All-atom molecular dynamics study of thermo-osmotic flow in Janus nanoslits

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Thermo-osmosis refers to fluid transport induced by a temperature gradient and typically occurs from the hot region to the cold region. It is known to be influenced by pressure gradients, surface tension, and other factors; however, under certain conditions, a reverse flow from the cold region to the hot region, known as negative thermo-osmosis, has also been reported [1]. Such phenomena are relevant to applications such as seawater desalination and energy conversion, and understanding thermo-osmotic transport at the nanoscale remains an important scientific challenge. In particular, the effects of surface wettability and interfacial interactions on the direction and magnitude of thermo-osmotic flow are not yet fully understood at the molecular level. In this study, the thermo-osmotic behavior of water was investigated using all-atom molecular dynamics simulations. Water molecules were modeled using the SPC/E water model, and a nanoslit with Janus walls having different wettabilities on each side was considered. A temperature difference was applied by varying the temperature inside the slit and the interaction between the walls and water molecules, in order to examine the influence of asymmetric surface properties on fluid transport. Pistons were placed in the reservoirs at both ends of the slit to maintain a pressure of 0.1 MPa, thereby eliminating the effects of pressure-driven flow. This setup allows for the analysis of fluid transport induced solely by the temperature gradient. From the simulation results, velocity profiles, density distributions, and the molecular structure of water near the solid surfaces were analyzed. In addition, the excess enthalpy near the interface was evaluated to investigate the relationship between interfacial energy distribution and thermo-osmotic flow. These analyses aim to clarify how asymmetric surface wettability affects thermo-osmotic transport of water under nanoconfinement.

Keywords:
Thermo-osmosis, Molecular dynamics simulation, Janus surfaces, Nanoconfined water

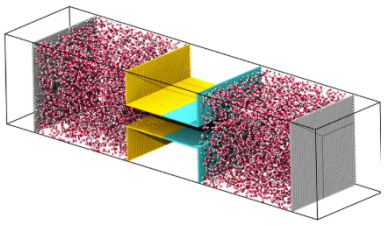

Fig.1 Simulation model of the Janus nanoslit system used for the thermo-osmotic flow study.

References:

[1] K.Qui et.al., Self-Sustained Flow in Janus Nanochannels Based on Thermo-Osmosis, J. Phys. Chem. B 129 (2025), 8043-8049