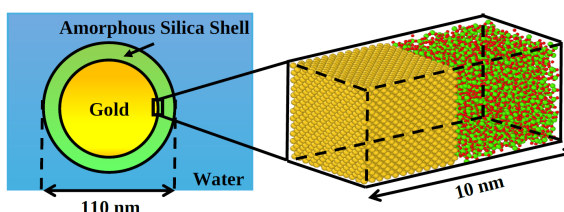


ATOMISTIC SIMULATIONS OF THERMAL TRANSPORT AT GOLD/SILICA INTERFACES FOR IMPROVED THERMOPLASMONIC APPLICATIONS

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Lumière Matière (iLM)
TEAM(S) : MMCI
CONTACT(S) : MERABIA Samy
CONTACT(S) DETAILS: samy.merabia[at]univ-lyon1.fr / Tel. 0472448339
KEYWORD(S) : MolecularDynamics / thermal transport / core-shell nanoparticles

SCIENTIFIC CONTEXT :

Nanoparticles immersed in water can be optically heated by hundredths of Kelvins on a picosecond time scale. This unique property opens the path to locally release heat in an aqueous environment, offering a host of opportunities for applications in nanomedicine [1]. Core-shell nanoparticles, particularly those having gold parts, have emerged as a highly promising class of materials due to their unique optical and thermal properties. We have recently pointed out the possibility to enhance heat transfer by coating gold nanoparticles with a silica layer [2,3].



Institute Light and Matter

MISSIONS :

The aim of the PhD project is to explore the possibility to optimize the thermal response of heterogeneous gold core-silica shell nanoparticles by playing with silica porosity. The recruited student will perform molecular dynamics possibly based on machine-learning potentials to predict accurately the thermal transport properties of gold-nanoporous silica heterojunctions and nanoporous silica-water interfaces. By training a potential based on ab-initio calculations, he/she will characterize the thermal resistance at the interface between nanoporous silica and gold/water, which will be used as input of the thermoplasmonic code developed in the group [3]. This code allows one to predict the thermal response of heterogeneous nanoparticles following pulse illumination. This PhD project offer should fit to a student interested in nanosciences, nanoscale thermal transfer and materials modeling. No prior deep knowledge of molecular dynamics is required, but motivation to run and analyze atomistic simulations is compulsory. The subject involves also collaborations with experimentalists at the ILM and in Montpellier.

To apply, please send a CV to samy.merabia@univ-lyon1.fr

OUTLOOKS :

Depending on the student tastes, ab-initio calculations may be envisaged

BIBLIOGRAPHY :

- [1] Muhi et al., « A review of heat transport in solvated gold nanoparticles: molecular dynamics modelling and experimental perspectives », *Nanoscale* (2025)
- [2] A. Alkurdi, J. Lombard, F. Detcheverry, S. Merabia, "Enhanced Heat Transfer with Metal-Dielectric Core-Shell Nanoparticles", *Phys. Rev. Appl.* (2020)
- [3] J. El Hajj, G. Ledoux and S. Merabia, "Thermoplasmonic of gold-silica core-shell nanoparticles under pulse illumination", *J. Phys. Chem C* (2025)

