ENERGY TRANSPORT ACROSS A SINGLE DNA CHAIN

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Lumière Matière

LEVEL : M1 / M2
TEAM(S) : MMCI
THEOCHEM

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KEYWORD(S) : MolecularSimulations / Thermal conductivity / DNA

SCIENTIFIC CONTEXT :

Understanding heat transfer within one-dimensional objects is a question that has haunted theorists since the work of Fermi, Pasta, Ulam and Tsingou. While there has been considerable progress in characterizing the thermal conduction of nanowires and nanotubes, the situation is much more contrasted for molecular junctions. One reason is the experimental difficulty of measuring thermal currents (in the order of picowatt/K) within a single molecule. Recently, this difficulty has been overcome with the development of near-field heat probes [1,2]. These recent advances open the way to exploring heat transfer within a large class of molecules and polymers. Very recently, ILM started to model thermal transport across a single DNA molecule in collaboration with an experimentalist group at the Institute Néel in Grenoble.

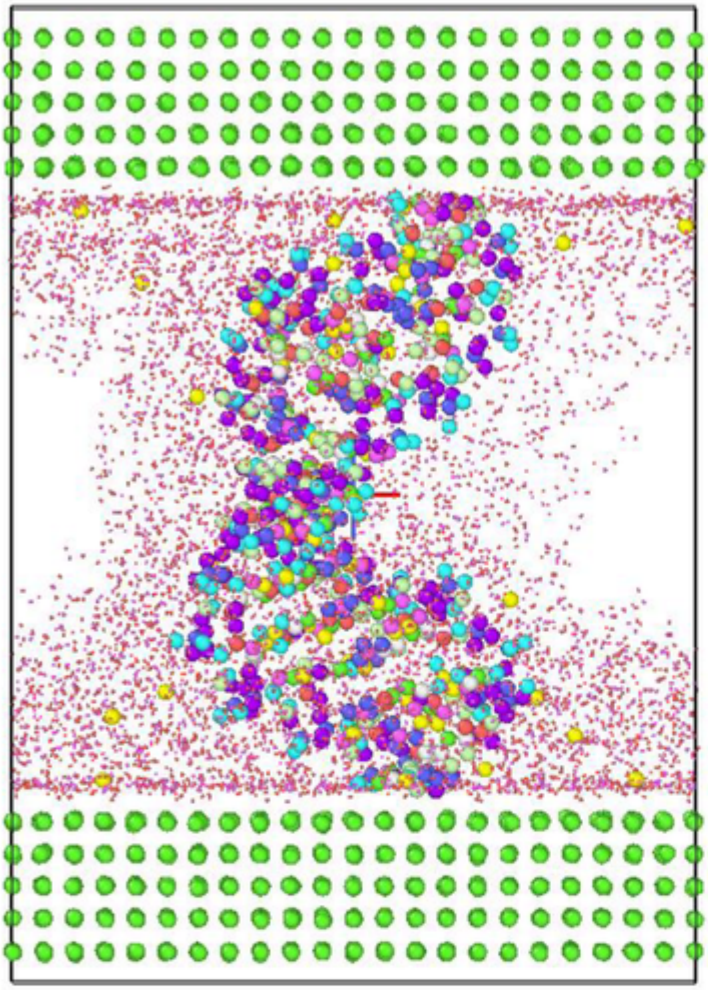

Fig. 1: Molecular dynamics of a DNA molecule junction

MISSIONS :

The student will investigate the thermal transport properties of DNA single molecules attached to gold surfaces using atomistic simulations. Molecular dynamics (MD) simulations will be employed to compute the local heat flux and thermal conductivity [3]. The successful candidate should hold a Master degree in Physics, Physical Chemistry or Material Science. He/she should have knowledge and a taste for nanosciences, modeling and basic programming (fortran or C or python). Good communication skills and english writing are requested. The student will work at the Institute Lumière Matière (ILM) in Lyon area, under the supervision of S. Merabia (CNRS) and C. Loison (CNRS) who has expertise in the modelling of biomolecules [4]. He/she will also interact with our experimentalist collaborators working at the Néel Institute. The internship can lead to a thesis on a related topic.

Interest candidates should send an email along with a resume to Samy Merabia (samy.merabia@univ-lyon1.fr) and Claire Loison (claire.loison@univ-lyon1.fr).

OUTLOOKS :

Informal enquiries are welcome.

BIBLIOGRAPHY :

[1] Cui, L. et al. Thermal conductance of single-molecule junctions. Nature (2019)

[2] Nico Mosso et al., Nano Letters (2019)

[3] Gemma, A. et al., Full thermoelectric characterization of a single molecule. Nat Commun (2023)

[4] Terrien, K. et al., Inviting C5-Trifluoromethylated Pseudoprolines into Collagen Mimetic Peptides, Biomacromolecules (2023)