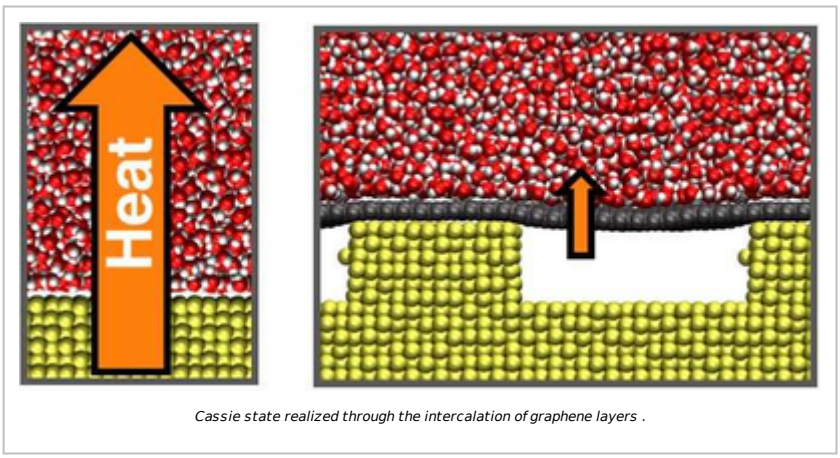
ATOMISTIC MODELLING BIOMIMETIC NANOSTRUCTURED INTERFACES FOR IMPROVED THERMAL DISSIPATION MANAGING

LABORATORY : Institut Lumière Matière

LEVEL : M2
TEAM(S) : MMCI
ENERGIE

KEYWORD(S) : Atomistic Simulations / nanostructured interfaces / nanoscale heat transfer

SCIENTIFIC CONTEXT :



Cassie state realized through the intercalation of graphene layers .

Managing heat dissipation at nano-scales is critical to prevent computers and smartphones from overheating. Within these devices, the heat is evacuated from the circuits to a refrigerant liquid. To delay the boiling crisis that leads to catastrophic heating, it is necessary to maximize the thermal resistance at solid/liquid interfaces. Recently, based on atomistic simulations, we propose an innovative solution to increase this resistance: insert graphene sheets between a metallic nanostructure and water [1]. Graphene makes it possible to achieve a robust suspended state (known as Fakir state), which, by minimizing the thermal contact between the nanostructure and the water, dramatically increases the thermal resistance. In the frame of this internship, we intend to reach even improved thermal dissipation by finding inspiration in nature.

MISSIONS :

The student will investigate the thermal transport properties of graphene coated nanostructures between gold and water inspired by biomimetic superhydrophobic and superhydrophilic interfaces as well. Molecular dynamics (MD) and ab-initio DFT calculations will be employed to build machine-learning potentials [2] to model the interfaces and compute local heat flux and thermal resistance [1]. The successful candidate should hold a Master degree in
Physics, Physical Chemistry or Material Science. He/she should have knowledge and a taste for surface physics, 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, under the supervision of C. Adessi (UCBL prof.) and S. Merabia (CNRS). He/she will also interact with our collaborators expertise in machine learning potentials for atomistic simulations [2].
Interest candidates should send an email along with a resume to Christophe Adessi (christophe.adessi@univ-lyon1.fr) and Samy Merabia (samy.merabia@univ-lyon1.fr). Informal enquiries are welcome.

OUTLOOKS :

The internship can lead to a funded thesis on a related topic.

BIBLIOGRAPHY :

[1] C. Herrero, L. Joly and S. Merabia, Ultra high liquid-solid thermal resistance using nanostructured gold surfaces coated with graphene, Appl. Phys. Lett. 120 (2022) 171601

[2] P Mirchi, C Adessi, S Merabia, A Rajabpour, Lattice thermal conductivity and mechanical properties of the singlelayer
penta-NiN 2 explored by a deep-learning interatomic potential, Phys. Chem. Chem. Phys. 26 (2024), 14216-14227

published on 29/11/2024