ATOMISTIC SIMULATIONS OF THERMAL TRANSPORT AT METAL/CARBON INTERFACES FOR THERMOPLASMONIC APPLICATIONS

LABORATORY : Institut Lumière Matière

LEVEL : M2
TEAM(S) : MMCI
ENERGIE

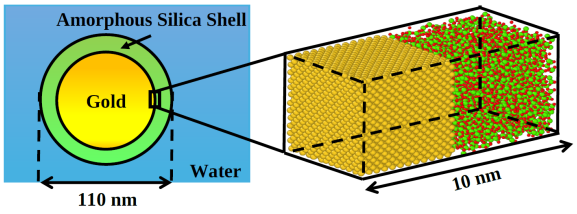
CONTACT(S) : ADESSI Christophe
BISSUEL Dylan
MERABIA Samy

CONTACT(S) DETAILS: christophe.adessi[at]univ-lyon1.fr / Tel. 0472431819
dylan.bissuel[at]univ-lyon1.fr / Tel. 0472448271
samy.merabia[at]univ-lyon1.fr / Tel. 0472448339

KEYWORD(S) : molecular dynamics simulations / nanoscale thermal transport / machine learning potentials

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 nanomedecine [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].



MISSIONS :

The aim of the internship is to explore the possibility to optimize the thermal response of heterogeneous gold core-shell nanoparticles based on carbon. The recruited student will perform molecular dynamics based on machine-learning potentials to predict accurately the thermal transport properties of gold-carbon heterojunctions. He/she will benefit for the experience of the group in the exploitation of machine learning potentials for thermal transfer problems [4]. By training a potential based on ab-initio calculations, he/she will characterize the thermal resistance of gold-carbon interfaces, which will be used as input of the thermoplasmonic code developed in the group [3]. This internship offer should fit to a student interested in nanosciences, nanoscale thermal transfer and materials modeling. No prior deep knowledge of machine learning potentials 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, dylan.bissuel@univ-lyon1.fr and christophe.adessi@univ-lyon1.fr

OUTLOOKS :

Possibility to continue with a funded phD on a related topic.

BIBLIOGRAPHY :

[1] M. A.M. Munchi et al., Nanoscale. (2025)

[2] A. Alkurdi et al., “Enhanced Heat Transfer with Metal-Dielectric Core-Shell Nanoparticles”, Phys. Rev. Appl. (2020)

[3] J. El Hajj et al., “Thermoplasmonic of gold-silica core-shell nanoparticles under pulse illumination”, J. Phys. Chem C (2025)

[4] A. Rajabpour et al., "Accurate estimation of interfacial thermal conductance between silicon and diamond enabled by a machine learning interatomic potentials", Int. Jour. Therm. Sci. (2025)

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