Title: Molecular Dynamics Simulation Insight into Water Condensation as a Function of Surface Hydrophobicity

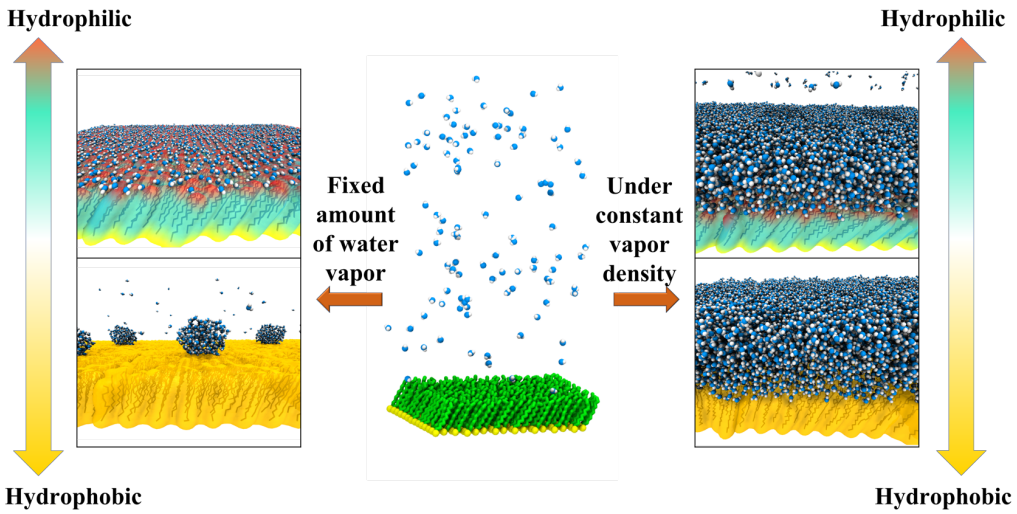
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Keywords: molecular dynamics, self assembled monolayer, water condensation, heat transfer, wettability, surface chemistry, hydrophobicity

Water condensation plays a major role in a wide range of industrial applications. Over the past few years, many studies have shown interest in designing surfaces with enhanced water condensation and removal properties; lotus leaf-like super-hydrophobic surfaces (SHS) and hydrophilic directional slippery rough surfaces (SRS) are some of the examples. To advance these designs a molecular scale understanding of the water behavior as a function of surface hydrophobicity is strongly needed. Since the approaches to quantify wetting at the macroscale do not always translate to the nanoscale, there is a need for new methods to characterize hydrophobicity at small scale. Using molecular dynamics computer simulations of well-characterized alkanethiol self- assembled monolayers with different head group chemistries, here we quantify the role of surface hydrophobicity on water condensation. We measured the water condensation rates on different surfaces and linked that behavior to well established surface characteristics to give a more complete picture of the role of surface hydrophobicity on the behavior of water. We showed that using our techniques, even small changes in the surface hydrophobicity are readily apparent. We also observed a remarkable correlation between our results and the role of surface hydrophobicity on the water compressibility, interfacial thermal conductance and contact angle when we compare data across different studies. Examining the total interaction energy between water and the surface, density fluctuations near the surface, the formation, growth mechanism and stability of water clusters, and the wetting process on the surface we are able to provide insight into the water condensation process on different surfaces as a function of surface hydrophobicity.



Reference:

(1) Ranathunga, D. T. S.; Shamir, A.; Dai, X.; Nielsen, S. O. Molecular Dynamics Simulations of Water Condensation on Surfaces with Tunable Wettability. *Langmuir* 2020, *36* (26), 7383–7391.

(2) Dai, X.; Sun, N.; Nielsen, S. O.; Stogin, B. B.; Wang, J.; Yang, S.; Wong, T. S. Hydrophilic Directional Slippery Rough Surfaces for Water Harvesting. *Sci. Adv.* 2018, *4* (3).

Biography:

Dineli T. S. Ranthunga is a young scientist with a PhD in computational chemistry from the University of Texas at Dallas, USA. Her doctoral work mainly explores the applications of molecular modeling techniques to understand the molecular behavior of mechanically and biologically important surfaces. During her PhD, she published more than 8 articles and has been serving as a peer reviewer in reputed journals. Before obtaining her PhD, she received a BSc in Chemistry (2014) from the University of Peradeniya, Sri Lanka and a Bachelor of Information Technology (2105) from the University of Colombo, Sri Lanka. From 2014 to 2016 she worked as a quality assurance analyst / tiger brewer at Heineken, Sri Lanka.

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Session name/ number: Young Scientist Award
Category: Oral /Poster