HIGH PERFORMANCE NANOFLUIDIC HEAT HARVESTING USING POLARIZED GRAPHENE SURFACES

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Lumière Matière (iLM)

LEVEL : M2
TEAM(S) : MMCI

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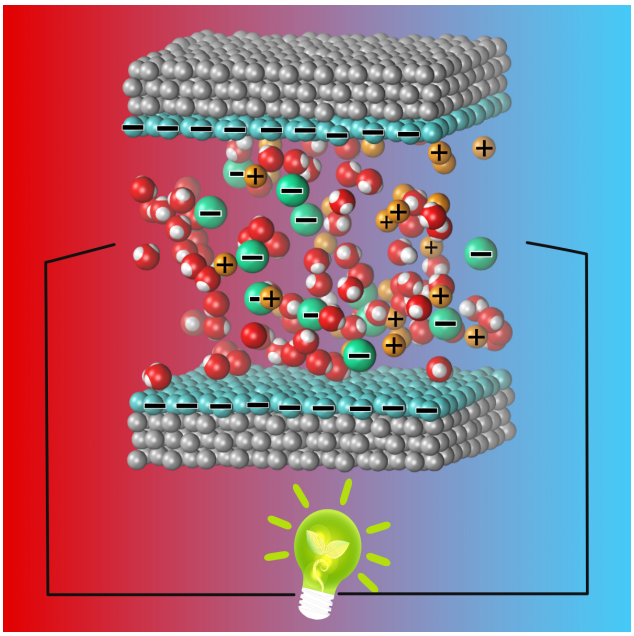
KEYWORD(S) : nanofluidics / Molecular Dynamics / Ionic systems

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.

In that context, we would like to identify promising surfaces with high conversion efficiency by studying thermoelectric energy conversion in graphene nanochannels, inspired by our recent work [3].



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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 and to explore a wide range of working conditions (surface charge, 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 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 intership can be followed by a PhD thesis (graduate school concours).

BIBLIOGRAPHY :

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

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

[3] M. Ouadfel, M. De San Feliciano, C. Herrero, S. Merabia and L. Joly, "Complex coupling between surface charge and thermo-osmotic phenomena", PCCP (2023)

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