**Molecular views on thermo-osmotic flows**

**Li Fu, Samy Merabia, Laurent Joly**

(Institut Lumière Matière, Université Lyon 1, France)

Waste heat harvesting is one of the greatest challenges of our society. Nanofluidic systems could play a role thanks to thermo-osmotic flows, generated at surfaces by temperature gradients. We used molecular dynamics simulations performed with LAMMPS to explore the underlying molecular mechanisms, and understand the effect of the wetting properties of the liquid on the solid surfaces [1]. We have shown the critical role of interfacial hydrodynamics, which can reverse the direction of the flow, and strongly amplify it. Notably, we predicted giant thermos-osmotic flows at the water-graphene interface. Following this prediction, we explored the practical implementation of waste heat harvesting with carbon-based membranes, focusing on model membranes of carbon nanotubes (CNT) [2]. We show that, despite viscous entrance effects and a thermal short-circuit mechanism, CNT membranes can generate very fast thermo-osmotic flows, which can be used to desalinate seawater.

[1] L. Fu, S. Merabia and L. Joly, Phys. Rev. Lett. 119, 214501 (2017)

[2] L. Fu, S. Merabia and L. Joly, J. Phys. Chem. Lett. 9, 2086 (2018)