## Enhanced Water Evaporation From Å-scale Graphene Nanopores

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The unusual effect of nanoscale confinement of water on its phase transition behaviour is of fundamental scientific interest. The evaporation rate of water from a classical interface can be described by the Hertz-Knudsen (HK) relationship.<sup>1</sup> However, this relationship breaks down for water confined in nanoscale spaces where enhanced evaporation rates exceeding the prediction of HK relationship have been observed.<sup>2</sup> The ultimate limit of nanoscale evaporation conduit is a nanopore with size commensurate to the water molecule, however, currently, there is no available experimental data on study of evaporation from nanopores down to the size of a water molecule. Here, we integrate oxygen-functionalized graphene nanopores into a macroscopic device in a controlled fashion as our model system (Figure 1A). The evaporation fluxes through graphene nanopores are characterized by an-order-ofmagnitude enhancement compared to an open liquid-vapor interface and exhibit a pore size dependence (Figure 1B). Molecular dynamics discloses that water molecules tend to leave the nanopores through the edge region, and this process is further dominant for smaller pores. The fast dynamics of hydrogen bonds forming between oxygen-containing functional groups and water molecules renders enhanced evaporation. Overall, this work helps to understand the evaporation kinetics at nanoscale and to develop energy-efficient vaporbased technologies.

## References

[1] Persad, A. H.; Ward, C. A. Chem. Rev. 2016, 116 (14), 7727–7767.

[2] Radha, B.; Esfandiar, A.; Wang, F. C.; Rooney, A. P.; Gopinadhan, K.; Keerthi, A.; Mishchenko, A.; Janardanan, A.; Blake, P.; Fumagalli, L.; Lozada-Hidalgo, M.; Garaj, S.; Haigh, S. J.; Grigorieva, I.V; Wu, H. A.; Geim, A. K. Nature **2016**, 538 (7624), 222–225.



**Figure 1:** (A) Schematic of the permeation set-up for water evaporation through nanoporous singlelayer graphene(N-SLG) and few high-resolution transmission electron microscope images. Scale bar: 1 nm. (B) Comparison of evaporation rate from open water aperture and from three different sizes of graphene nanopores and their  $O_2$  plasma treatment conditions.

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