Équipe MMCI
(modélisation de la matière condensée & interfaces)
Nanothermique

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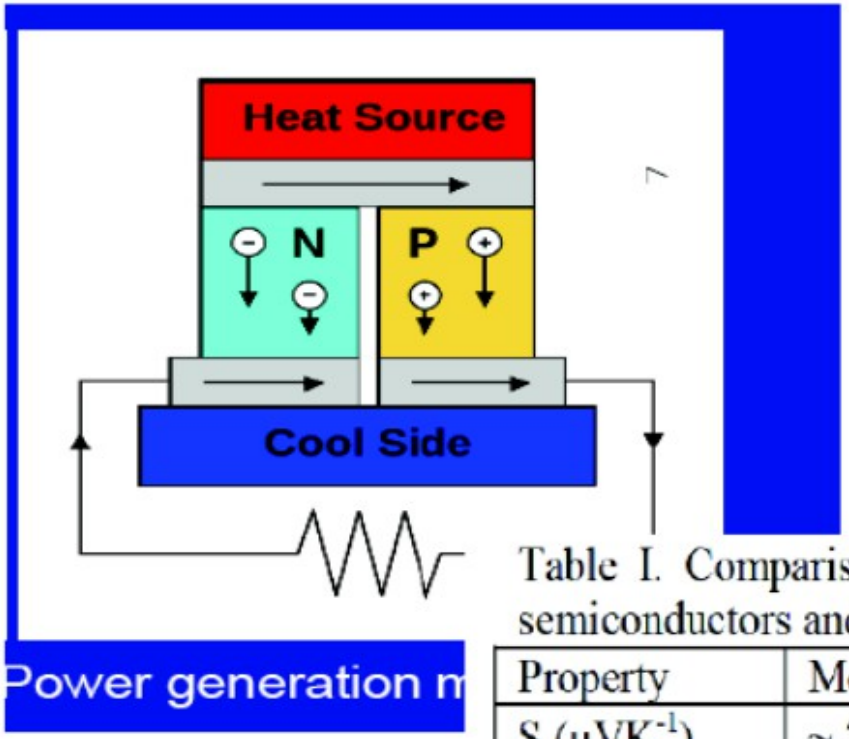
Permanents : C. Adessi, T. Albaret, T. Biben, L. Joly, S. Merabia, A. Tanguy

Doctorants : A. Alkurdi, T. Damart

Réunion du LRA Nanothermique, Lyon 16 Avril 2015

Thermoelectricity



Efficiency : figure of merit

$$Z \equiv \frac{\alpha^2}{KR}$$

`Figure of merit' (Note: Z.T dimensionless)

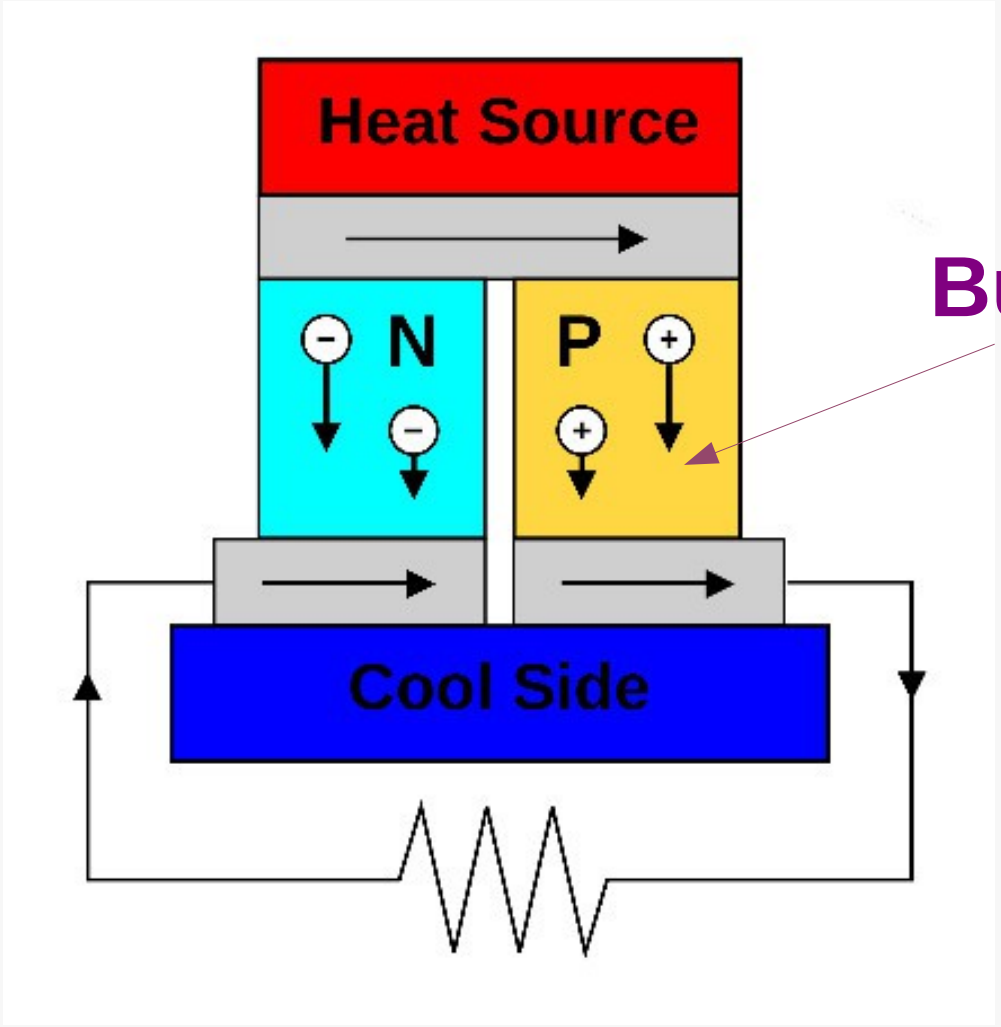
α : coefficient Seebeck

K : conductivité thermique

Table I. Comparison of thermoelectric properties of metals, semiconductors and insulators at 300K. (after ref. [2])

Property	Metals	Semiconductors	Insulators
S (μVK^{-1})	~ 5	~ 200	~ 1000
σ ($\Omega^{-1}cm^{-1}$)	~ 10^6	~ 10^3	~ 10^{-12}
Z (K^{-1})	~3×10^{-6}	~2×10^{-3}	~5×10^{-17}

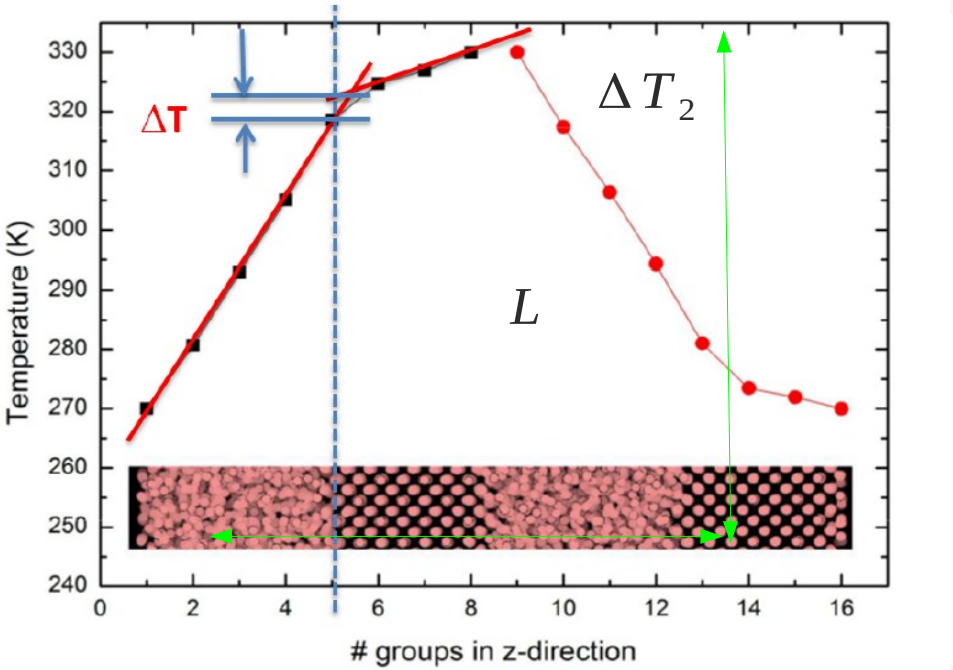
Thermoelectricity

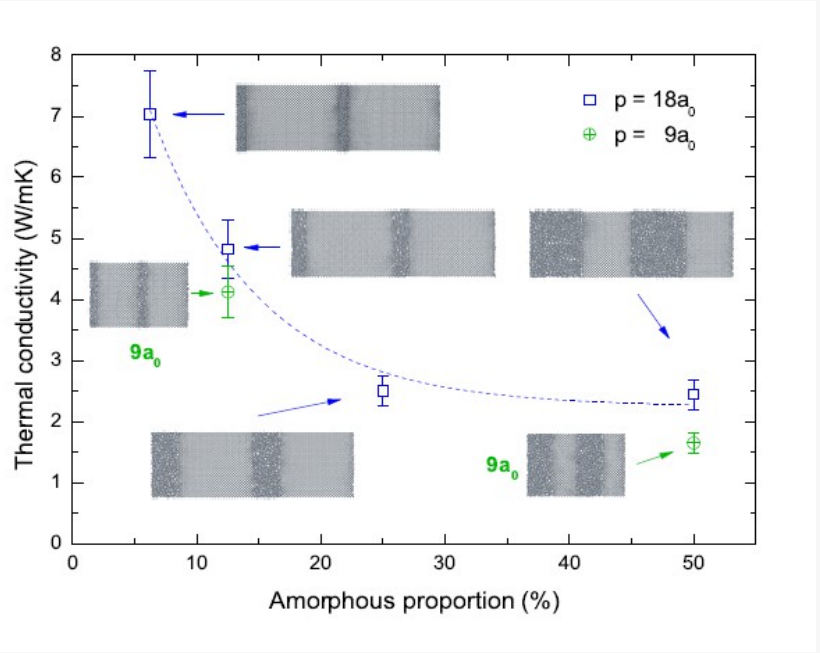


Bulk material

Amorphous-crystalline structures for thermoelectricity

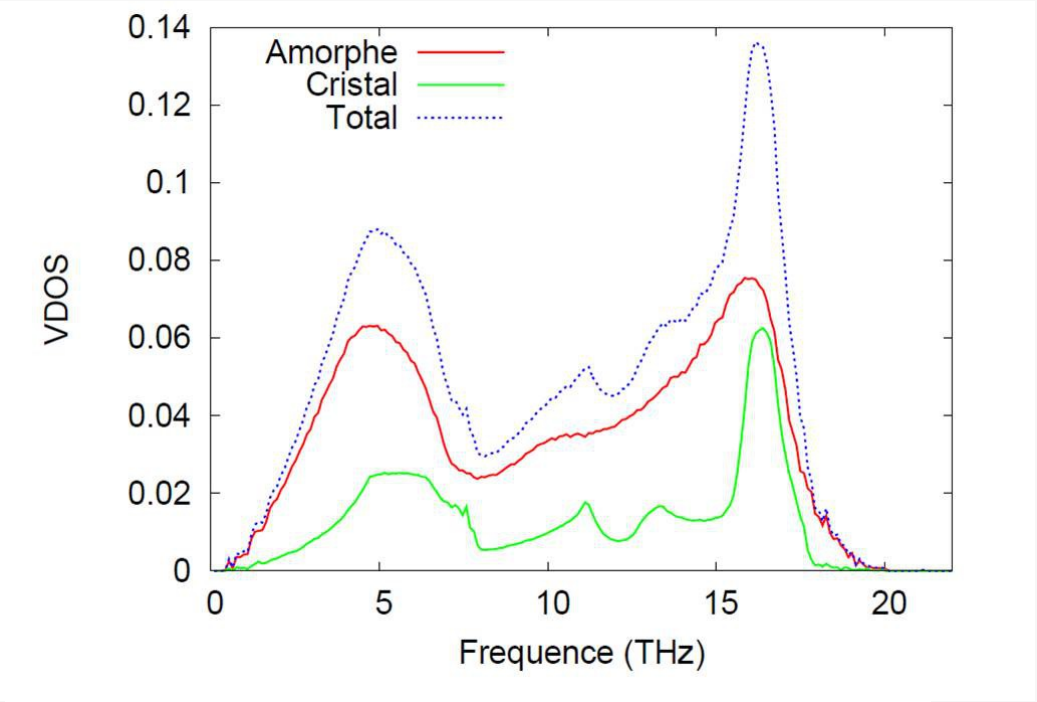
Collaboration LEMTA Nancy
T. Albaret, S. Merabia

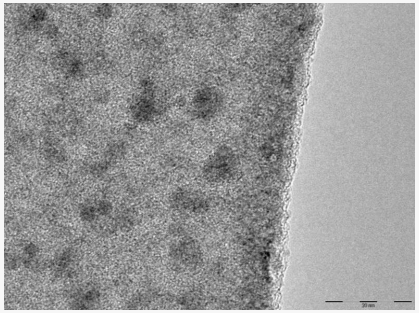


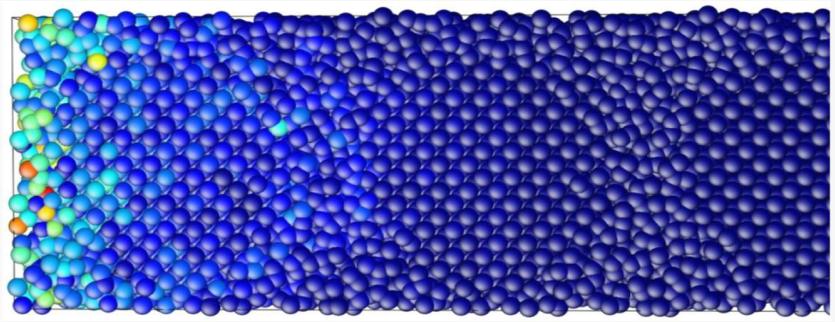


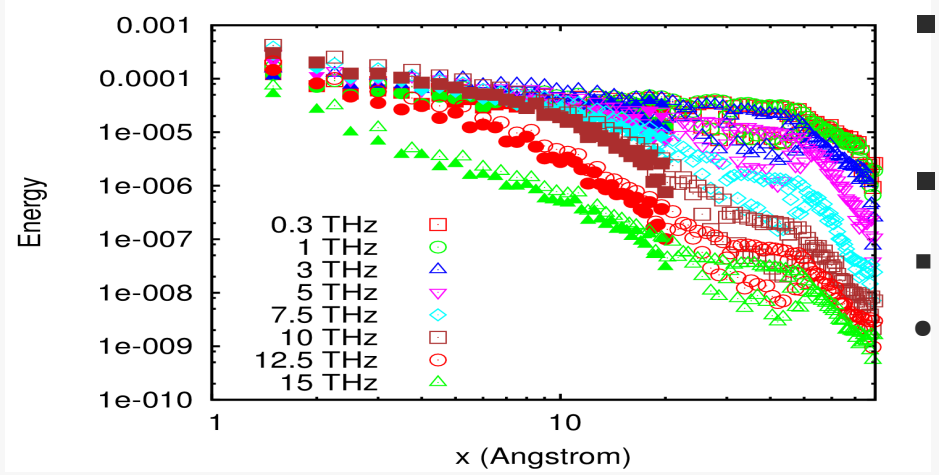
dynamique moléculaire

Verre métallique avec nano-inclusions cristallines





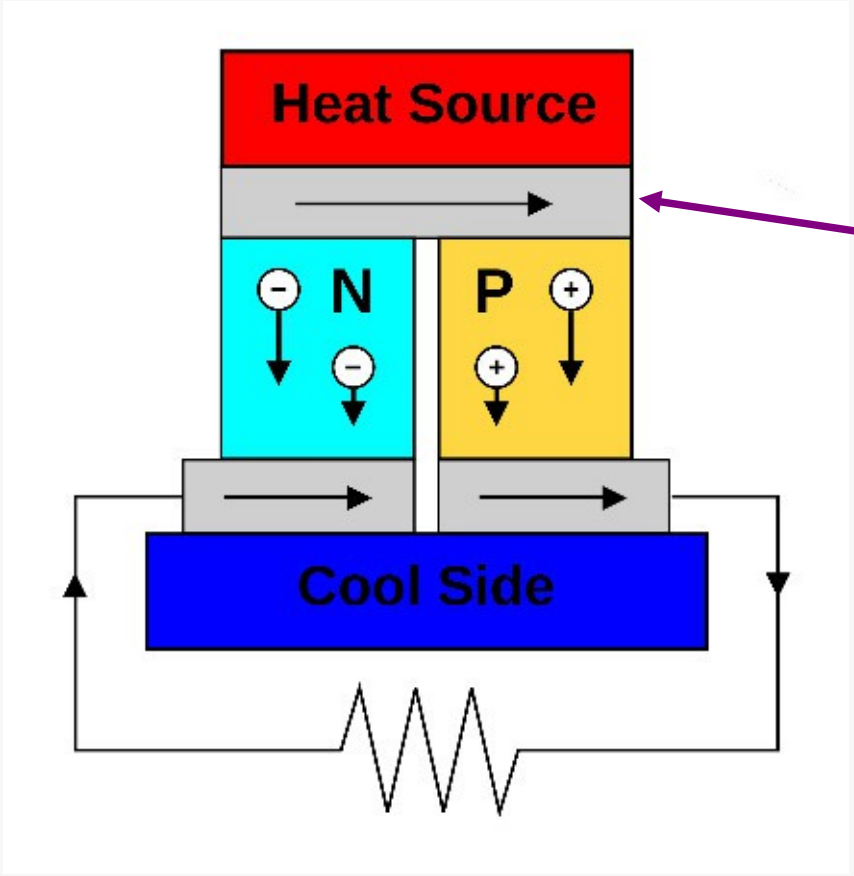




- T. Damart, V. Giordano, S. Merabia, S. Pailhès, A. Tanguy
- Thèse A. Tlili (ARC ENERGIE – région Rhône-Alpes)
- Collaboration équipe ENERGIE (IL

Heat transfer at interfaces

ANR Mascoth -équipe Energie
Coll. R. Viennois Montpellier



Pertes thermiques ?
Interface électrode/module

Résistance thermique
D'interface ?

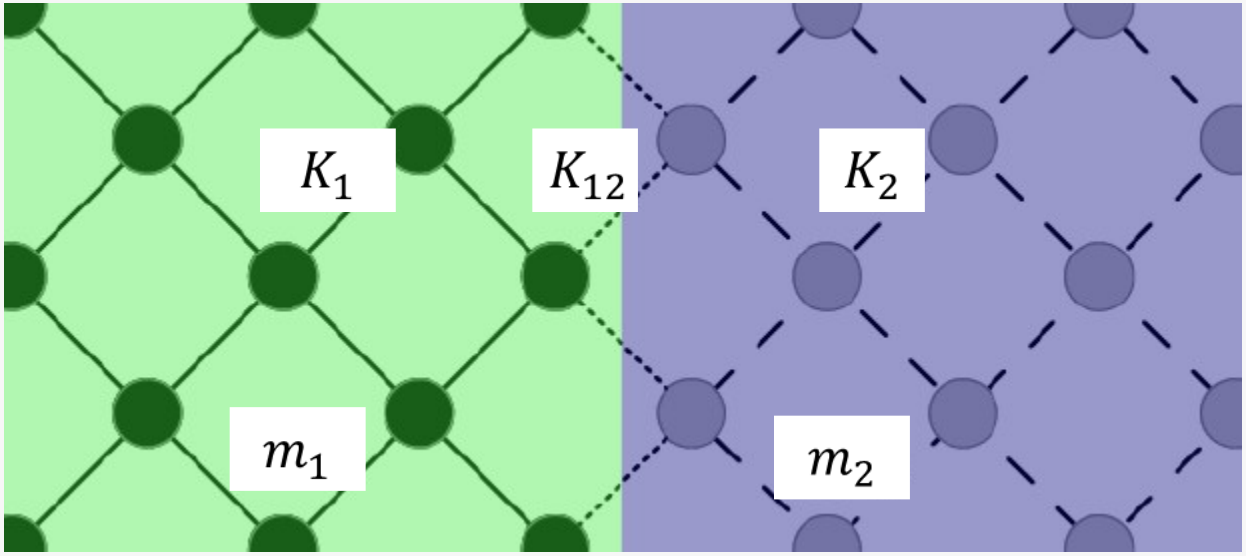
Peu de travaux dans la littérature...

Ab-initio lattice dynamics

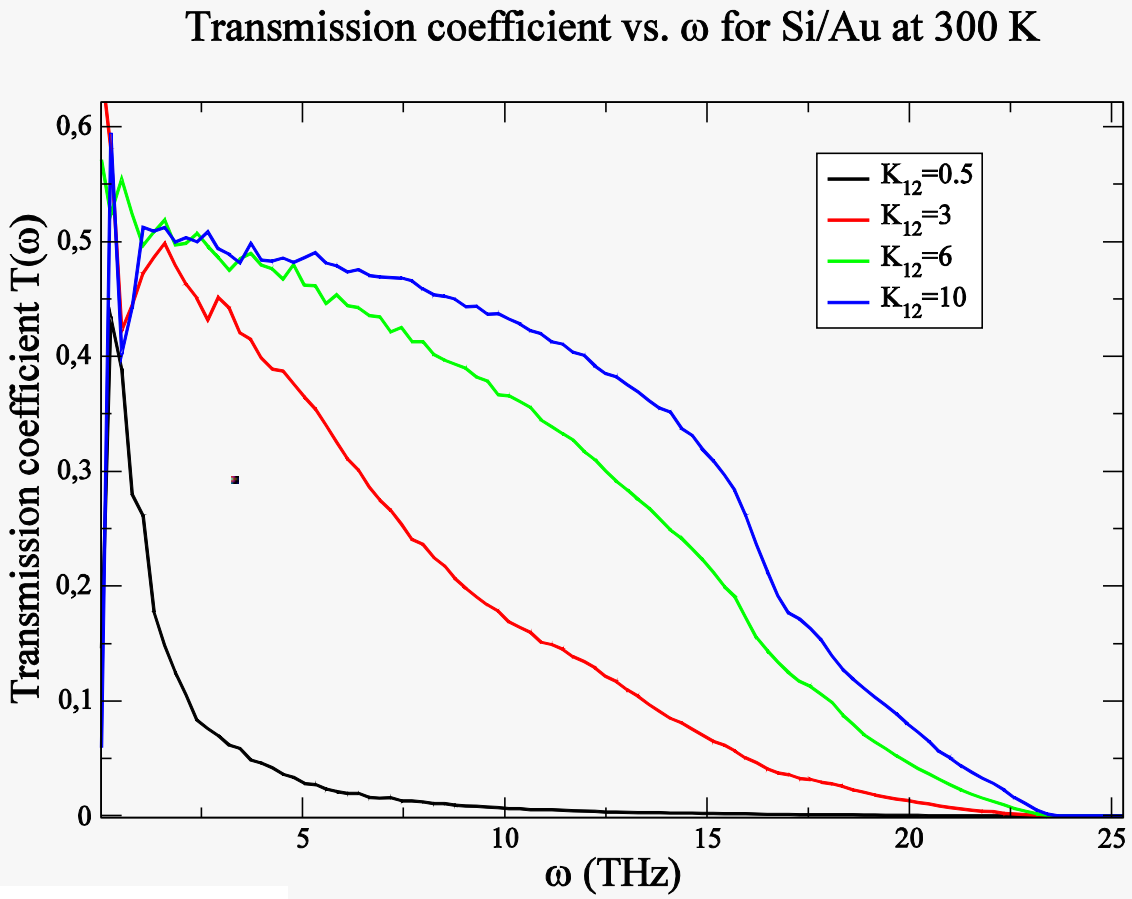
Thèse A. Alkurdi, C. Adessi

Harmonic Hamiltonian : $H = H_0 + \frac{1}{2}\sum_{i,j} C_{ij}^{\alpha\beta} u_i^{\alpha} u_j^{\beta}$

2nd order spring constant



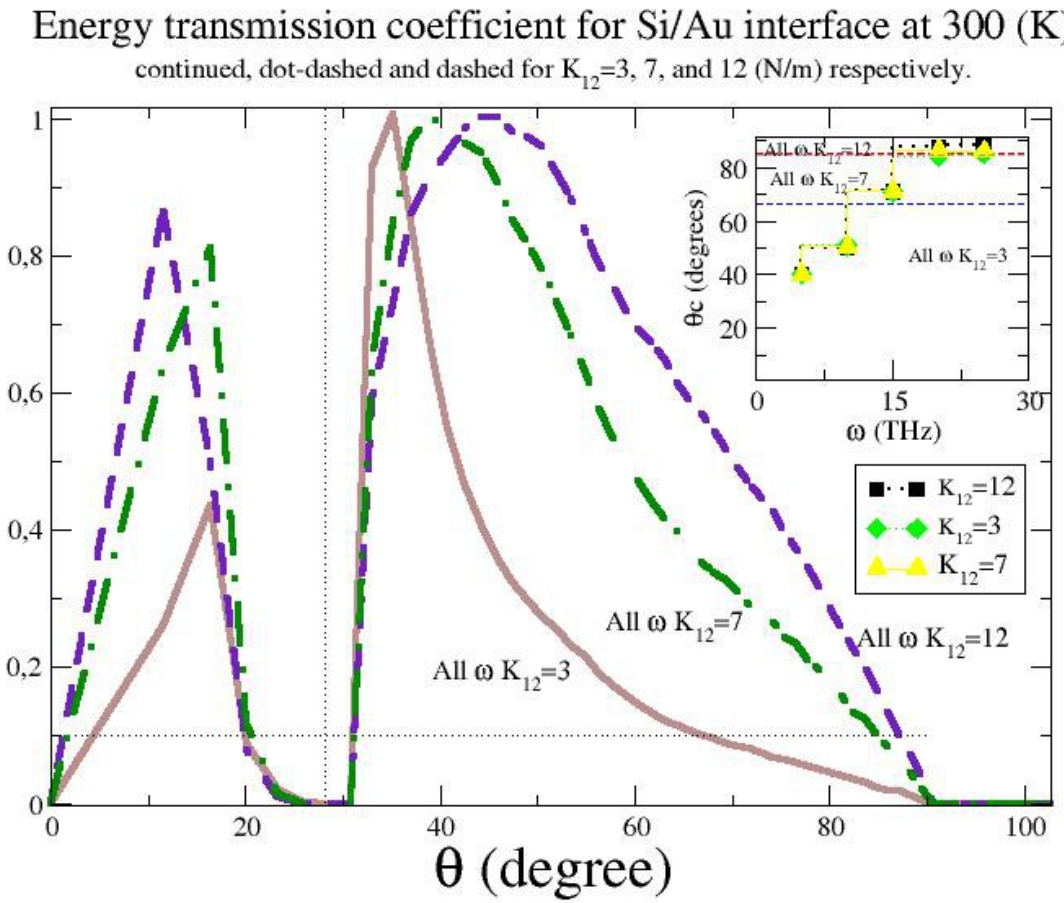
Phonon transmission coefficient

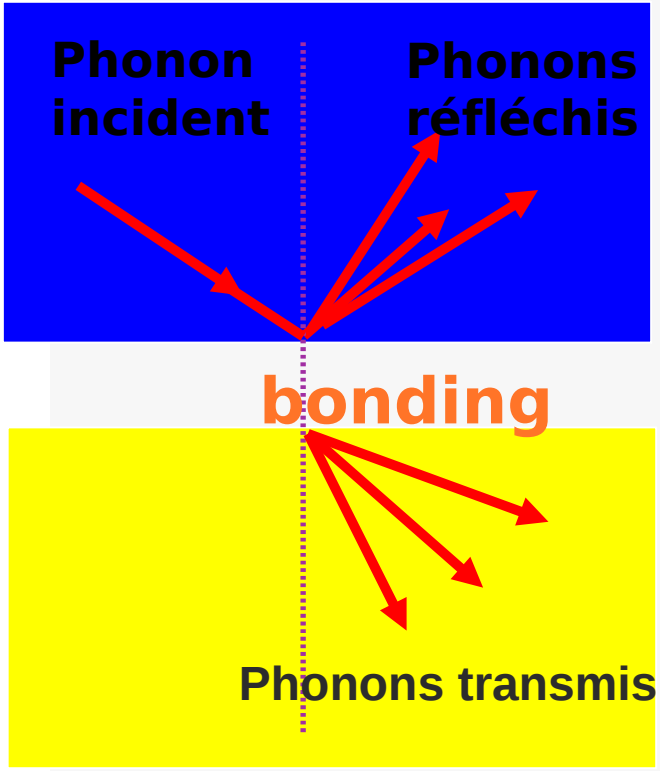


$$t_{1\to 2} = \frac{\rho_{m,2}}{\rho_{m,1}} \sum_{q=4}^{6} \frac{v^z_{g,q} \cdot |A_q|^2}{v^z_{g,0} \cdot |A_0|^2}$$

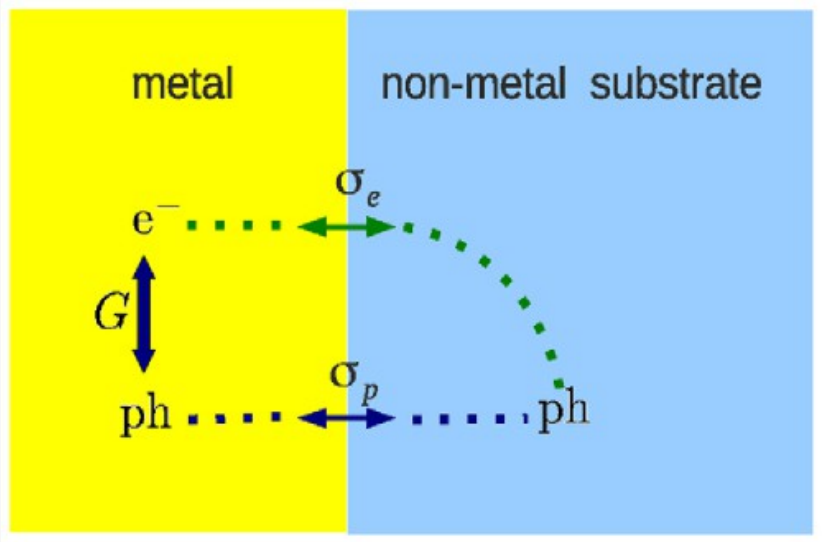
Angular transmission coefficient

Si/Au interface





Electron-phonon interfacial heat transfer



Two temperature model

$$c_e\,\partial_t T_e = k_e\,\partial_{xx}^2 T_e - G(T_e - T_p),$$

$$c_p\,\partial_t T_p = k_p\,\partial_{xx}^2 T_p + G(T_e - T_p),$$

$$c_s\,\partial_t T_s = k_s\,\partial_{xx}^2 T_s.$$

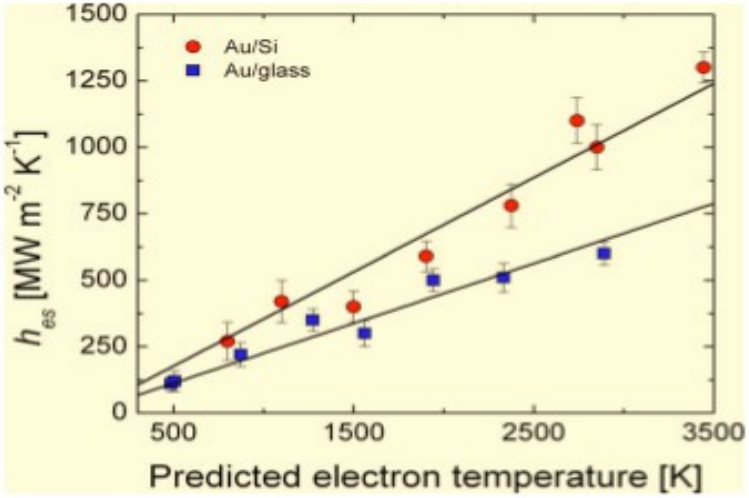
+ boundary conditions

$$-k_s\,\partial_x T_s = \sigma_e(T_e - T_s) + \sigma_p(T_p - T_s),$$

$$= -k_e\,\partial_x T_e - k_p\,\partial_x T_p.$$

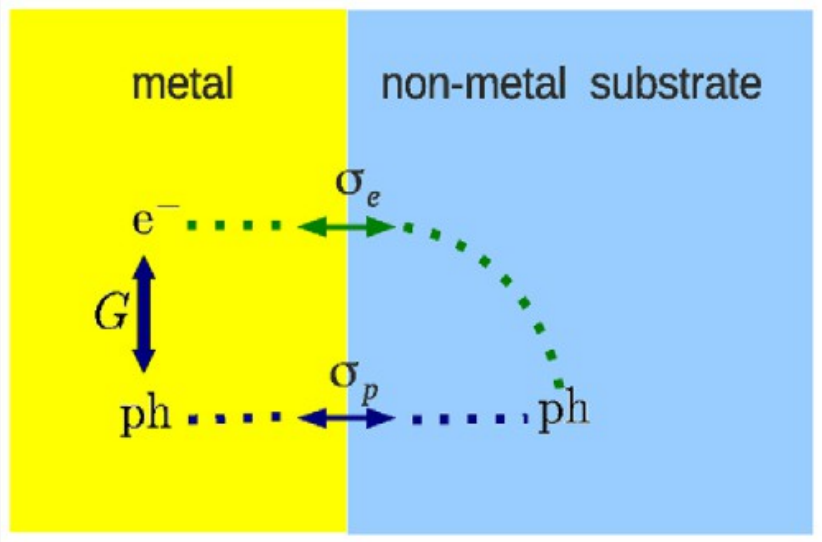
Effective conductance :

$$1/\sigma_{eff} = 1/Gh + 1/(\sigma_e + \sigma_p).$$

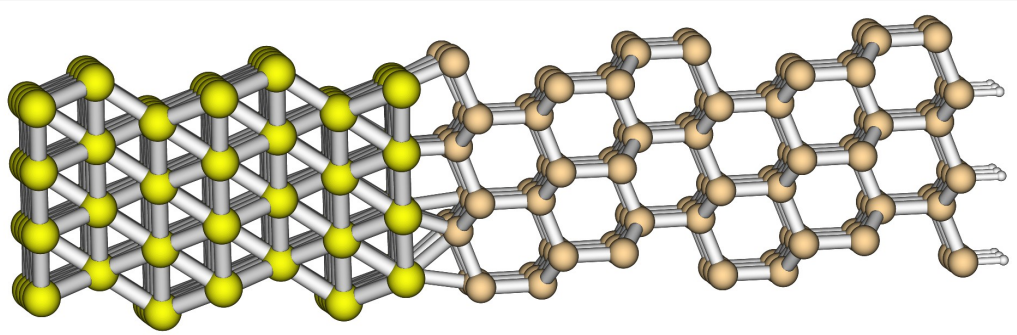


Electron-phonon interfacial heat transfer

C. Adessi

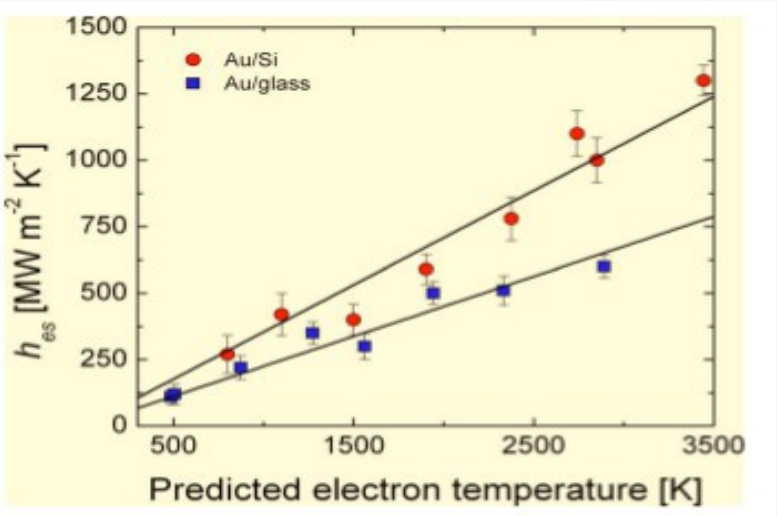


Ab-initio calculations



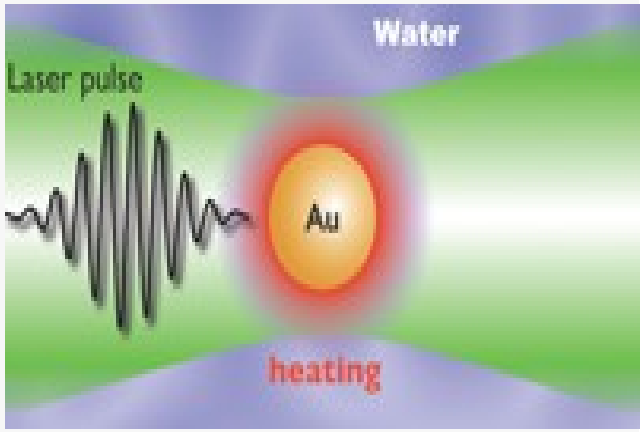
Effective conductance :

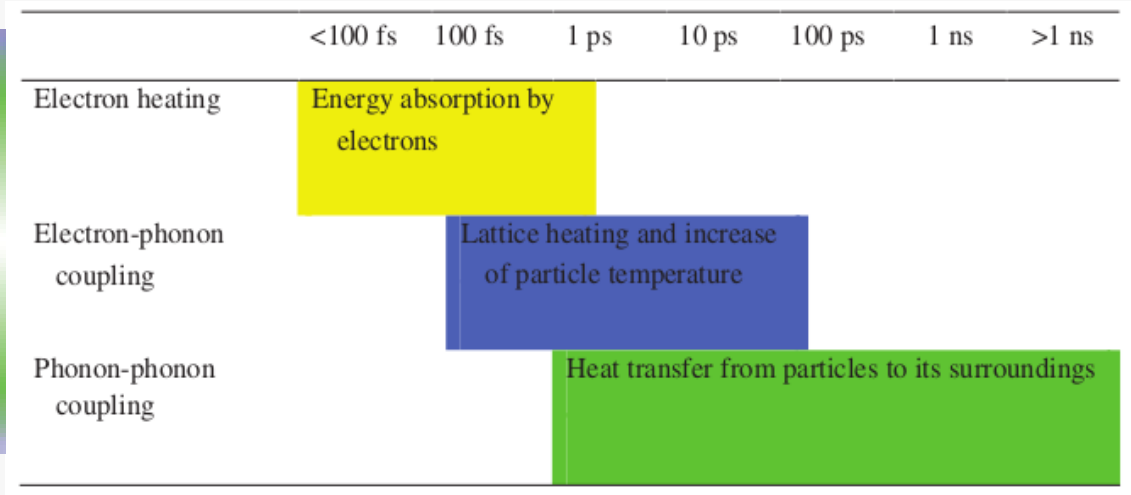
$$1/\sigma_{\text{eff}} = 1/Gh + 1/(\sigma_e + \sigma_p).$$



Biomedical applications

T. Biben, L. Joly, S. Merabia, J. Lombard

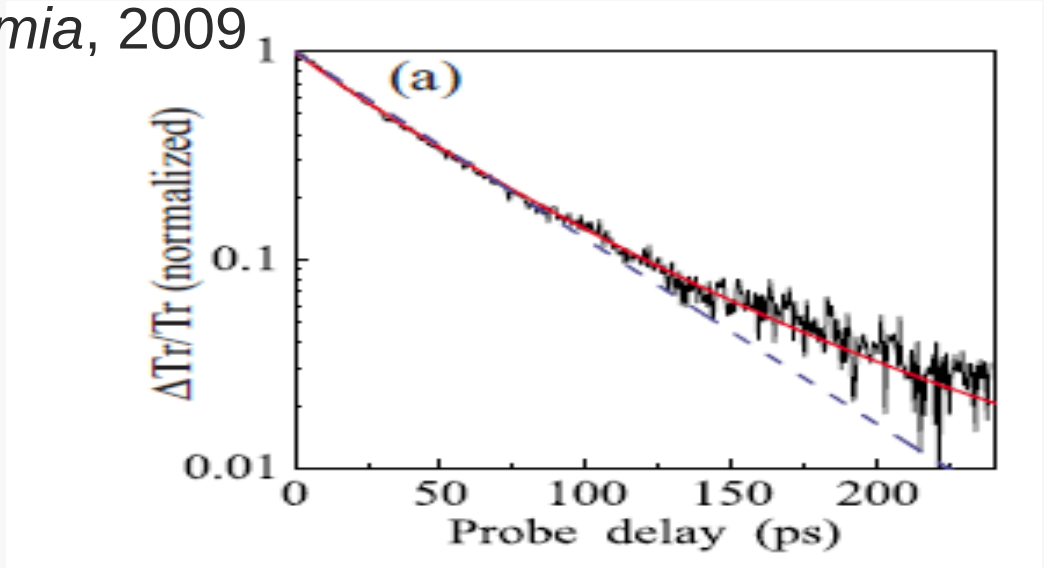




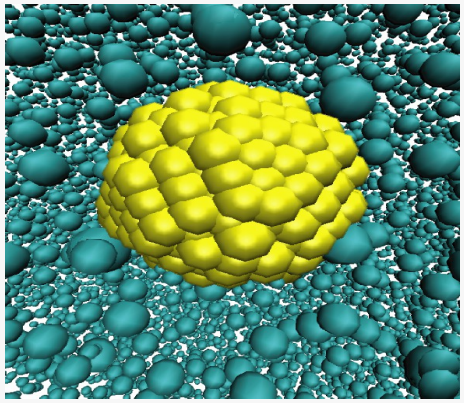
Wen, *Int. J. Hyperthermia*, 2009

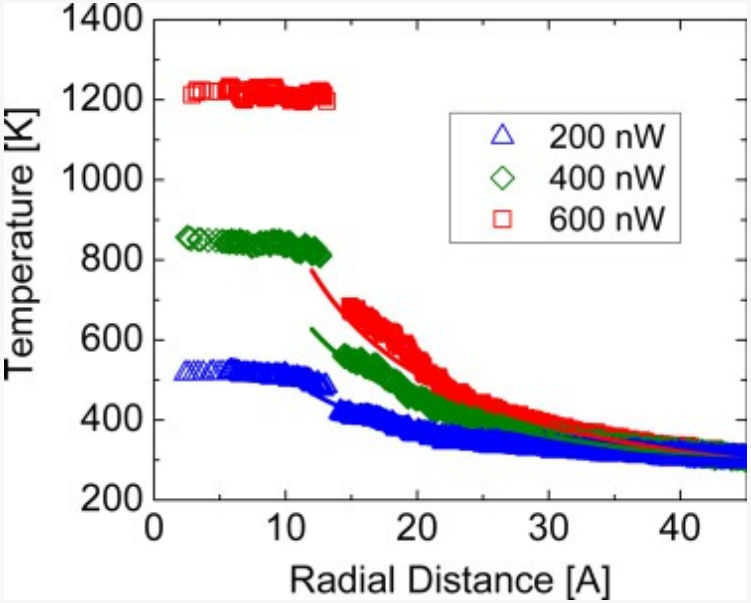
$$\frac{\partial T_p(t)}{\partial t} = -\frac{3G}{Rc_p}[T_p(t) - T_m(R,t)],$$

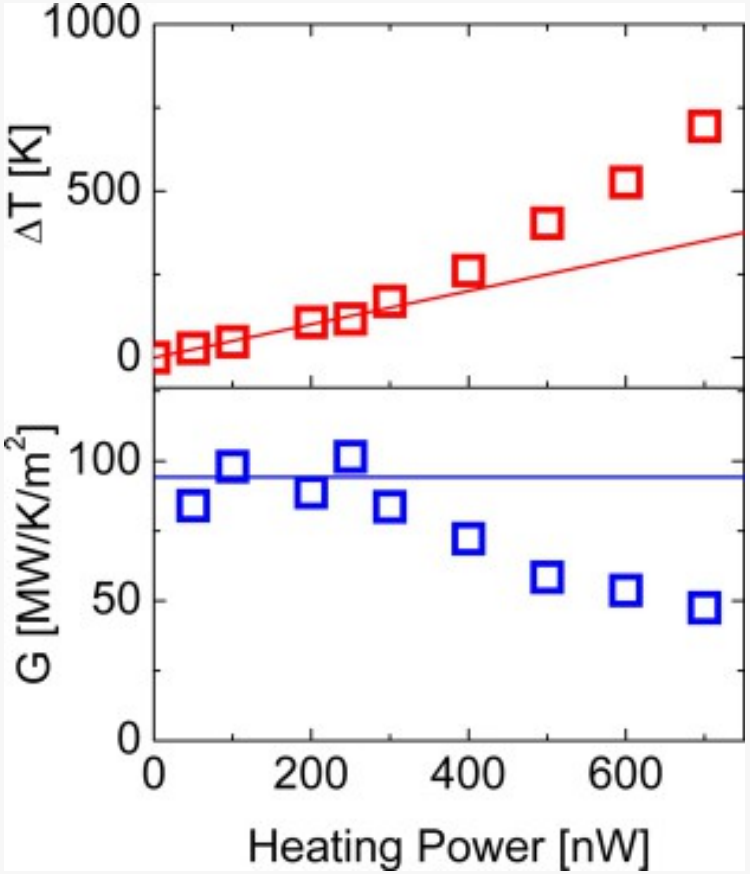
$$c_m \frac{\partial T_m(r,t)}{\partial t} = \Lambda_m \frac{1}{r}\frac{\partial^2}{\partial r^2}[rT_m(r,t)],$$



Gold nanoparticles in liquid water



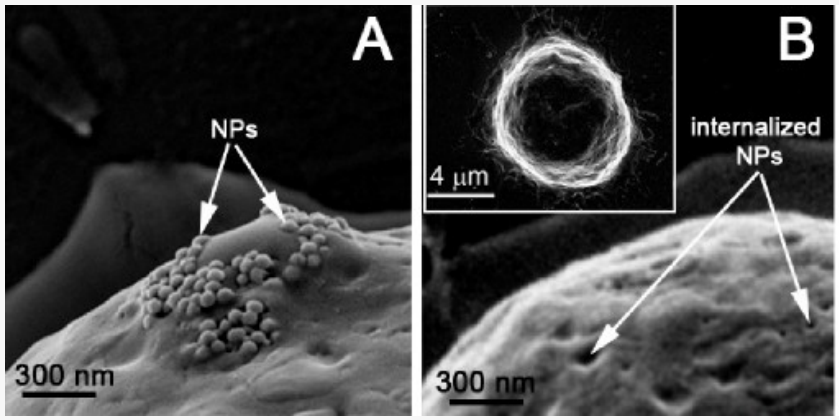


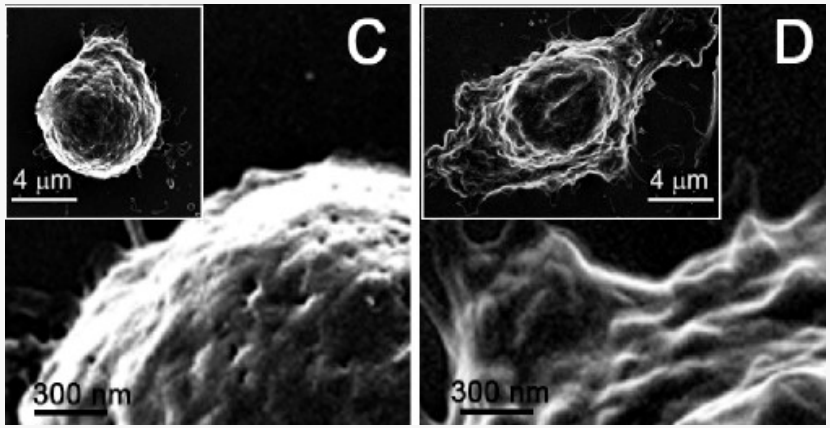


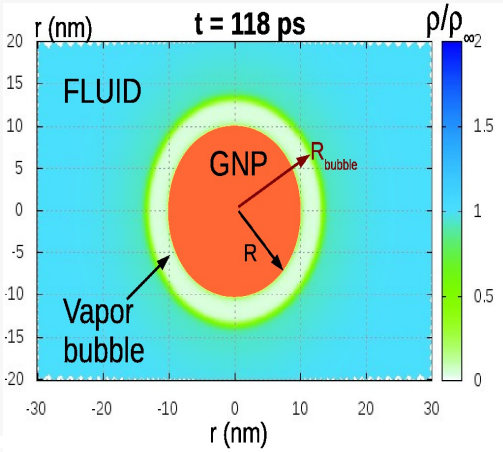
molecular dynamics + analytical work

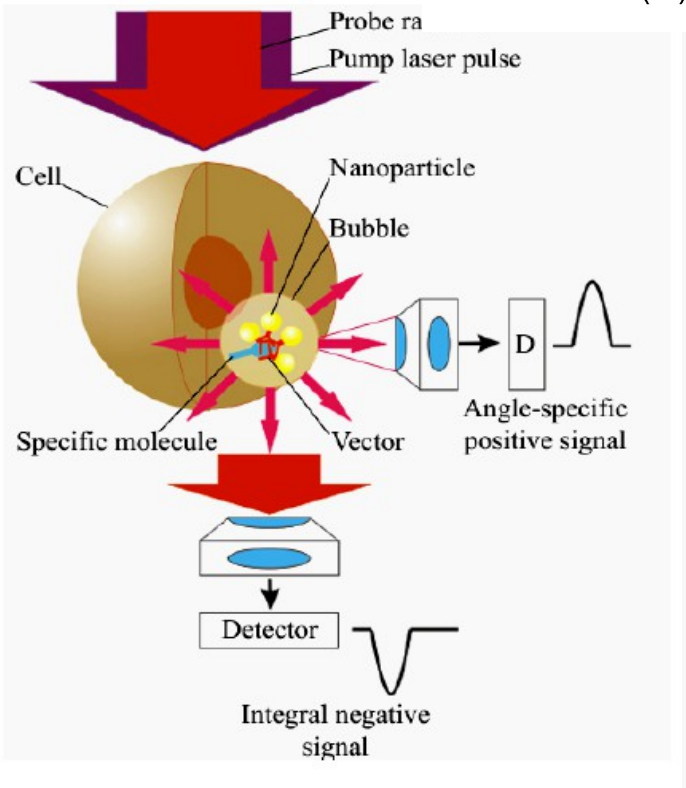
Biomedical applications

Diagnostic and tumor therapy





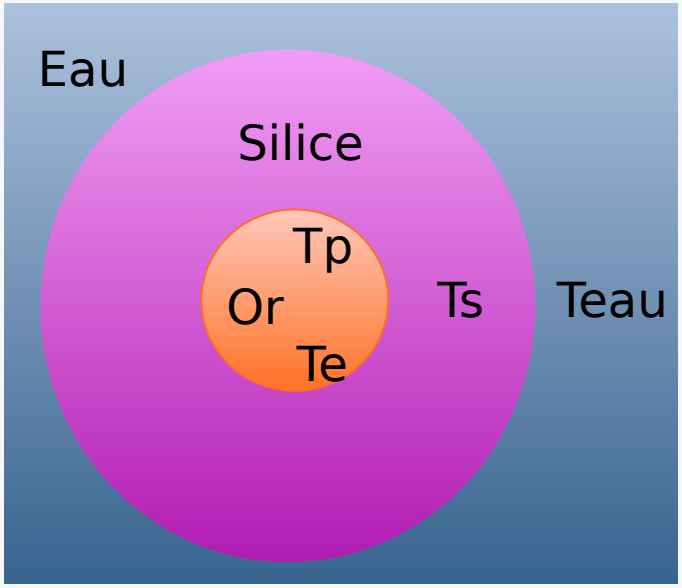


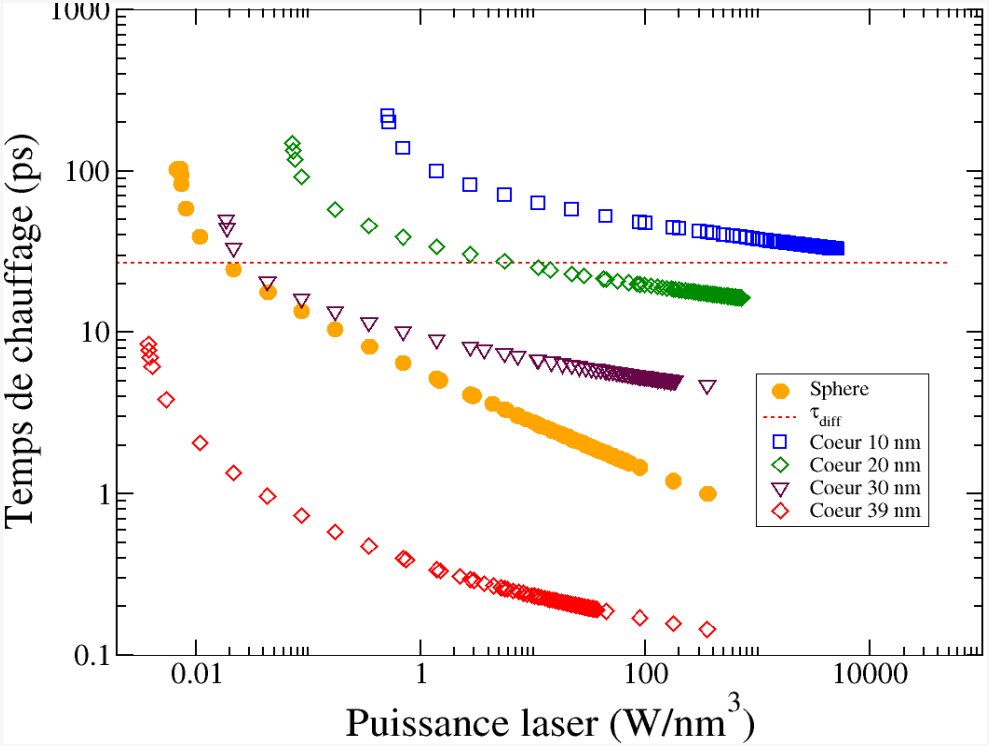


Lapotko et al., *ACS Nano* (2010) Collaboration Institut Curie

Lapotko, Cancer (2011)

Core-shell nanoparticles





Thèse A. Alkurdi, J. Lombard