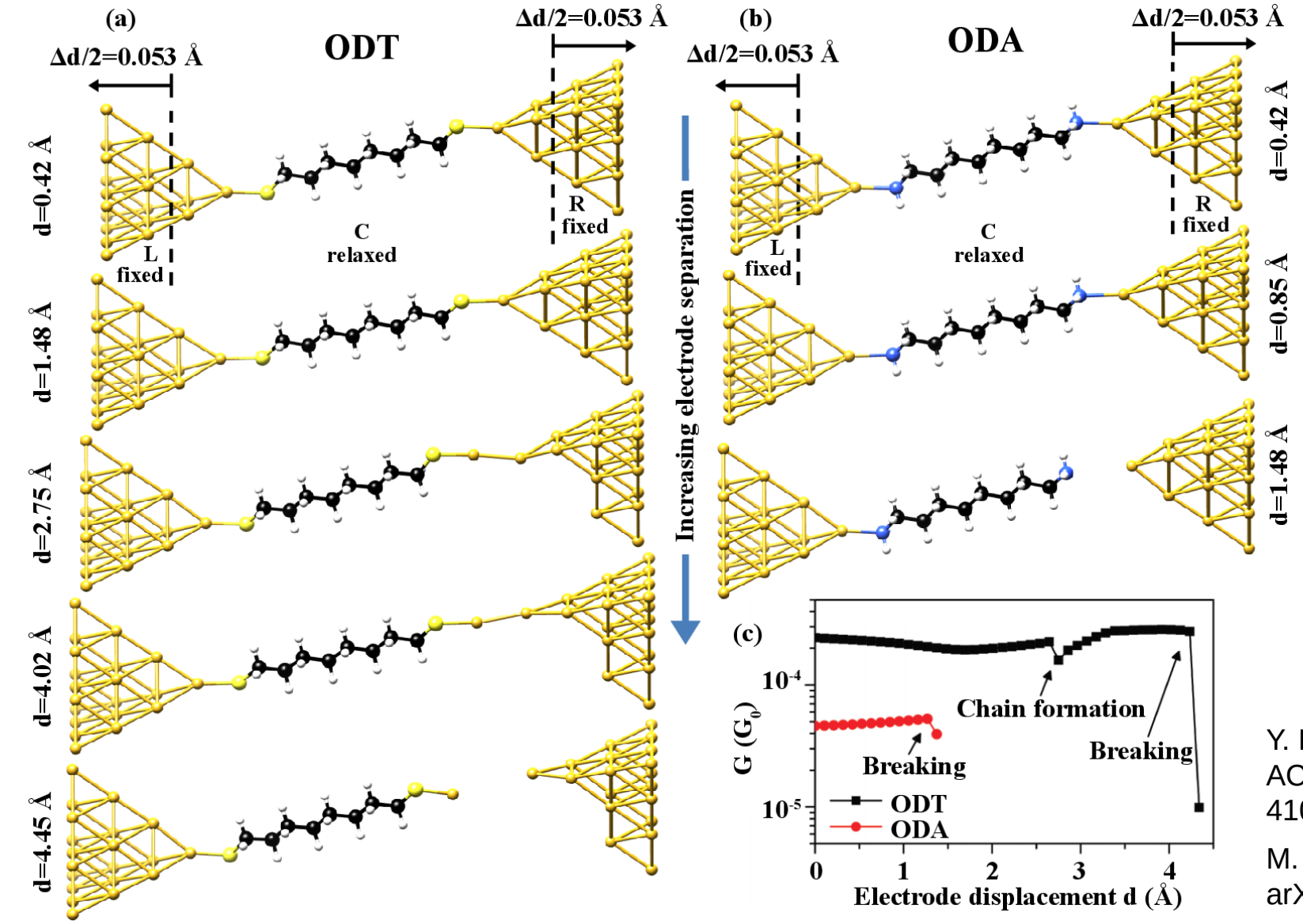
Elastic transport in octane-based junctions



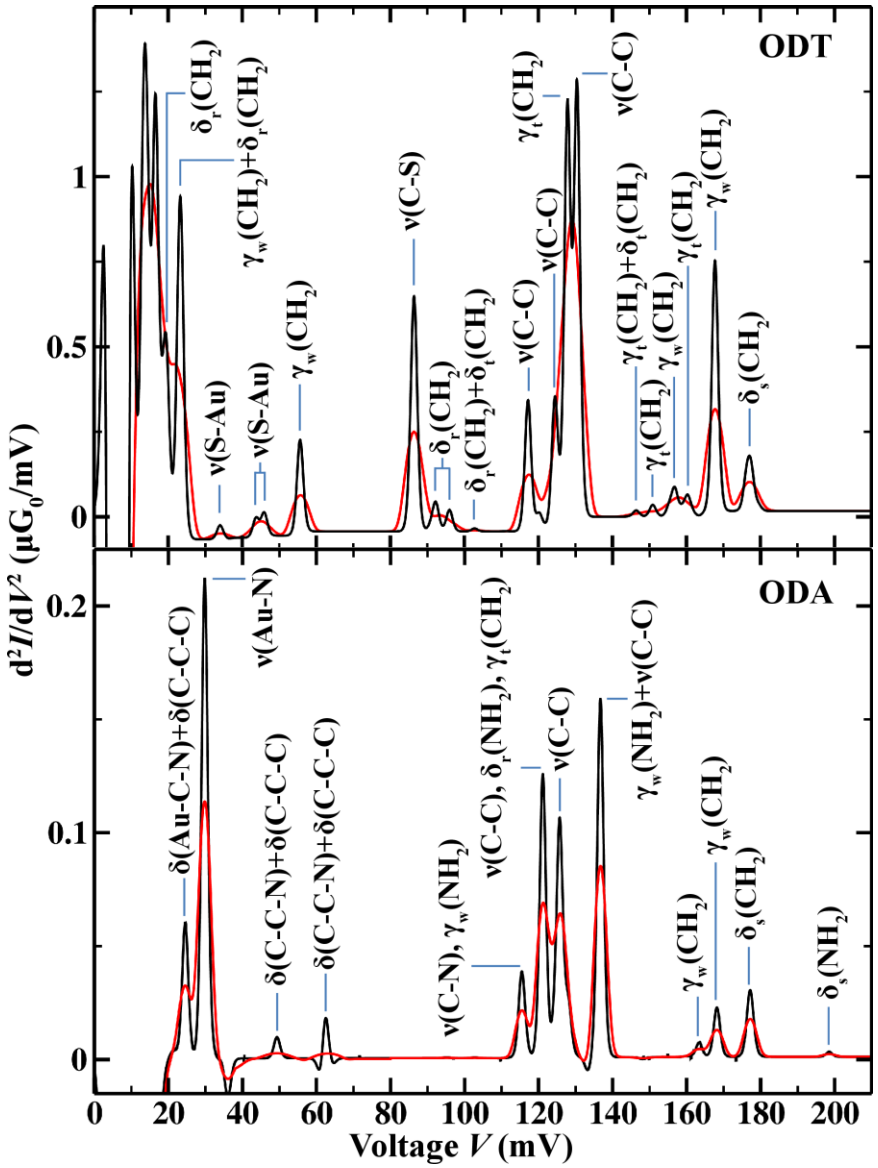
Y. Kim et al., ACS Nano 5, 4104 (2011)

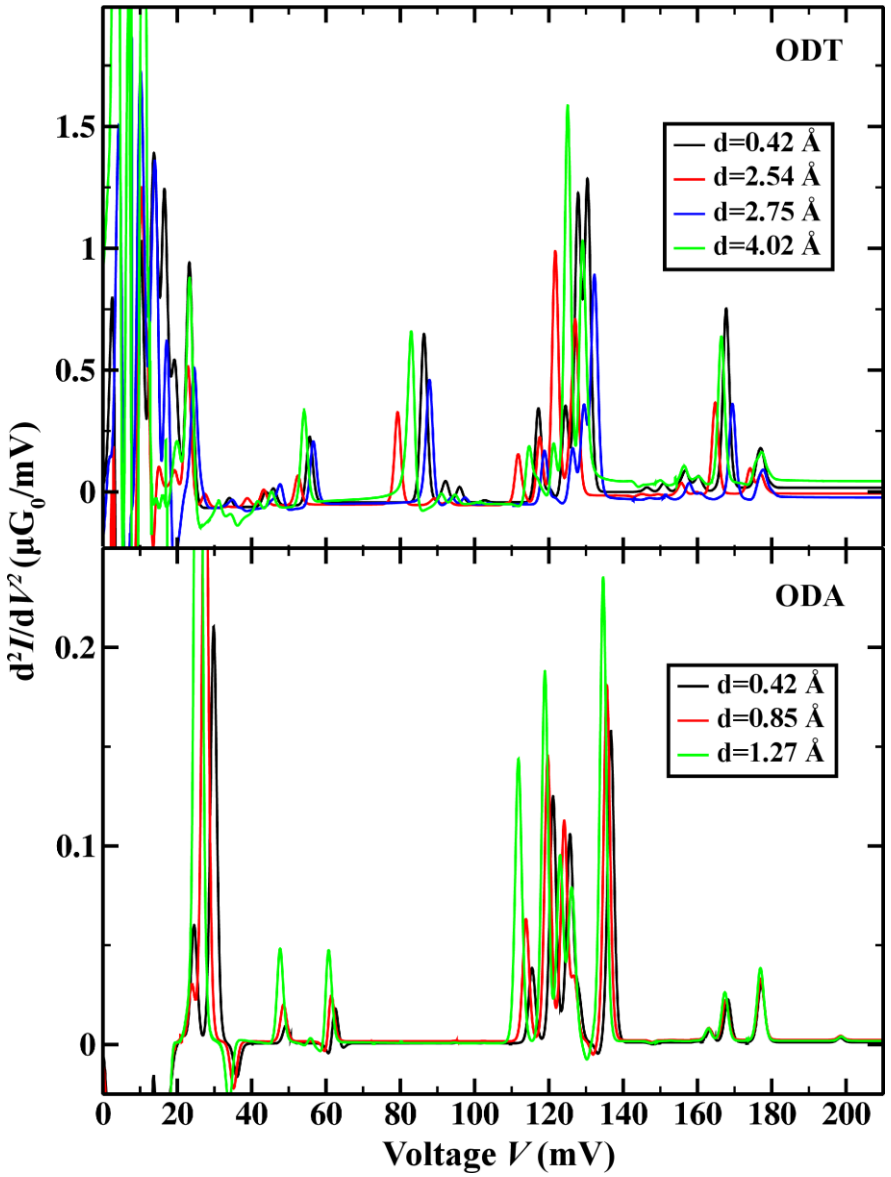
M. Bürkle et al., arXiv:1309.4552

Inelastic transport in octane-based junctions

Universität Konstanz

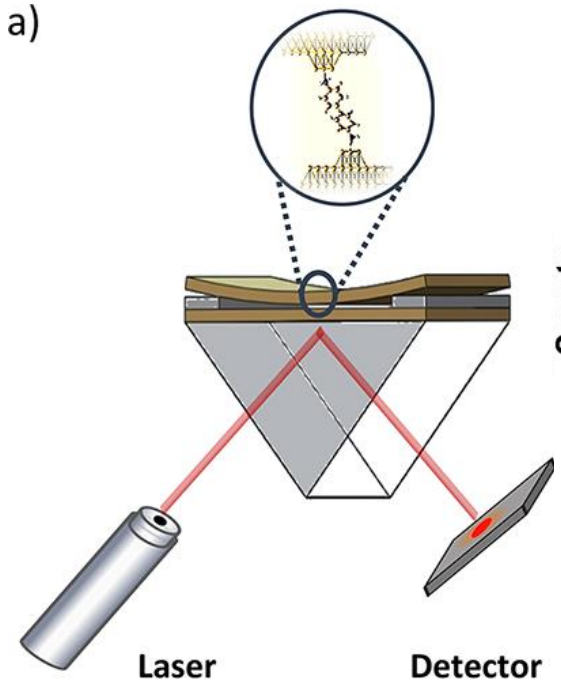
M. Bürkle *et al.*, arXiv:1309.4552

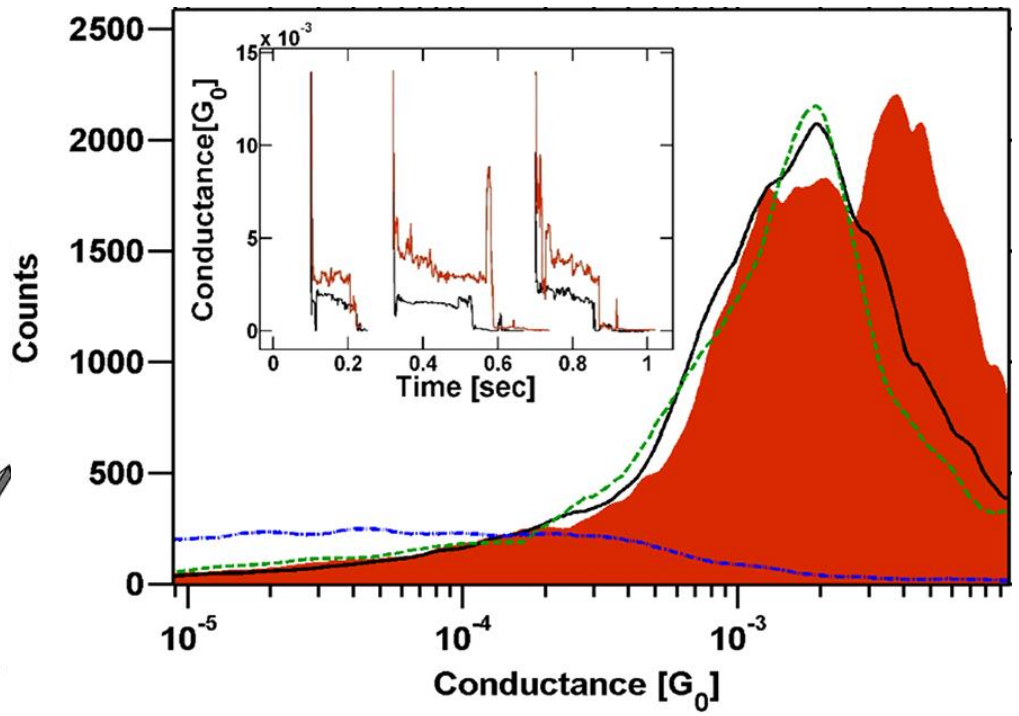


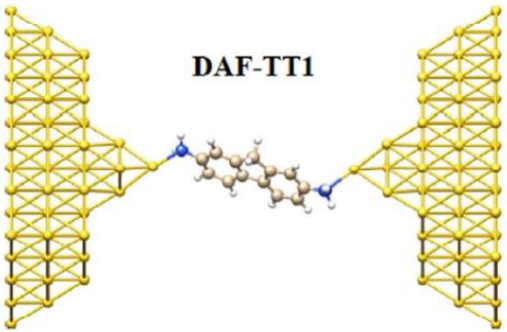


Miscellaneous

Plasmon-induced conductance enhancement







Conductance histogram of Au-DAF-Au

— no light

■ 781 nm, p-polarized light

– – – 781 nm, s-polarized light

–·–·– pure solvent

M. Vadai, N. Nachman, M. Bürkle, F. Pauly, J. C. Cuevas, and Y. Selzer, J. Phys. Chem. Lett. 4, 2811 (2013)

Plasmon-induced conductance enhancement

Universität Konstanz

Radiation creates oscillating bias voltage V_{AC} on top of V_{DC} due to plasmonic response.

P. K. Tien and J. P. Gordon, Phys. Rev. 1963
J. K. Viljas *et al.*, Phys. Rev. B 75, 075406 (2007)
N. Ittah *et al.*, Nano Lett. 9, 1615 (2009)

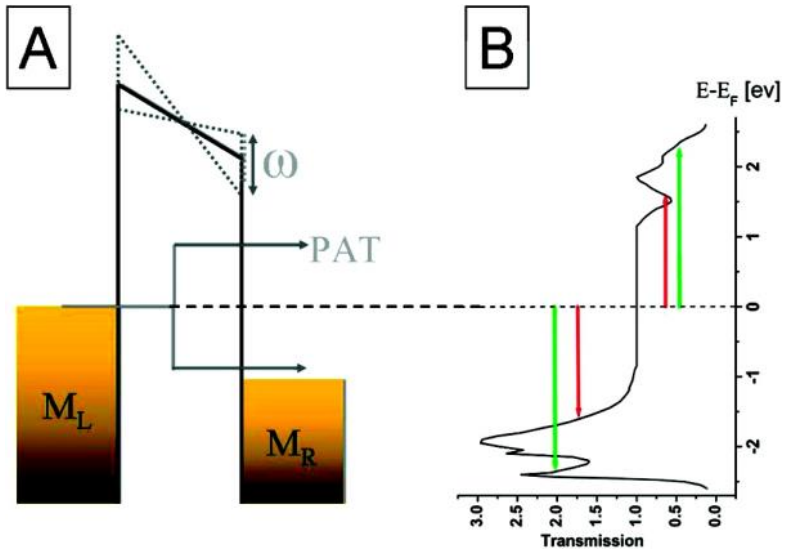
$$G_{dc}(\omega) = G_0 \sum_{n=-\infty}^{\infty} J_n^2(\alpha)\tau(E_F + n\hbar\omega)$$

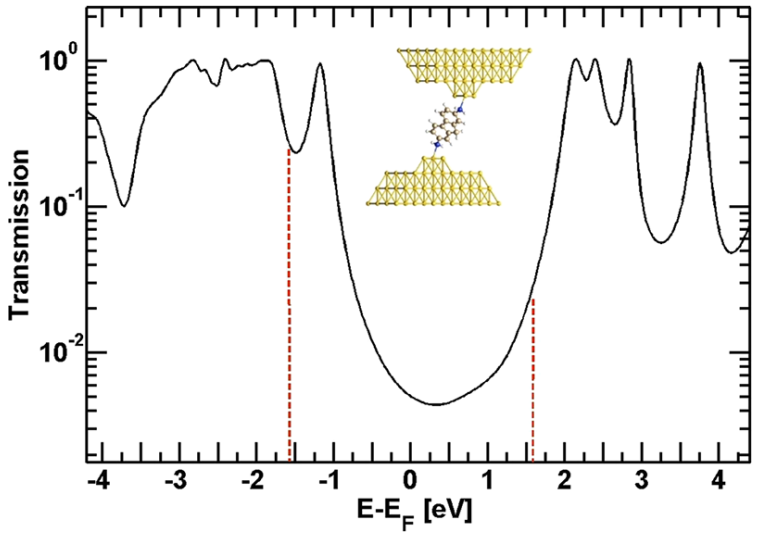
with $\alpha = eV_{ac} / \hbar\omega$

$$\alpha \ll 1 \text{ and } \tau(E_F), \tau(E_F + \hbar\omega) \ll \tau(E_F - \hbar\omega)$$

$$eV_{ac} = 2\hbar\omega \sqrt{\frac{G_{dc}(\omega) - G_{dc}(0)}{G_0 \tau(E_F - \hbar\omega)}}$$

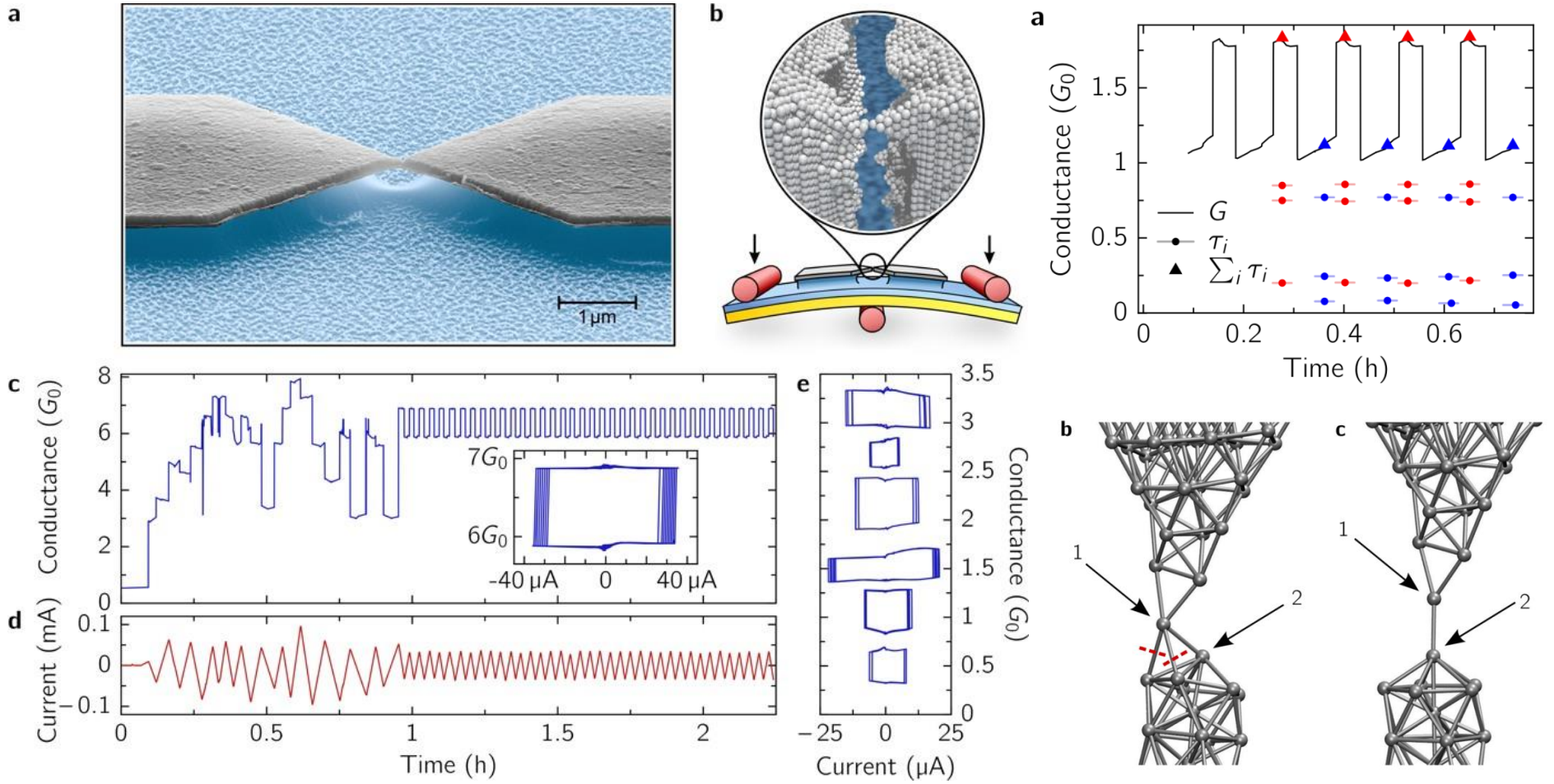
$V_{ac} \approx 0.17$ V; field enhancement ≈ 1100





M. Vadai, N. Nachman, M. Bürkle, F. Pauly, J. C. Cuevas, and Y. Selzer, J. Phys. Chem. Lett. 4, 2811 (2013)

A current-driven single-atom memory



C. Schirm, M. Matt, F. Pauly, J. C. Cuevas, P. Nielaba, and E. Scheer, Nature Nanotechnology 8, 645 (2013)

See also News & Views: S. J. van der Molen, Nature Nanotechnology 8, 622 (2013)

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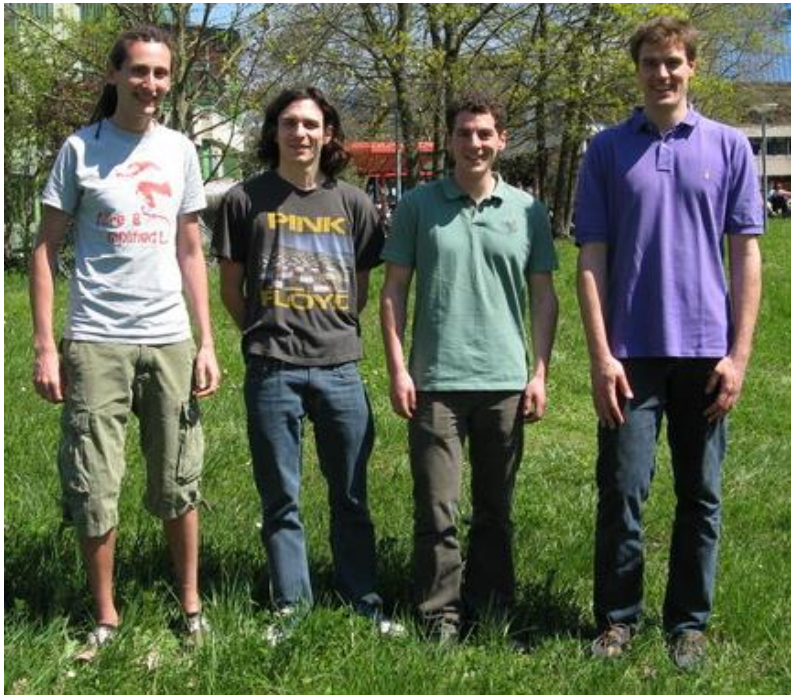
- Marcel Mayor & Group (U Basel)
- Thomas Wandlowski & Group (U Bern)
- Pramod S. Reddy & Group (U Michigan)



Open position:
1 Postdoc/PhD

?

MB (Japan)

TH

… and funding agencies

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Baden-Württemberg
MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST

Summary

- **Heat dissipation and thermopower in atomic-scale junctions**
- **Influence of vibrations on electron transport**
  - Gold junctions
  - Octane-based junctions
- **Miscellaneous**
  - Plasmon-induced conductance enhancement in single-molecule junctions
  - A current-driven single-atom memory

→ Improved understanding of charge transport at smallest scale by measurement of several quantities: Conductance, IETS, thermopower, heating, …

Outlook

- **Phonon transport**
  - Realistic *ZT*, including more than just electronic contributions