Understanding the effect of interfacial hydrodynamics on thermo-osmosis using molecular dynamics

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The fundamental influence of thermal gradients on the flux has received scanty attention until only the past decades. Thermophoretic phenomena were firstly studied for numerous applications such as optothermal DNA trap [1] or disease-related protein aggregates [2]. On the other hand, thermo-osmosis at solid-liquid interfaces is the least studied among the osmotic phenomena. It is usually interpreted as a thermal gradient-induced Marangoni flow, but the molecular level understanding is still lacking. Using molecular dynamics simulations, we measured the thermo-osmosis coefficient by both mechanocaloric and thermo-osmosis routes, against different solid-liquid interfacial energies. We show 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 [3]. Following this prediction, we explored the practical implementation of waste heat harvesting with carbon-based membranes, focusing on model membranes of carbon nanotubes (CNT) [4]. 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.

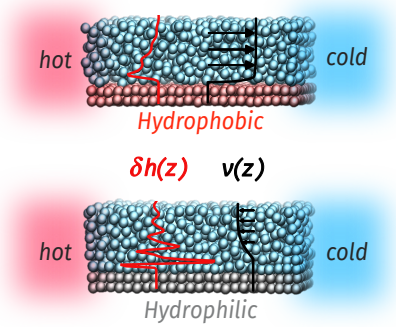

Figure 1: Illustration of the role of surface wettability on thermo-osmotic flows

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[2] M. Wolff, J. J. Mittag, T. W. Herling, E. De Genst, C. M. Dobson, T. P. J. Knowles, D. Braun, and A. K. Buell, Scientific Reports 6, 22829 (2016).

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