HIGH PERFORMANCE NANOFLUIDIC THERMOELECTRICITY USING SMOOTH POLARIZED SURFACES

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : TU Darmstadt

LEVEL : M2
TEAM(S) : MMCI

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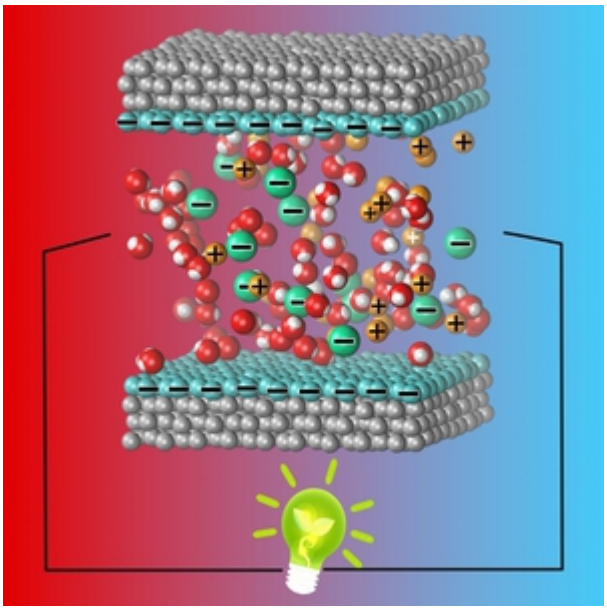
KEYWORD(S) : thermoelectricity / nanofluidics / modeling

SCIENTIFIC CONTEXT :

Nanofluidic systems offer great promises for new energy harvesting technologies. In particular, charged nanochannels filled with salted water could produce electricity from waste heat, with an efficiency reaching that of the best solid-state thermoelectric materials [1], when boosted by liquid-solid slip arising on low-friction surfaces. However, high performance also requires high surface charge, which is detrimental to slip. Nevertheless, we have recently shown that smooth polarized surfaces -especially graphene- display a favorable charge-slip coupling [2]; consequently, these surfaces could provide excellent thermoelectric conversion perfomances.



Nanofluidic devices with smooth polarized walls can convert waste heat into electricity

In that context, we would like to identify especially promising configurations with high conversion efficiency by studying thermoelectric energy conversion in graphene nanochannels, in collaboration with the group of S. Hardt in Darmstadt, Germany (smoothE project, funded by the ANR). To develop a comprehensive picture of thermoelectricity in nanofluidic channels, we will use a multiscale approach, combining atomistic simulations in Lyon [1,2], to capture molecular effects in the nanometric vicinity of the interface, and continuum-mechanical simulations in Darmstadt [3], to describe the entire system at a larger scale.

The internship, which can be followed by a PhD (funded by the ANR), will focus on the atomistic modeling part of the project.

MISSIONS :

The objectives of the internship are: to understand at the nanometric scale the generic molecular mechanisms of thermoelectricity at liquid-solid interfaces; to investigate the specificities of polarized graphene (fluctuating surface charge, role of defects); and to explore a wide range of working conditions (polarization potential, salt type and concentration) to identify cases with optimal performance.

The student will use molecular dynamics (MD) simulations, based on empirical interaction potentials. The thermoelectric response will be measured with different non-equilibrium MD setups, and related to static and dynamical properties of the interface computed independently, using semi-analytical descriptions (e.g. modified Poisson-Boltzmann equation).

OUTLOOKS :

The internship can be followed by a PhD thesis (fully funded by an ANR project).

BIBLIOGRAPHY :

[1] L. Fu, L. Joly, S. Merabia: "Giant thermoelectric response of nanofluidic systems driven by water excess enthalpy", Phys. Rev. Lett. 123, 138001 (2019);

[2] Y. Xie, L. Fu, T. Niehaus, L. Joly: "Liquid-solid slip on charged walls: dramatic impact of charge distribution", Phys. Rev. Lett. 125, 014501 (2020);

[3] M. Dietzel and S. Hardt, "Thermoelectricity in Confined Liquid Electrolytes", Phys. Rev. Lett. 116, 225901 (2016).

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