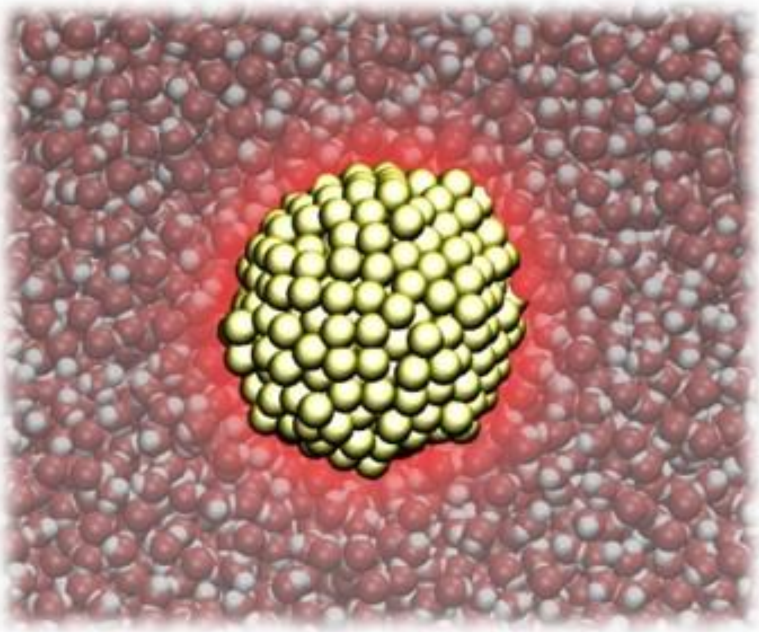
Thermal transport at solid-liquid interfaces: nanoparticles and graphene coated gold nanostructures

O. Gutiérrez, C. Herrero, R. Santamaria, L. Joly
and Samy Merabia

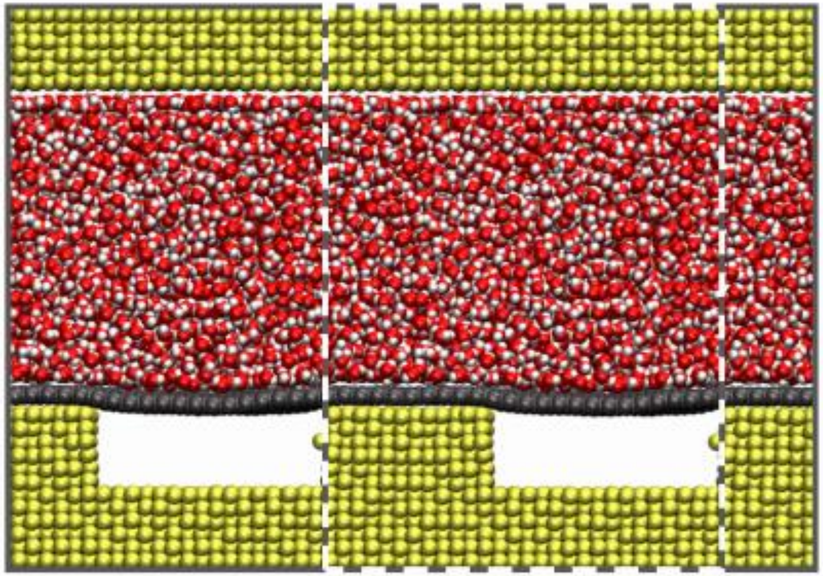
ILM-Institute Light and Matter
CNRS and Université Lyon 1

Outline

Thermal transport around plasmonic nanoparticles

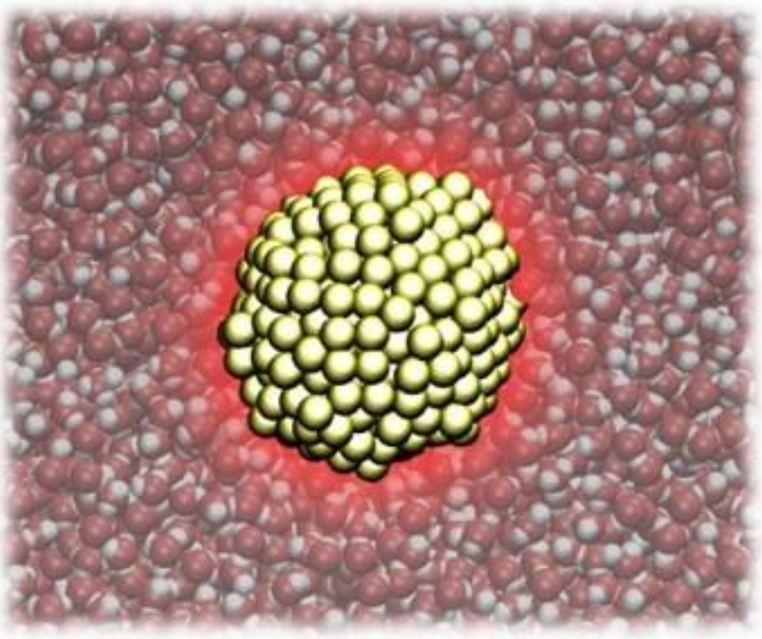


Thermal transport at nanostructured interfaces

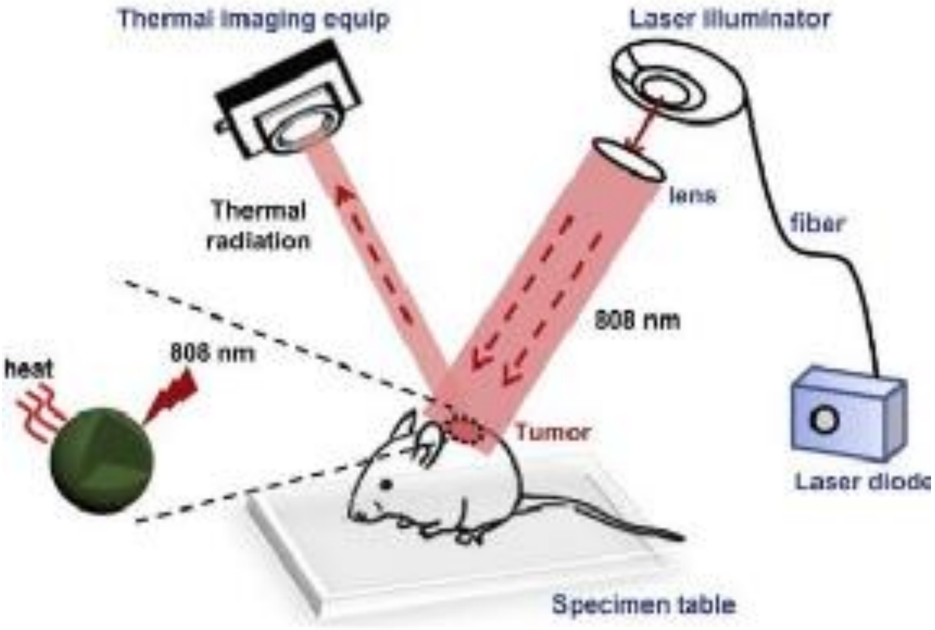


Outline

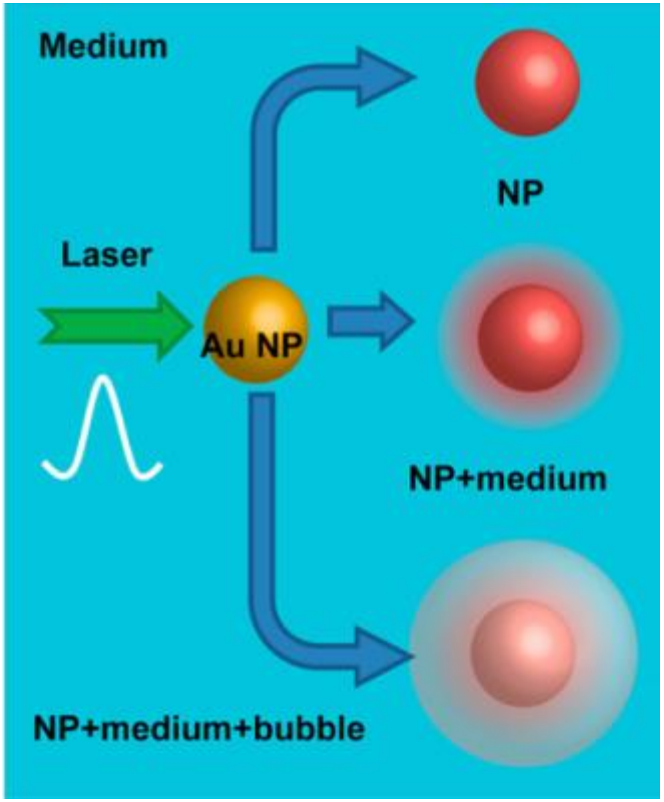
Thermal transport around plasmonic nanoparticles



Motivations



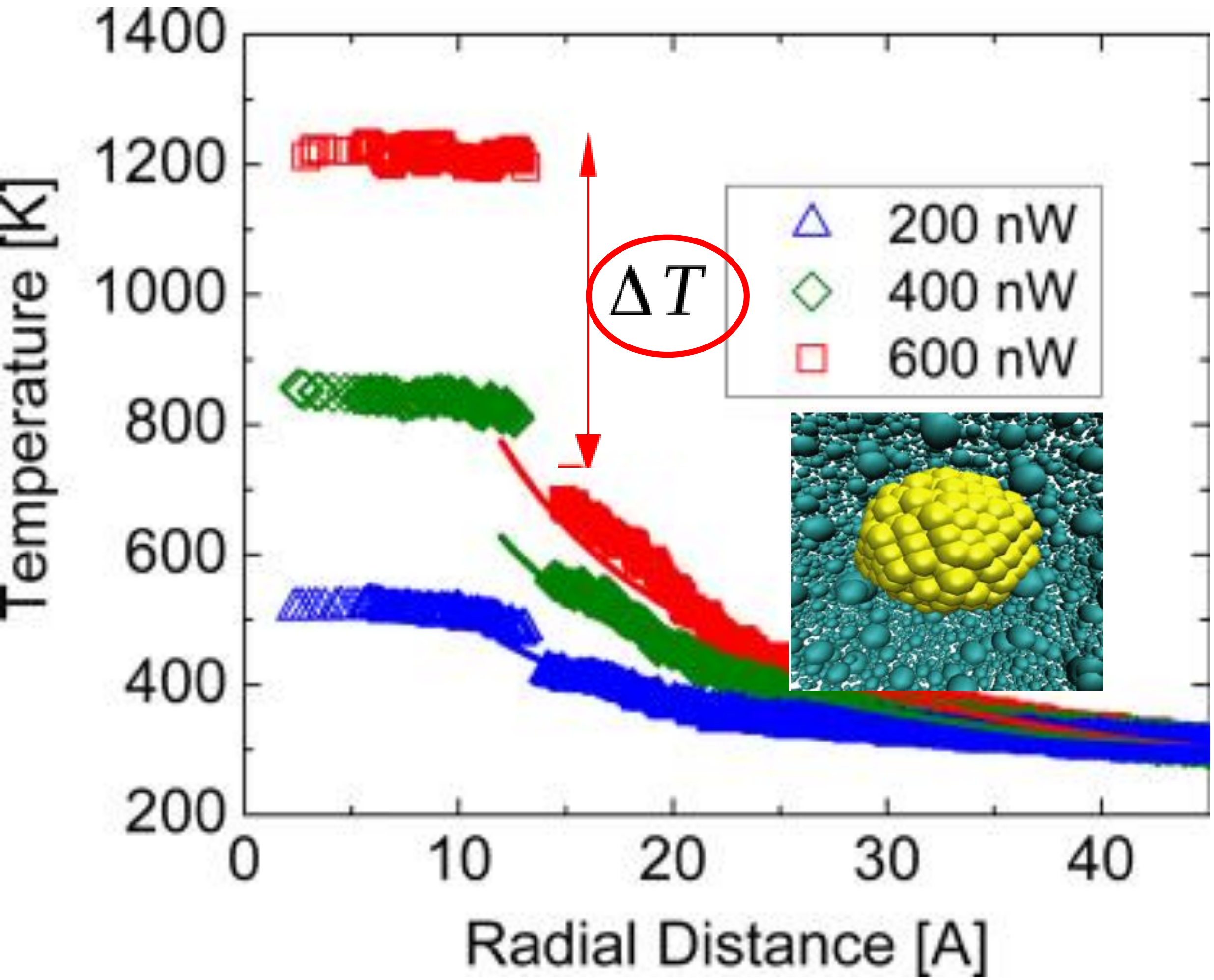
Biomaterial 34 (2013) 9584

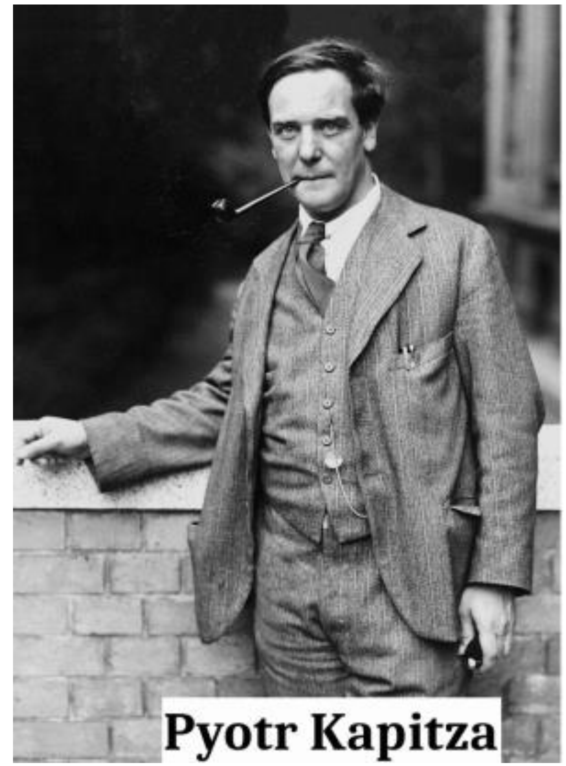


Plasmonic nanoparticles show some promise for photothermal cancer therapies

In pulsed laser conditions local levels of heating depend on the interface thermal conductance at the nanoparticle-water interface

Kapitza conductance





$$R = \frac{1}{G} = \frac{(T_2 - T_1)}{q}$$

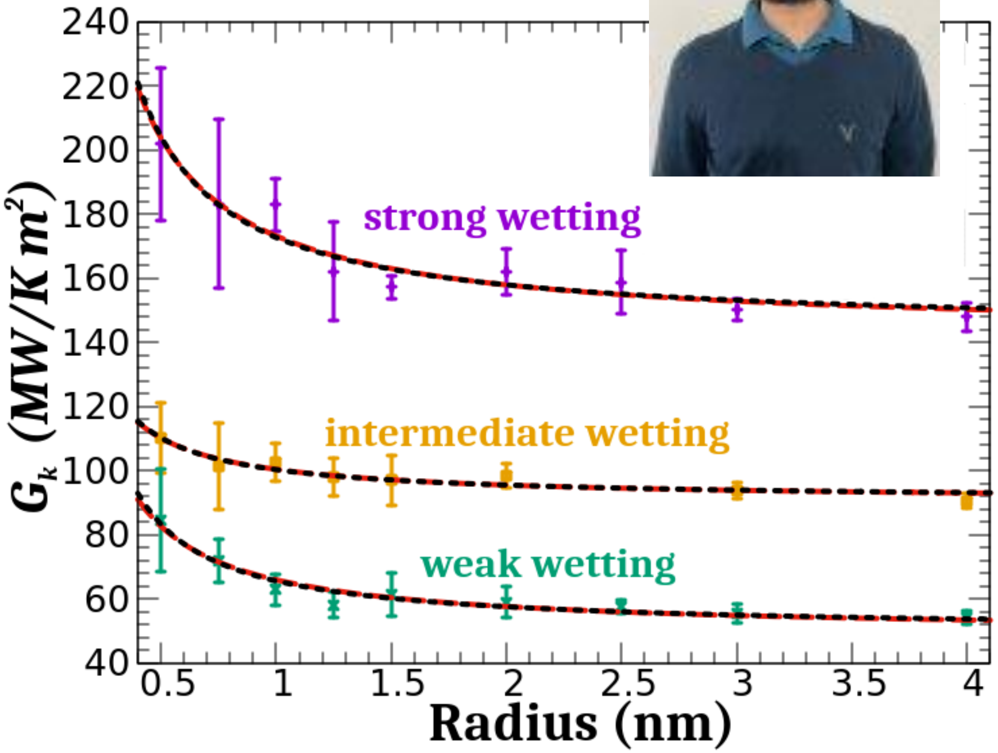
S. Merabia, L. Lewis, P. Keblinski and J.-L. Barrat, *Phys. Rev. E* (2009)

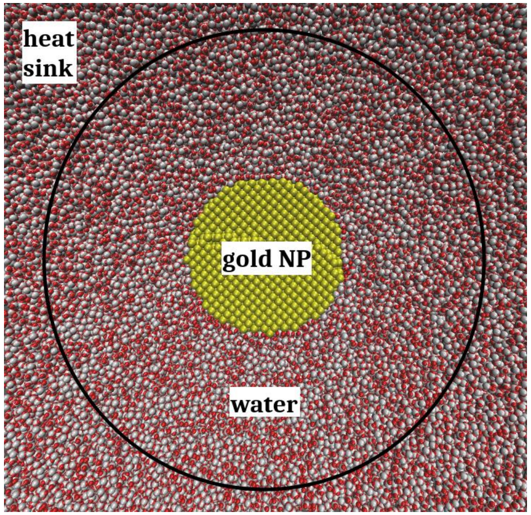
How does the Kapitza conductance depend on the nanoparticle size ?

What happens for very strong heating ?

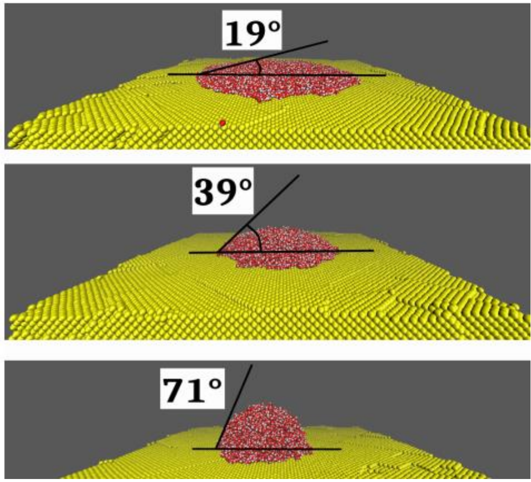
Size dependent thermal conductance

O. Gutiérrez-Varela





Strong wetting

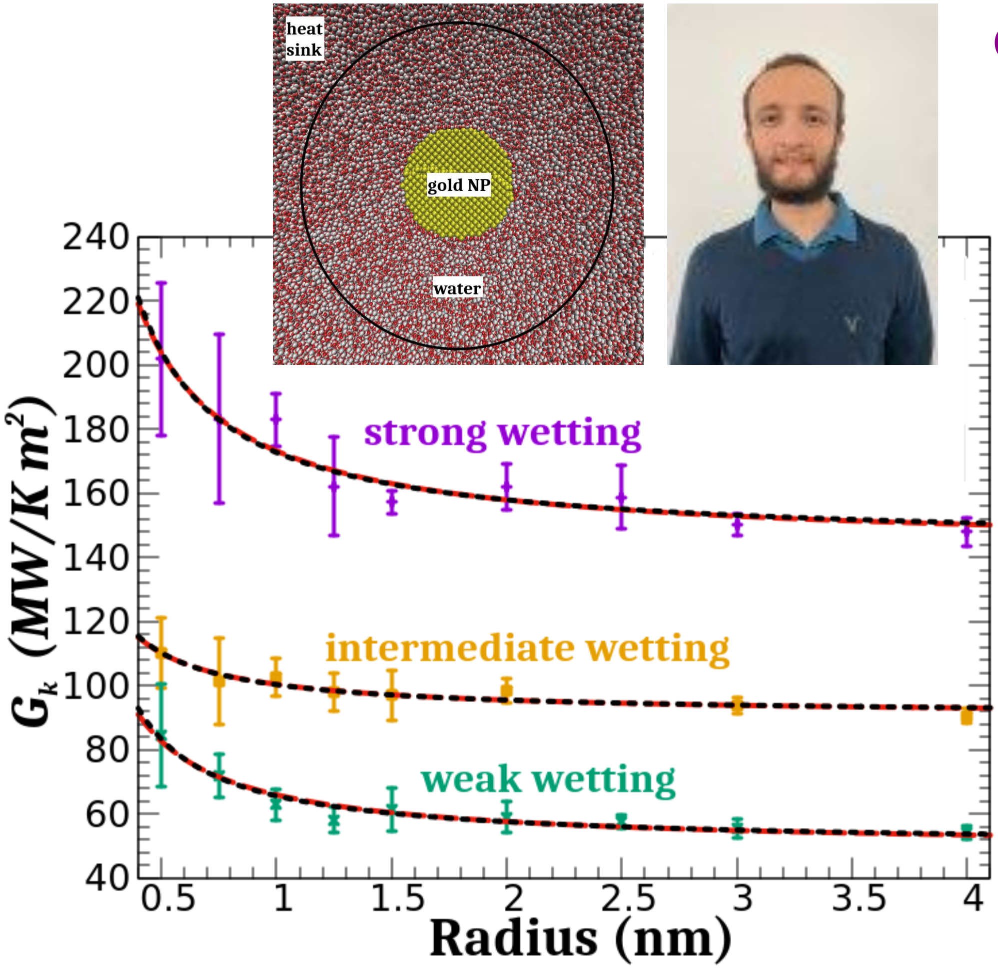


Weak wetting

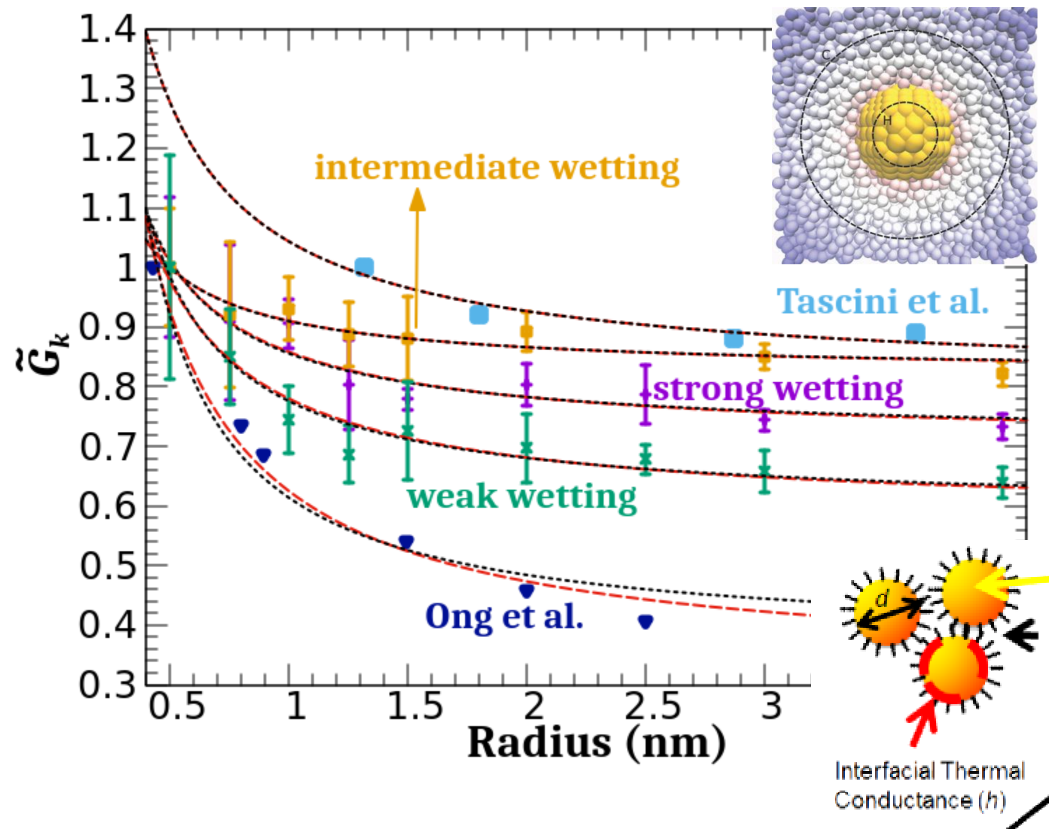
The interface thermal conductance increases with the nanoparticle curvature

O. Gutiérrez, S. Merabia and R. Santamaria, *J. Chem. Phys.* (2022)

Size dependent thermal conductance



O. Gutiérrez-Varela



The interface thermal conductance increases with the nanoparticle curvature

O. Gutiérrez, S. Merabia and R. Santamaria, *J. Chem. Phys.* (2022)

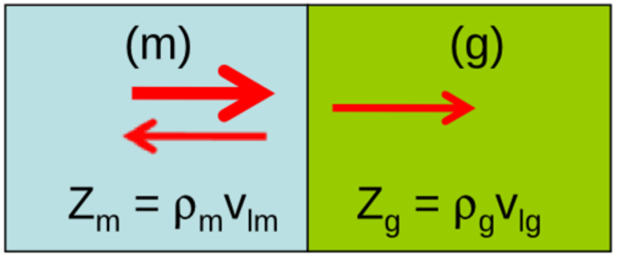
Generalized acoustic mismatch model

Thermal conductance

$$G_k = \sum_p \int_0^{\omega_{\max}} k_B g_p(\omega) v_p(\omega) \tau_p(\omega) d\omega$$

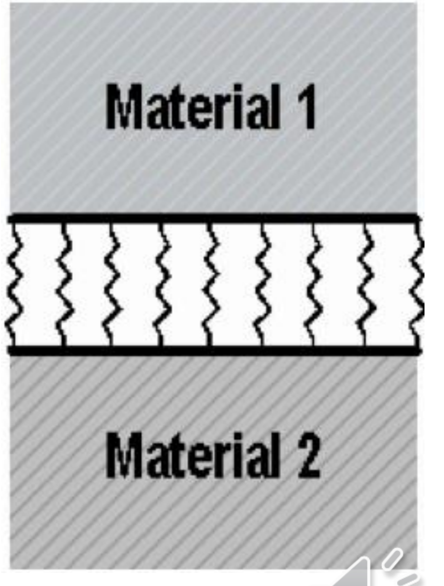
Acoustic mismatch model

Based on continuum acoustics, no scattering



Transmission coefficient

$$\tau_p(\omega) = \frac{Z_{\rm np}(\omega) Z_{\rm wat}(\omega)}{(Z_{\rm np}(\omega) + Z_{\rm wat}(\omega))^2 + \frac{\omega^2}{K^2(R_{\rm np})}(Z_{\rm np}(\omega) Z_{\rm wat}(\omega))^2}$$

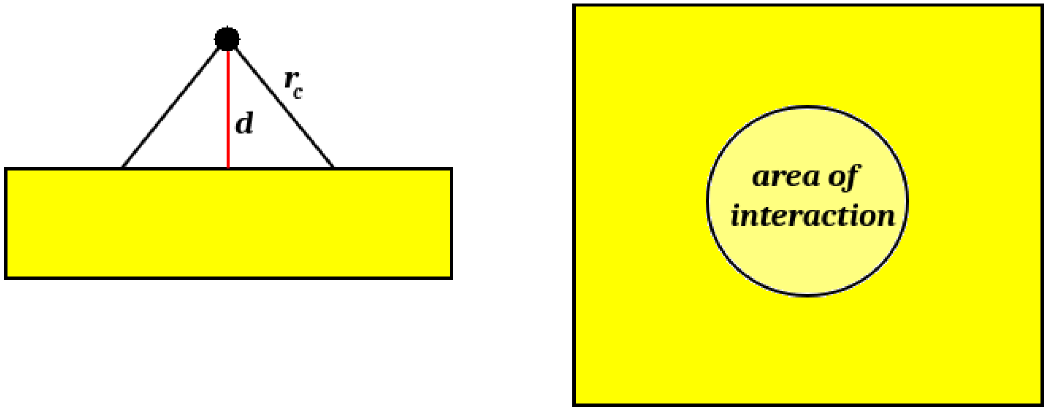


Bonding stiffness

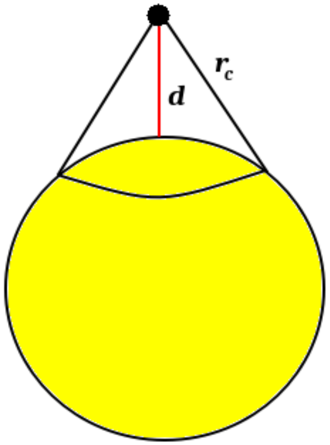
$$K(R_{np}) = \sigma(R_{np}) * \frac{d^2V}{dr^2}$$

R. Prasher, *Appl. Phys. Lett.* (2009)
S. Merabia, A. Alkurdi and J. Lombard, *Int. J. Heat Mass Transf.* (2016)

Effect of the curvature



Area of interaction for a planar surface



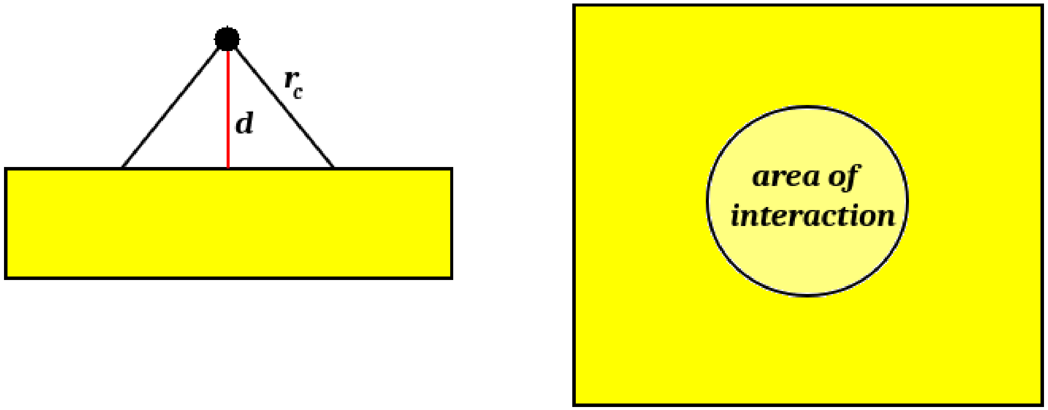
Area of interaction for a spherical surface

Molecular footprint

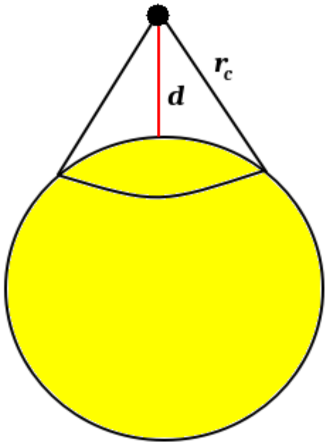
$$s_{R_{\rm np}\to\infty}(d) = \pi(r_c^2 - d^2)$$

$$s_{R_{\rm np}}(d) = \pi\frac{(r_c^2 - d^2)}{(1 + d/R_{\rm np})}.$$

Effect of the curvature



Area of interaction for a planar surface



Area of interaction for a spherical surface

Molecular footprint

$$s_{R_{\mathrm{np}}\to\infty}(d) = \pi(r_c^2 - d^2)$$

$$s_{R_{\mathrm{np}}}(d) = \pi\frac{(r_c^2 - d^2)}{(1 + d/R_{\mathrm{np}})}.$$

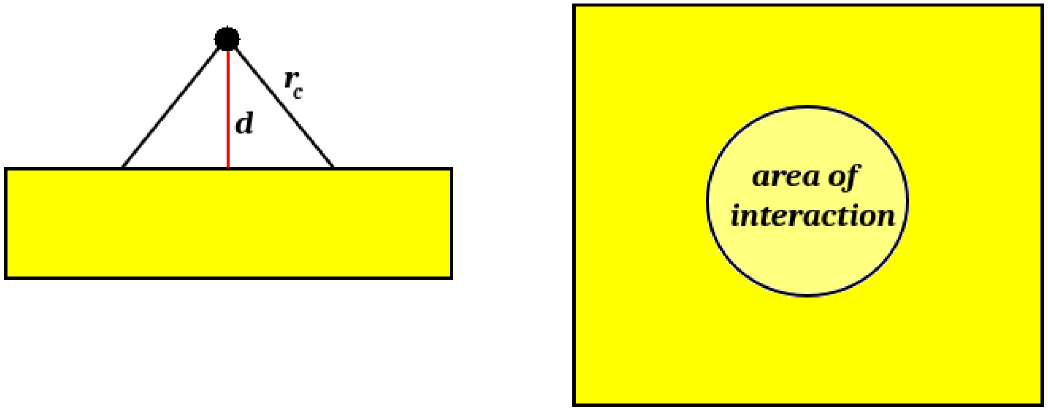
Surface density

$$\sigma(R_{\mathrm{np}}) = 1/s_{R_{\mathrm{np}}}(\delta) = \sigma(\mathrm{R}_{\mathrm{np}} \to \infty)(1 + \delta/R_{\mathrm{np}})$$

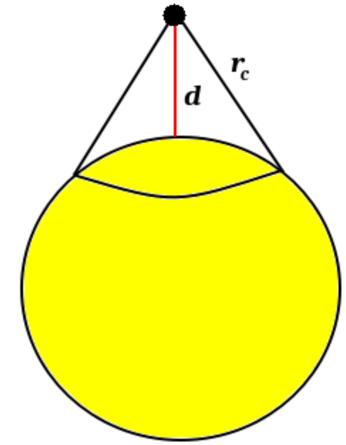
Interface bonding

$$K(R_{\mathrm{np}}) = K(\mathrm{R}_{\mathrm{np}} \to \infty)(1 + \delta/R_{\mathrm{np}})$$

Effect of the curvature



Area of interaction for a planar surface



Area of interaction for a spherical surface

Molecular footprint

$$s_{R_{\mathrm{np}}\to\infty}(d) = \pi(r_c^2 - d^2)$$

$$s_{R_{\mathrm{np}}}(d) = \pi\frac{(r_c^2 - d^2)}{(1 + d/R_{\mathrm{np}})}.$$

Surface density

$$\sigma(R_{\mathrm{np}}) = 1/s_{R_{\mathrm{np}}}(\delta) = \sigma(\mathrm{R_{np}} \to \infty)(1 + \delta/R_{\mathrm{np}})$$

Interface bonding

$$K(R_{\mathrm{np}}) = K(\mathrm{R_{np}} \to \infty)(1 + \delta/R_{\mathrm{np}})$$

Phonon transmission

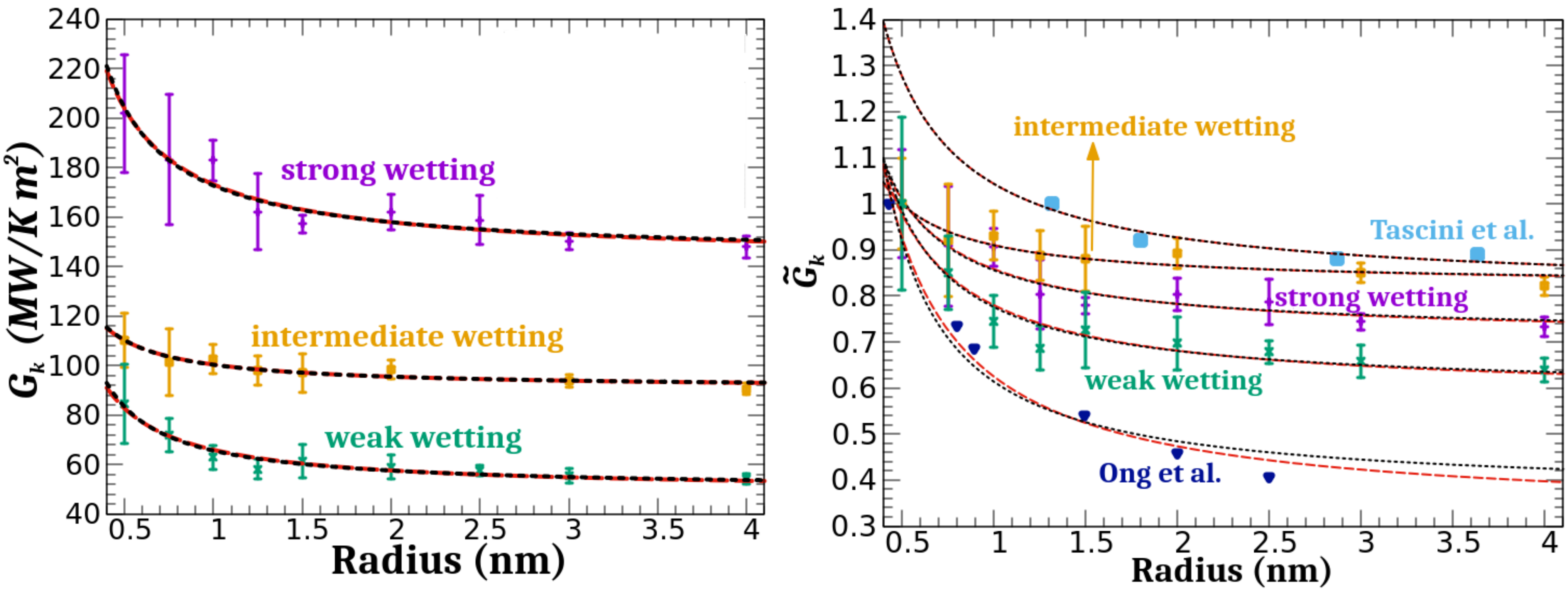
$$\tau_p(\omega) \simeq K^2(R_{\mathrm{np}})/\omega^2 \propto (1/\omega^2)(1 + \delta/R_{\mathrm{np}})^2$$

Thermal conductance

$$G_k(R_{\mathrm{np}}) \simeq G_k(\infty)\left(1 + \frac{\delta}{R_{\mathrm{np}}}\right)^2$$

Size dependent thermal conductance

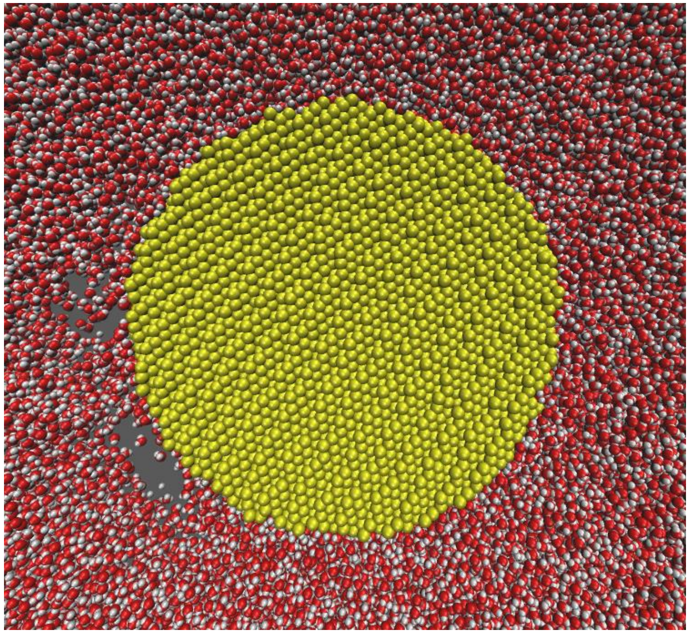
$$G_k(R_{\mathrm{np}}) \simeq G_k(\infty)\left(1 + \frac{\delta}{R_{\mathrm{np}}}\right)^2 \qquad \delta = 0{,}3\ nm$$

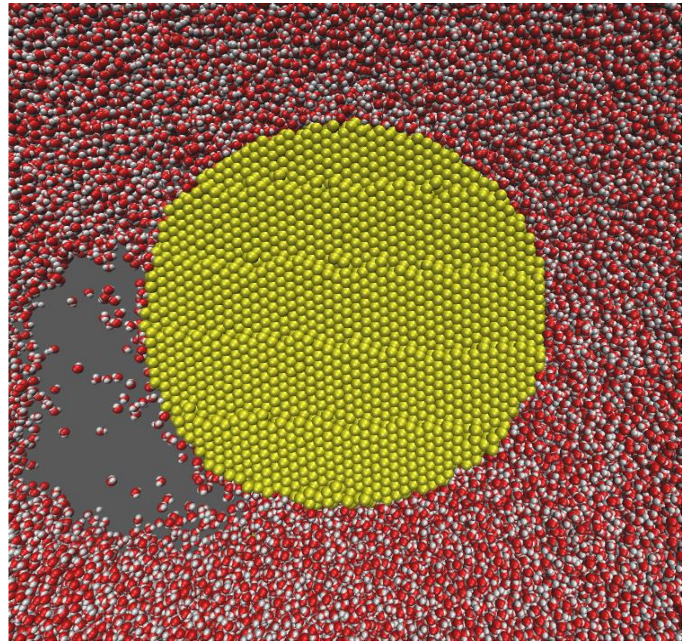


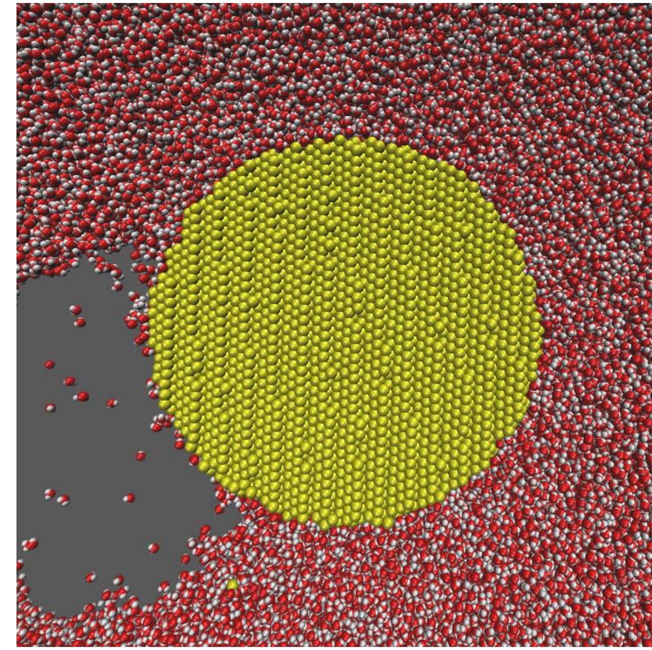
The quadratic model describes well the nanoparticle curvature dependence

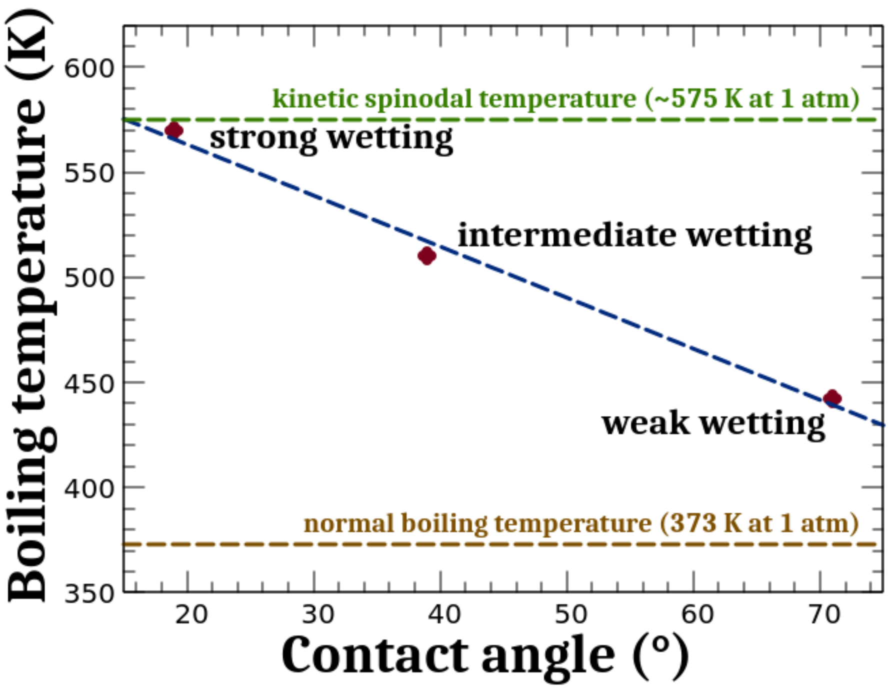
O. Gutiérrez, S. Merabia and R. Santamaria, *J. Chem. Phys.* (2022)

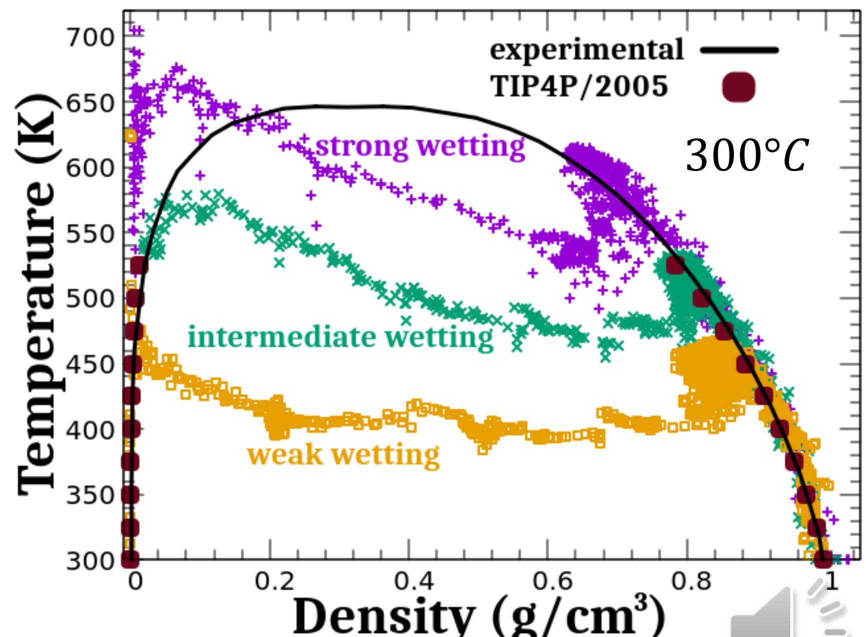
Nanoscale boiling







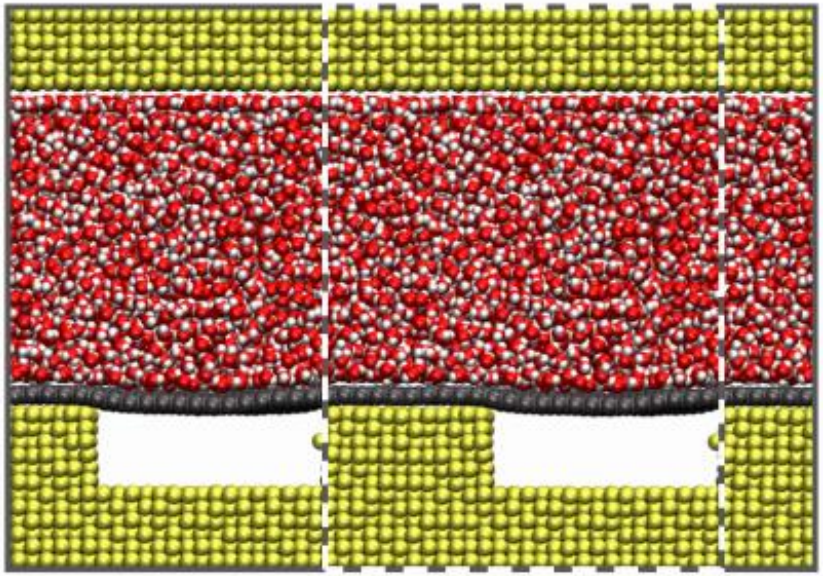




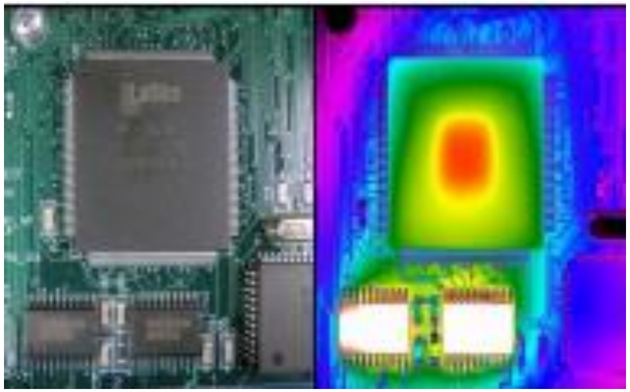
Gutiérrez, Lombard, Biben, Santamaria, Merabia, *arxiv* 2209.07900

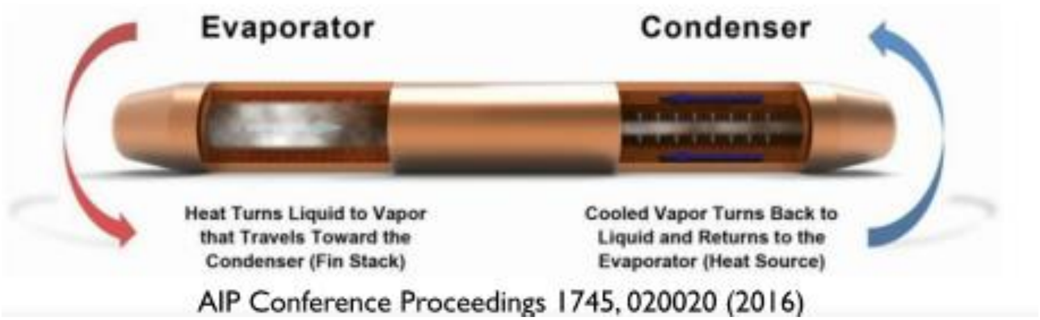
Outline

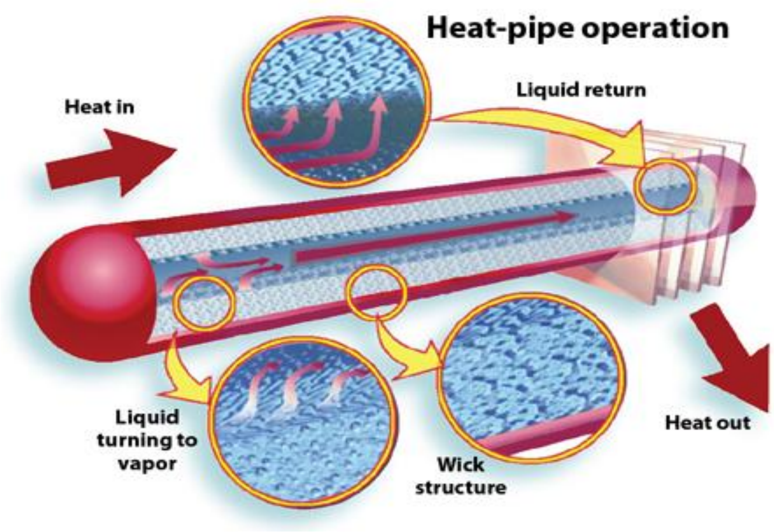
Thermal transport at nanostructured interfaces



Motivations





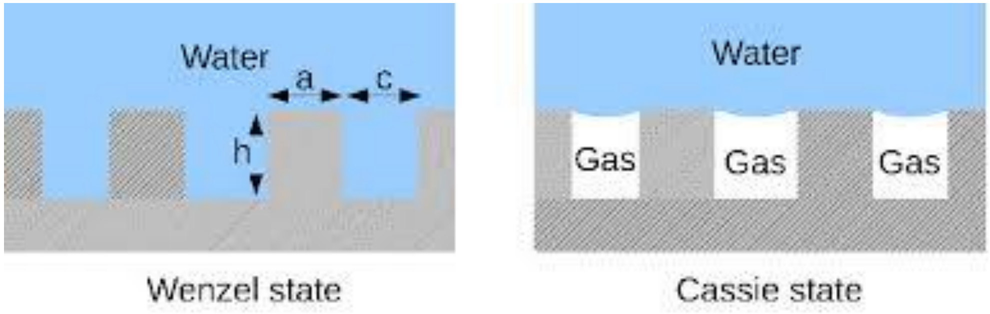


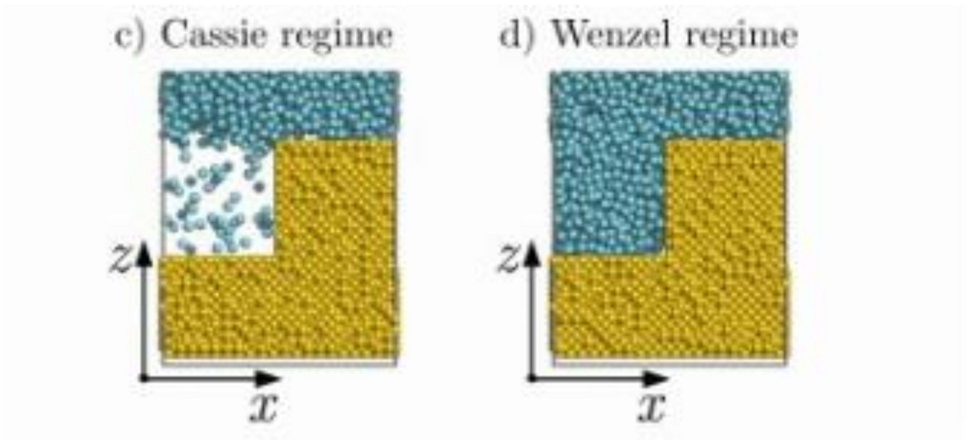
How to increase Kapitza resistance at solid-liquid interfaces ?

Minimizing heat transfer at solid-liquid interfaces

The objective: realizing a Cassie state

Casssie Wenzel states

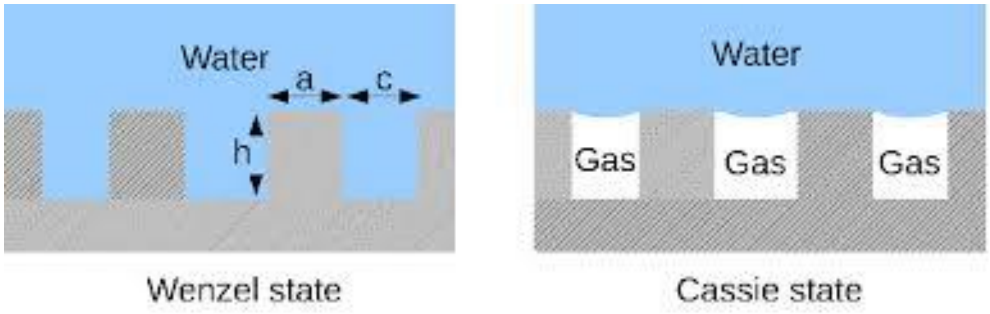


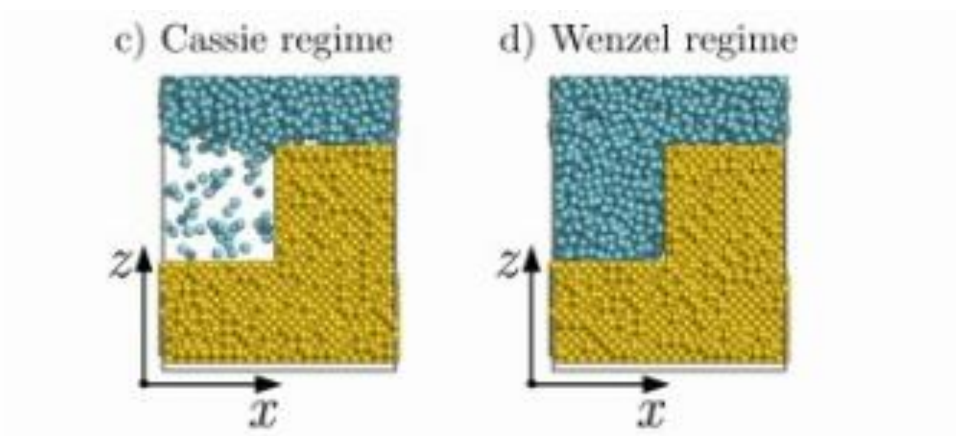


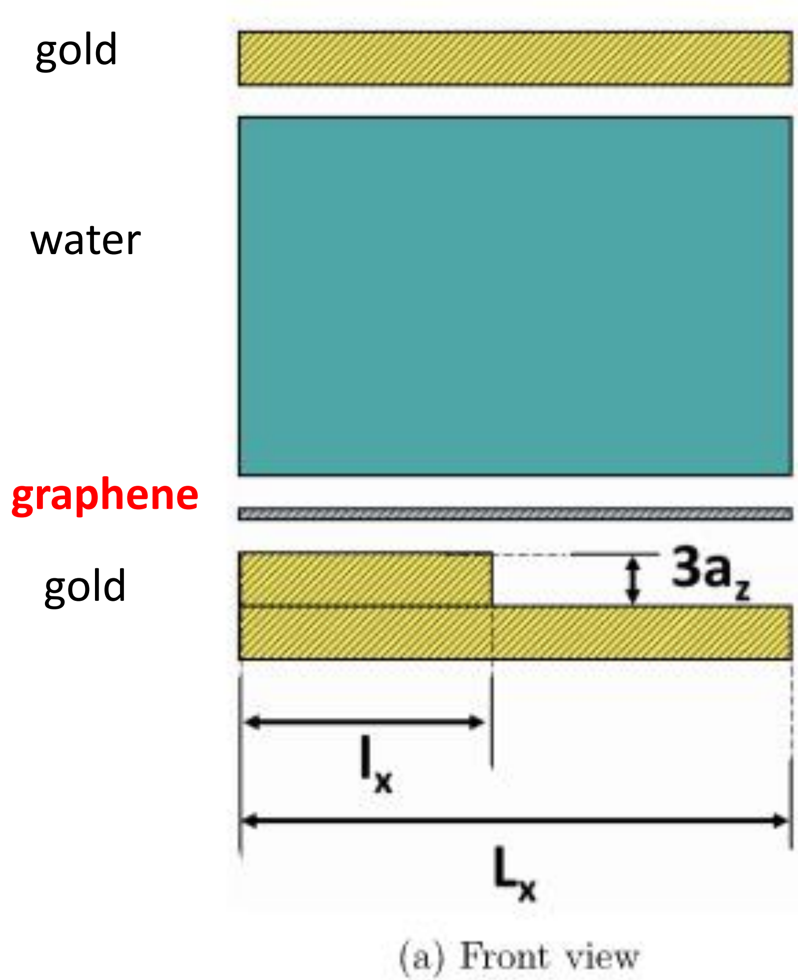
Donatas, Ohara, *J. Chem. Phys.* 2019

Minimizing heat transfer at solid-liquid interfaces

Casssie Wenzel states



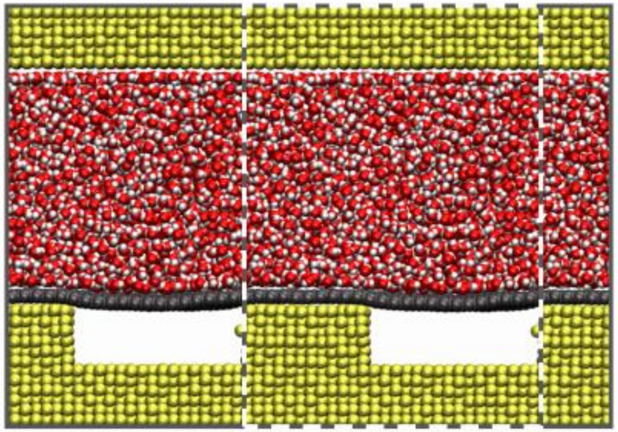




Donatas, Ohara, *J. Chem. Phys.* 2019

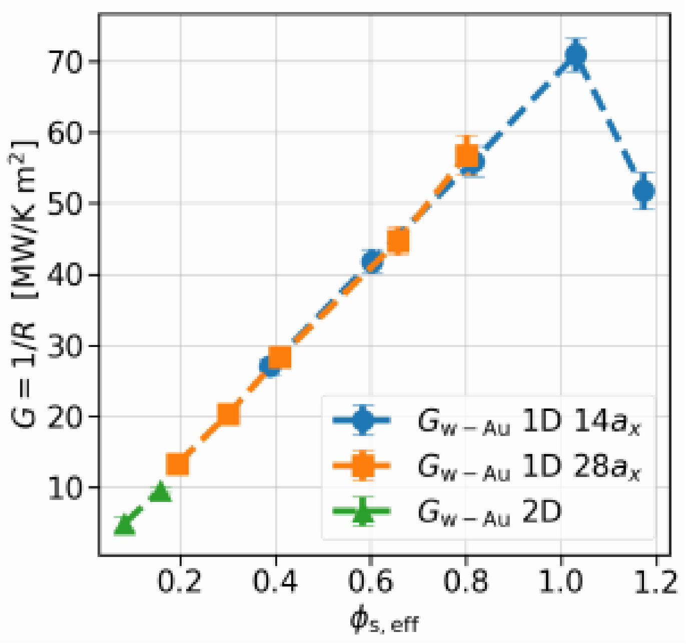
Herrero, Joly, Merabia, *Appl. Phys. Lett.* 2022

Heat transport on nanostructured graphene

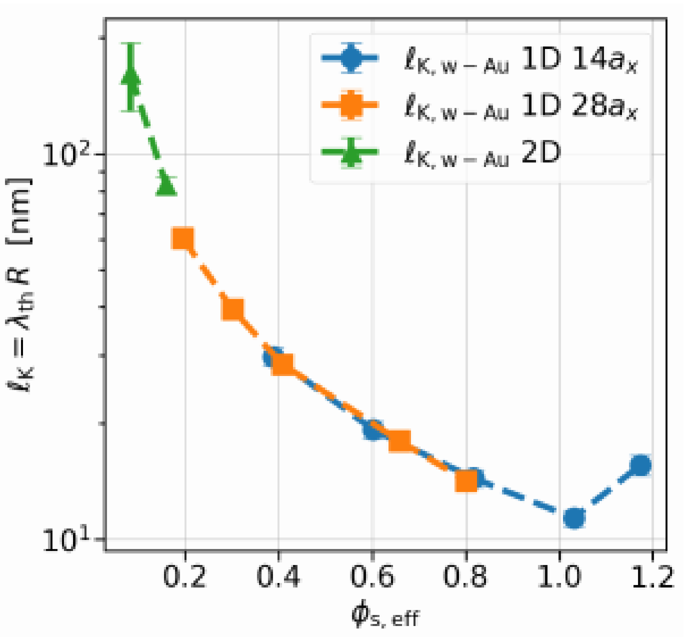


C. Herrero

Conductance



Kapitza length



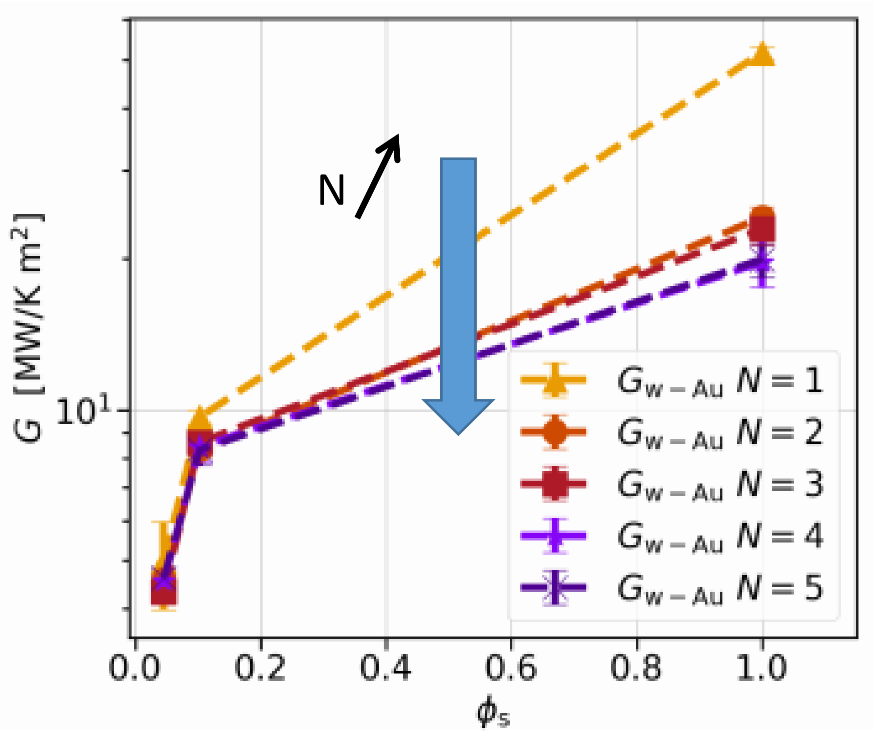
resistance $R_{\mathrm{w-Au}} = R_{\mathrm{w-C}} + \frac{R_{\mathrm{C-Au}}}{\phi_{\mathrm{s,eff}}}$

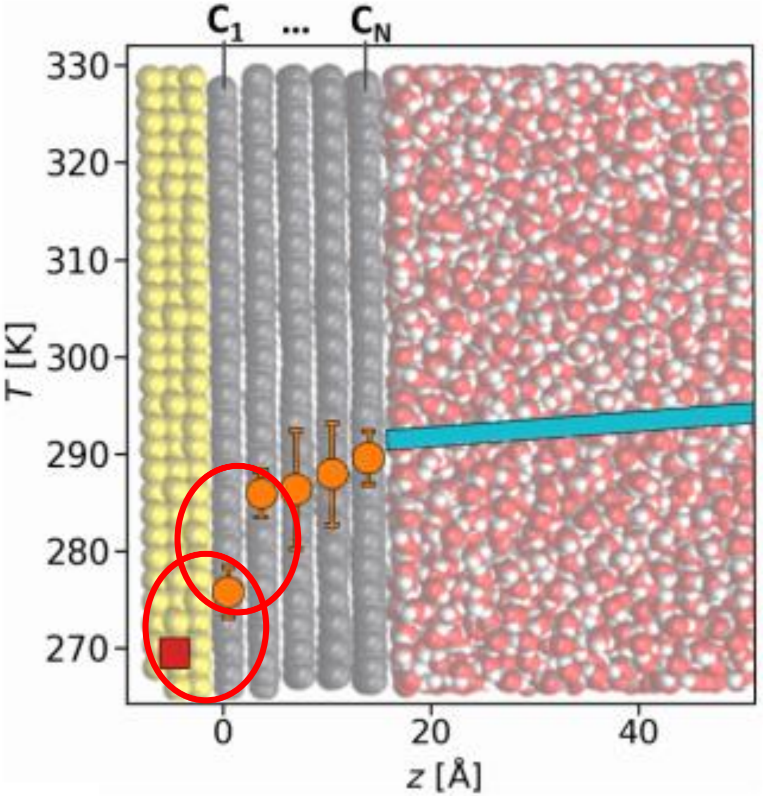
effective surface $\phi_{\mathrm{s,eff}} = \frac{l_x + 2r_c}{L_x}$

The Kapitza conductance increases linearly with the pillar effective surface fraction

Herrero, Joly, Merabia, *Appl. Phys. Lett. 120* (2022) 171620

Effect of the number of graphene layers





Effective resistance

$$R_{\mathrm{w-Au}} = R_{\mathrm{w-C}_N} + \sum_{i>1}^{N-1} R_{\mathrm{C}_{i+1}-\mathrm{C}_i} + R_{\mathrm{C}_2-\mathrm{C}_1} + \frac{R_{\mathrm{C}_1-\mathrm{Au}}}{\phi_{\mathrm{s,eff}}}.$$

$$R_{\mathrm{w-Au}} \simeq R_{\mathrm{C}_2-\mathrm{C}_1} + \frac{R_{\mathrm{C}_1-\mathrm{Au}}}{\phi_{\mathrm{s,eff}}}$$

Herrero, Joly, Merabia, Joly, *Appl. Phys. Lett.* 120 (2022) 171620

Conclusions

The thermal conductance of nanoparticle/water interfaces increases with the nanoparticle curvature as explained by generalised acoustic models

Intercalating graphene sheets between nanostructure gold and water help increase spectacularly the Kapitza resistance

Gutiérrez, Merabia, Santamaria, *J. Chem. Phys*., 157 (2022) 084702

Gutiérrez, Lombard, Biben, Santamaria, Merabia, *arxiv* 2209.07900

Herrero, Joly, Merabia, *Appl. Phys. Lett.,* 120 (2022) 171601

iLM
INSTITUT LUMIÈRE MATIÈRE

O. Gutiérrez-Varela

C. Herrero

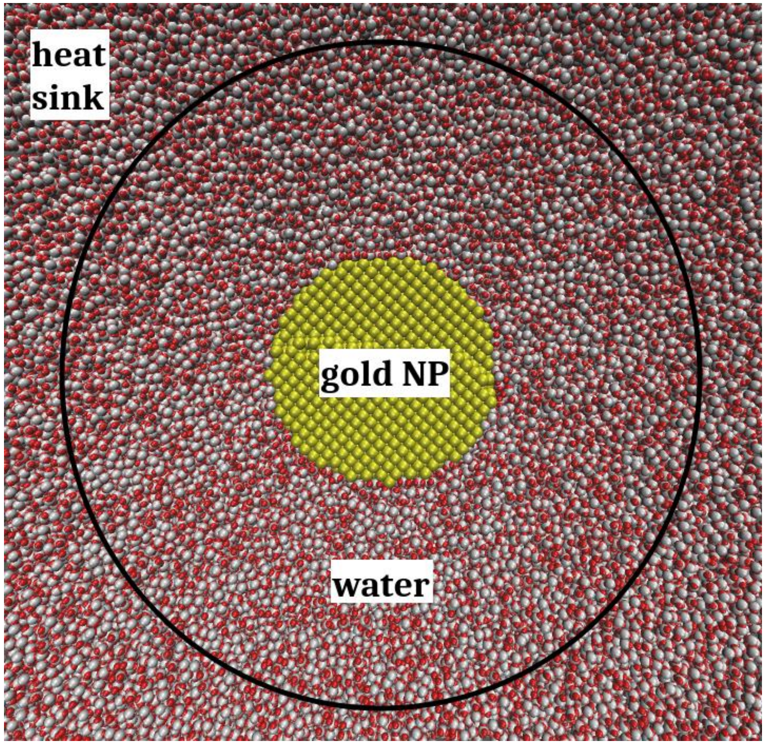
T. Biben

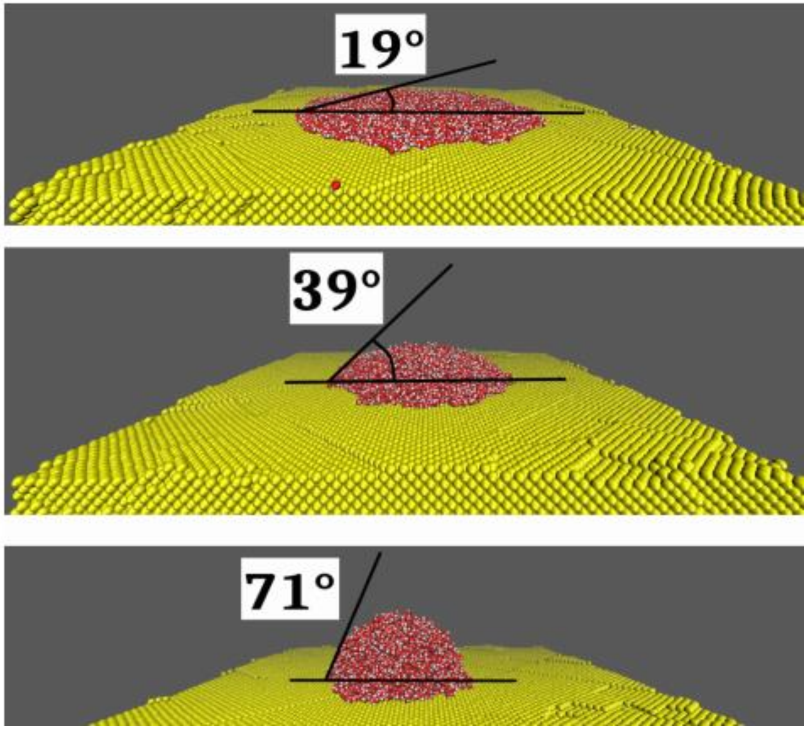
L. Joly

R. Santamaria

Thank you for your attention !

Methodology





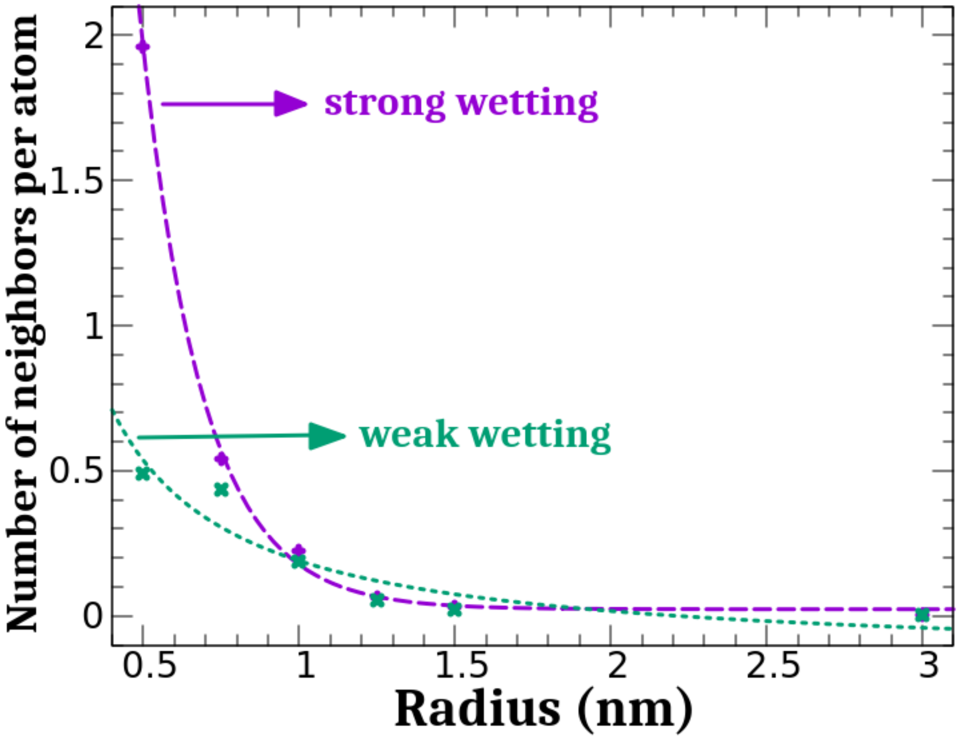
O. Gutiérrez-Varela

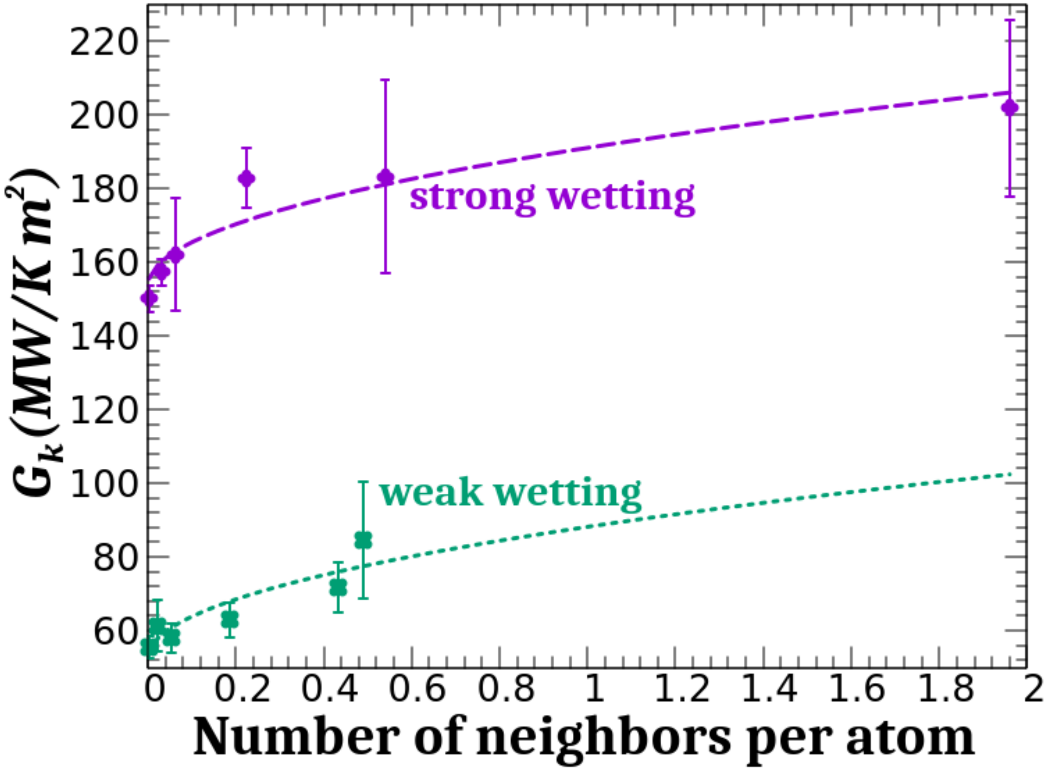
Non equilibrium molecular dynamics simulations

TIP4P2005 flexible for water; Heinz potential for gold

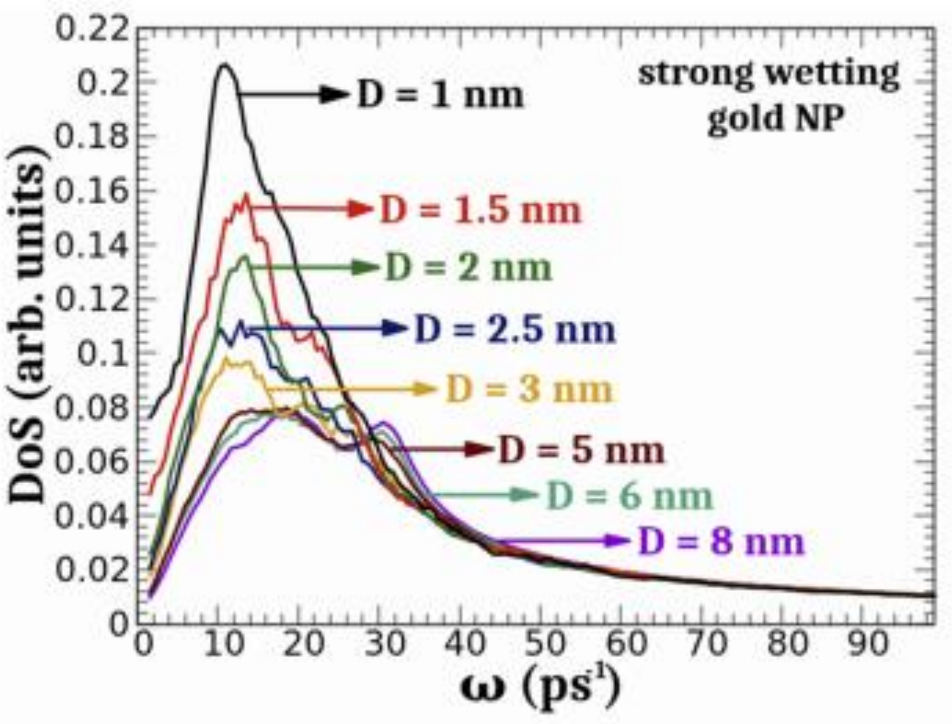
Nanoparticle of tunable wettability

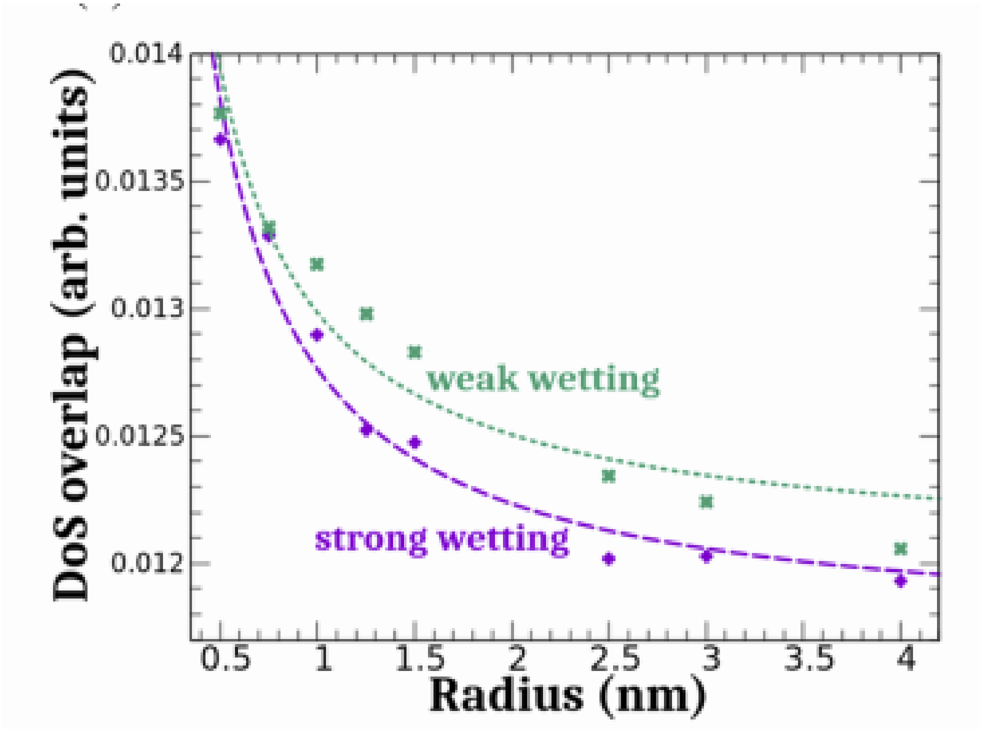
Size dependent thermal conductance

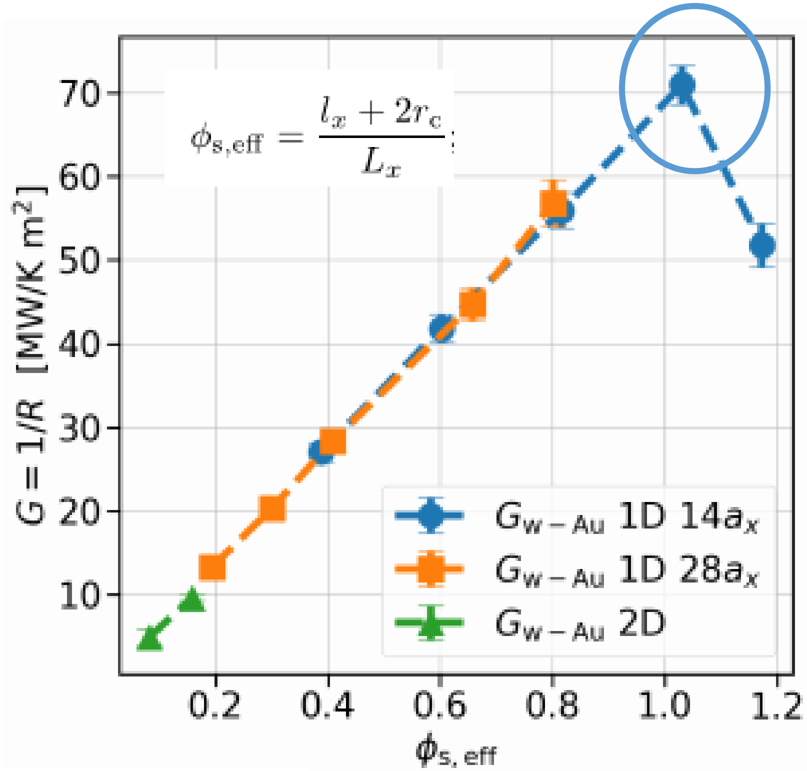


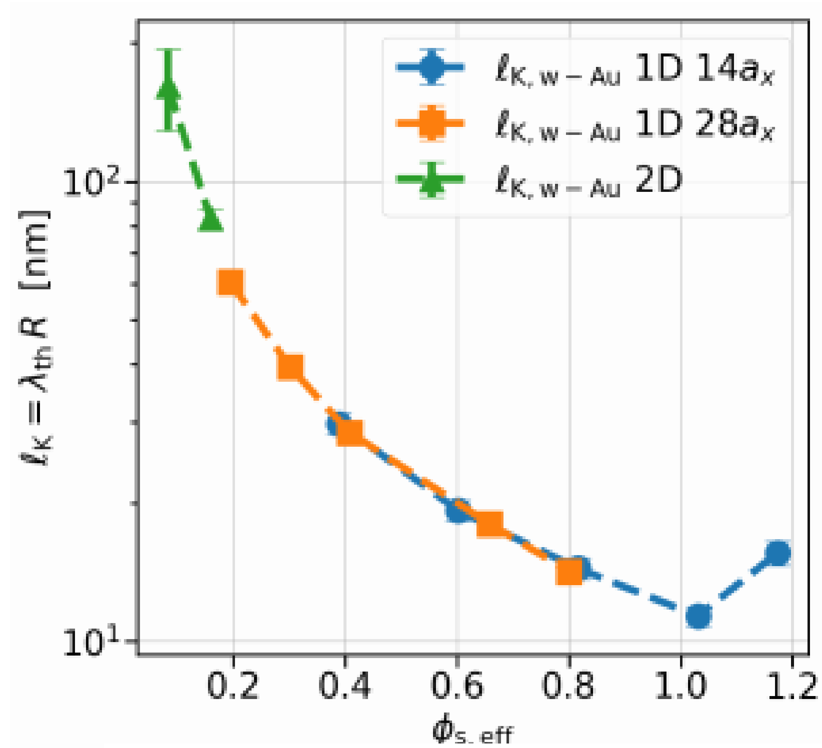


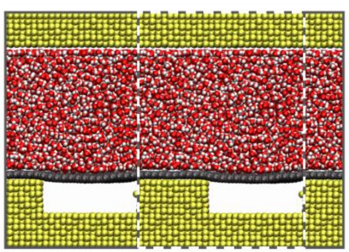
Vibrational properties of the nanoparticles











$$\phi_{s,\mathrm{eff}} = \frac{l_x + 2r_c}{L_x};$$

PHYSICAL REVIEW B **82**, 115427 (2010)

Flexural phonons and thermal transport in graphene

L. Lindsay,[1,2] D. A. Broido,[1] and Natalio Mingo[3,4]