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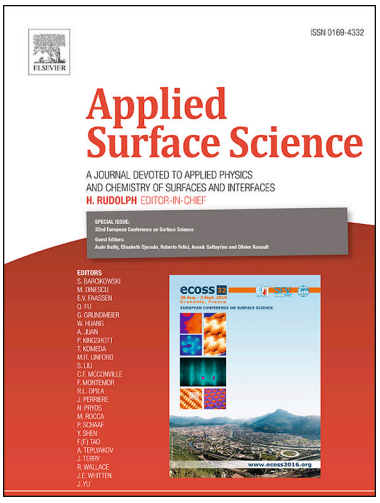

Full Length Article

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Molecular dynamics study of water evaporation enhancement through a capillary graphene bilayer with tunable hydrophilicity

Hieu Trung Kieu,[a,b] Bo Liu,[a,c] Hui Zhang,[a,b] Kun Zhou,*[a,c] Adrian Wing-Keung Law*[a,d]

[a] *Environmental Process Modelling Centre, Nanyang Environment and Water Research Institute, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

[b] *Interdisciplinary Graduate School, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

[c] *School of Mechanical and Aerospace Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

[d] *School of Civil and Environmental Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

HIGHLIGHTS

- The capillary evaporation of water when being confined in a vertically aligned graphene mesopore at the atomistic scale has been investigated via molecular dynamics simulations.
- Significant evaporation enhancement is observed when the pore surface is tuned from hydrophobic to hydrophilic.
- A high temperature is found to further facilitate the capillary effect, thus improves the evaporation rate.
- The pore size also affects the evaporation enhancement in a nonmonotonic manner, controlled by the morphology of the liquid-gas interface and the interaction energy between the water molecules and the graphene surface.

Abstract

The rate of water evaporation as fundamental phase-change phenomenon is critically important to thermal processes in various industrial and manufacturing applications. With the development of nanotechnology, significant acceleration of evaporation rate process is now potentially feasible, which can lead to much higher efficiency, for example for thermal desalination. Recently, hollow and porous nanostructures have exhibited promising potential in the evaporation enhancement due to their capillary effect. However, the mechanism of water vapor transport through a capillary media at the nanoscale and the effect of surface properties remain unexplored. The present study investigates the evaporation behavior of water through the capillary channel of a vertically aligned graphene bilayer using molecular