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TOPICAL REVIEW — Water at molecular level

# Evaporation of nanoscale water on solid surfaces*

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The evaporation of water is essential in the macroscopic world. Recent researches show that, on solid surfaces, the evaporation of nanoscale water is quite different from that on bulk water surfaces. In this review, we show the theoretical progress in the study of nanoscale water evaporation on various solid surfaces: the evaporation rate of nanoscale water does not show a monotonic decrease when the solid surface changes from hydrophobic to hydrophilic; the evaporation of nanoscale water on hydrophobic–hydrophilic patterned surfaces is unexpectedly faster than that on uniform surface; the evaporation of nanoscale water on patterned graphene oxide is faster than that on homogeneous one; how temperature affects the evaporation of nanoscale water on solid surface; how ions affect the evaporation of nanoscale water on graphene oxide.

**Keywords:** water evaporation, nanoscale, solid surface

**PACS:** 66.90.+r, 68.03.Fg, 87.90.+y, 89.40.Cc **DOI:** 10.1088/1674-1056/abc0d3

## 1. Introduction

The evaporation of water plays a key role in the global water circulation,[1] affecting many processes in nature and industry, e.g., transpiration,[2,3] thermoregulation,[4] soil salinization,[5] chip manufacturing,[6,7] printing,[8] and spray cooling.[9,10] The evaporation of water from bulk water surfaces such as lakes or rives is a classical topic and has already been extensively studied.[11,12] However, the nanoscale water on solid surfaces, such as those of leaves,[13] skin,[14] soil,[5] or a surface for printing,[8] are ubiquitous in nature. The evaporation rate of nanoscale water from those surfaces may cause obvious effects, e.g., plant withering, dehydration, desertification of soil, or improved efficiency for printing. In 2015, Chen *et al.* demonstrated an electricity generator that rests on nanoscale water while harvesting its evaporation to power a light source,[15] they proposed that natural evaporation of water could be a reliable renewable energy resource.[16] Thus, understanding the evaporation of such nanoscale water on solid surfaces is essential for many phenomena. Recent studies show that, the evaporation of such nanoscale water is quite different from the evaporation on bulk water surfaces.[17] Shin *et al.* experimentally investigated the evaporation of water droplets on hydrophobic and hydrophilic surfaces, and concluded that the evaporation rate is highly affected by the surface characteristics.[18] In 2011, Lee and his co-workers studied the evaporation of water droplets from nanoporous microcantilevers and stated that the dynamics of water evaporation under hydrophobic and hydrophilic conditions are very different.[19] In 2012, Sobac *et al.* found that the evaporation rate appears to be clearly influenced by the thermal effectivity of the substrate.[20] These all indicate that the characteristics of solid surface play an important role in the evaporation of nanoscale water. In this paper, we give a brief review of our recent theoretical progress in the study of nanoscale water evaporation on various solid surfaces.

## 2. Evaporation of nanoscale water on surfaces with different wetting properties

The substrate we used is assigned by positive and negative charges (each has a same magnitude $q$).[21] The total numbers of positive and negative charges are the same, which keeps the substrate neutral. The substrate changes from hydrophobic to hydrophilic as $q$ increases from 0 to $0.8e$. By molecular dynamics (MD) simulations, we found that, the evaporation rate of nanoscale water increased first, and then decreased after it reached a maximum value as the substrate changed from hydrophobic to hydrophilic (Fig. 1). Here, the evaporation rate $R$ represents the number of water molecules evaporating from the substrate per nanosecond. Such effect of the surface wettability on the evaporation rate of nanoscale water is the competition of two different mechanisms: on one hand, the surface wettability affects the shape of the liquid–gas surface; on the other hand, the attraction from the sub-

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strate of different wettability changes the escape probability of surface water molecules. When the substrate is not enough hydrophilic, the water molecules on the substrate accumulate into the form of a sessile spherical cap. The liquid–gas surface area of the droplet is the main factor that influences the evaporation rate of nanoscale water. Since the liquid–gas surface area of a droplet increases as the contact angle decreases, the evaporation rate of nanoscale water increases as the substrate becomes more hydrophilic. Meanwhile, when the substrate is enough hydrophilic, the water molecules spread to form a monolayer on the substrate, and the shape of the water aggregation almost remains the same. In this situation, the attraction from the substrate that prevents the water molecules from running off becomes stronger as the substrate becomes further hydrophilic, which results in the decreasing of the evaporation. Thus, the maximum evaporation rate of nanoscale water corresponds to the hydrophilic surface, on which the water molecules just spread to form a monolayer.[22]

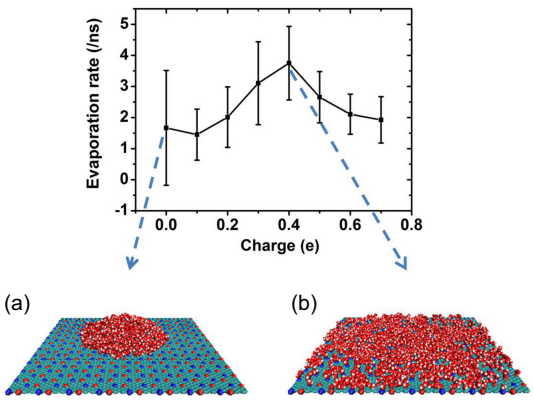



**Fig. 1.** The evaporation rate of nanoscale water versus assigned charge $q$. (a) Snapshot of water molecules forming a droplet on the substrate that is quite hydrophobic. (b) Snapshot of water molecules spreading to form a monolayer when the evaporation rate reaches a maximum value (red and blue spheres represent the atoms with positive and negative charges, respectively).

## 3. Faster water evaporation on hydrophobic–hydrophilic patterned surface

Most surfaces are not uniformly hydrophobic or hydrophilic in nature. For example, soil surfaces with a mixture of components, the back of a desert beetle,[23,24] and the surface of a leaf[25,26] all have patterns with different wettabilities. The patterned structure usually brings new properties, e.g., superhydrophobicity,[27–30] or wetting state change of a droplet.[31,32] How do these patterns influence the evaporation of nanoscale water?

We used a nanoscale triangular hydrophobic–hydrophilic pattern as a model to study the evaporation of nanoscale water. By MD simulation, we found that the evaporation of nanoscale water from certain hydrophobic–hydrophilic patterns was faster than that from any surface with uniform wettability, even though the water film only covered half of the substrate. Most water molecules were confined to the hydrophilic region of the substrate, and were separated into several films surrounded by the hydrophobic region. On the hydrophilic region, compared with the uniform surface, the thickness of the water film increased obviously due to the reduction of the hydrophilic area, and the evaporation rate per nm$^2$ increased sharply with the water thickness, which partly compensated for the effect of the decreased hydrophilic area. Meanwhile, water molecules also diffused out of the hydrophilic region across the contact lines that coincide with the pattern boundaries and evaporated from the hydrophobic region. This part of evaporation rate from the hydrophobic region was almost proportional to the total length of the contact lines (Fig. 2). The considerable evaporation rate from the hydrophobic region together with the slight decrease in evaporation rate from the hydrophilic region resulted in the enhancement of nanoscale water evaporation.[33]

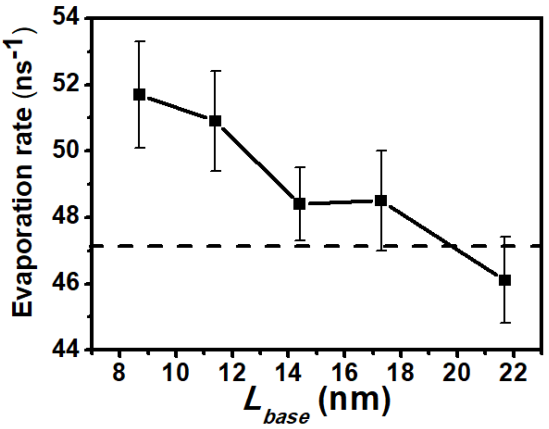



**Fig. 2.** The evaporation rate $R$ of nanoscale water on patterned surfaces with different $L_{\text{base}}$ (the base line of the regular triangle), together with the evaporation rate of the same amount of water on the maximal-evaporation uniform surface (dashed line).

Graphene is a star in materials science, which has excellent mechanical, electrical, thermal, and optical properties.[34–36] Graphene oxide (GO) has also received extensive interest[34,37–43] for the good dispersibility of GO in many solvents[35,44,45] and the tenability of its physicochemical properties.[34,45,46] The polar oxygen functional groups of GO render it strongly hydrophilic.[34,35] Both experiments[47–49] and theoretical calculations[40,50] showed the coexistence of both large unoxidized and oxidized regions on GO. The unoxidized region has the same wetting properties of graphene, which is hydrophobic. In our simulations, we used nanoscale model graphene with rectangular patterns of oxidized and unoxidized regions. By MD simulations, we found that most of water molecules were confined on the oxidized regions, and the evaporation of nanoscale water from certain patterned GO was faster than that from homogeneous one (Fig. 3). The evaporation rate of nanoscale water was quite stable until the oxidation degree of the oxidized regions became too weak to confine the water. The water film spread to the unoxidized regions and the evaporation rate dropped.

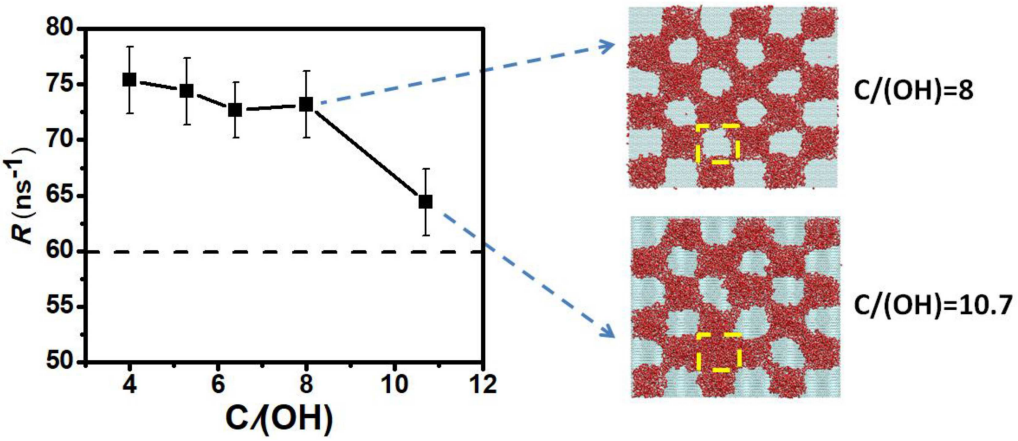



**Fig. 3.** Total evaporation rate on patterned GO with different degrees of oxidation, the dash line shows the evaporation rate of the same amount of water on homogeneous GO. The snapshots on the right show the distribution of water on the patterned GO with C/(OH) = 8 and 10.7. The yellow dashed rectangle outlines the unoxidized region which is covered by water film when C/(OH) = 10.7. C/(OH) is the ratio of carbon atoms and hydroxyl on the oxidized regions of GO.

For the outmost water molecules on the oxidized region, although the decrease of oxidation degree observably weakened the attraction between these water molecules and the solid surface, the correspondingly regulated water–water interaction compensated such loss and resulted in a very limited variation on the total interaction. When the oxidation degree became too low, the water film spread over some unoxidized region, the thickness of the water film decreased. The decrease in water thickness enhanced the attraction between the solid surface and the outmost water molecules. The life time of hydrogen bonds for these water molecules was extended, which made the outmost water molecules more difficult to evaporate.[51]

## 4. Evaporation of nanoscale water with ions on GO

Ions have been proved to affect the evaporation on bulk water and macro scale droplets.[52,53] Former studies showed that the presence of impurities in atmospheric or industrial conditions actually slows down the evaporation of macroscopic water.[54–56] By MD simulations, we studied the evaporation of nanoscale water with ions on GO surfaces. In simulation, both water molecules and ions were distributed only on the oxidized regions. The total evaporation rates on patterned and homogenous GO surfaces both decreased as the concentration of ions increased. The evaporation rate of nanoscale water on patterned GO decreased more than that on homogenous GO. We found that $Na^+$ was closer to the contact line than Cl. The propensity of $Na^+$ had greatly lengthened the H-bonds lifetime of each water molecule near the contact line, and reduced the number of water molecules diffusing from the oxidized regions to the unoxidized regions. Moreover, the effect of ions on the water evaporation does not change much when the variations of oxidation degree are in a certain range.[57] This indicates that the effect of ions on the evaporation of nanoscale water can be greatly affected by the morphology of the substrate.

## 5. Evaporation of nanoscale water at different temperature

Among many factors that can affect the evaporation of water on substrate,[18–20,58,59] temperature is an important parameter which controls a variety of macroscopic properties at interfaces.[60–62] Previous studies showed that, the evaporation rate of bulk water has an exponent relation to the temperature because of the Maxwell model.[63] By MD simulations, we studied the evaporation of nanoscale water film on a uniformly complete wetting surface at different temperatures (Fig. 4(a)).

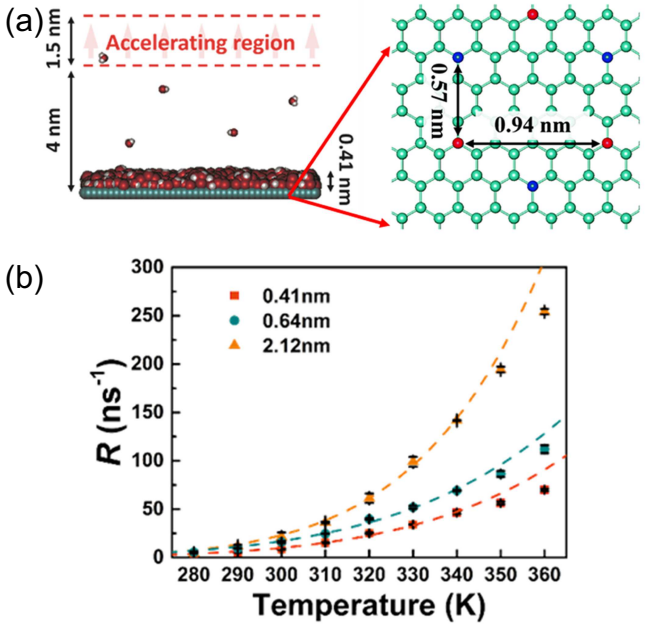



**Fig. 4.** (a) Model system and detailed geometry of the solid substrate. The blue and red spheres represent the atoms of solid with positive and negative charges. (b) The evaporation rate $R$ versus temperature $T$. The red squares with error bars represent the evaporation rates $R$ of water film with thickness of 0.41 nm. The dark cyan circle and the orange triangle with error bars represent the evaporation rates $R$ of water film with thickness 0.64 nm and 2.12 nm, respectively. The red, dark cyan, and orange dash lines are the exponential fits.

We found that, water evaporation rates increased almost exponentially with the temperature when the temperature was roughly below 340 K. This is conformed to the previous studies. But when the temperature was roughly over 340 K, the evaporation rate of water was obviously below the value of the exponential curve. The evaporation rate of monolayer water film was much slower than that of the thicker water film (Fig. 4(b)). Further analysis showed that, although the total interaction energy for each outmost water molecule decreased slowly with temperature, the H-bond lifetime and orientational autocorrelation time of each outermost water molecule decreased more slowly with temperature. The H-bond lifetime and orientational autocorrelation time for water molecules in the thinner film were much longer than those in the thicker one. This suggested that the lower evaporation rate of monolayer water film mainly came from the obvious limit to the rotation of water by the uniformly complete wetting surface.[64]

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## References

[1] Kohler M A and Parmele L H 1967 *Water Resour. Res.* **3** 997
[2] Leuning R, Kelliher F M, Depury D G G and Schulze E D 1995 *Plant Cell Environ.* **18** 1183
[3] Evaristo J, Jasechko S and McDonnell J J 2015 *Nature* **525** 91
[4] Fiala D, Lomas K J and Stohrer M 1999 *J. Appl. Physiol.* **87** 1957
[5] Zarei G, Homaee M, Liaghat A M and Hoorfar A H 2010 *Journal of Hydrology* **380** 356
[6] Dugas V, Broutin J and Souteyrand E 2005 *Langmuir* **21** 9130
[7] Chang S T and Velev O D 2006 *Langmuir* **22** 1459
[8] Park J and Moon J 2006 *Langmuir* **22** 3506
[9] Duursma G, Sefiane K and Kennedy A 2009 *Heat Transf. Eng.* **30** 1108
[10] Cheng W L, Zhang W W, Chen H and Hu L 2016 *Renew. Sust. Energ. Rev.* **55** 614
[11] Eames I W, Marr N J and Sabir H 1997 *International Journal of Heat and Mass Transfer* **40** 2963
[12] Ramanathan V, Crutzen P J, Kiehl J T and Rosenfeld D 2001 *Science* **294** 2119
[13] Jones R L 1957 *Physiologia Plantarum* **10** 281
[14] Potts R O and Francoeur M L 1990 *Proc. Natl. Acad. Sci. USA* **87** 3871
[15] Chen X, Goodnight D, Gao Z H, Cavusoglu A H, Sabharwal N, DeLay M, Driks A and Sahin O 2015 *Nat. Commun.* **6** 7346
[16] Cavusoglu A H, Chen X, Gentine P and Sahin O 2017 *Nat. Commun.* **8** 617
[17] Elbaum M and Lipson S G 1994 *Phys. Rev. Lett.* **72** 3562
[18] Shin D H, Lee S H, Jung J Y and Yoo J Y 2009 *Microelectronic Engineering* **86** 1350
[19] Lee M, Lee D, Jung N, Yun M, Yim C and Jeon S 2011 *Appl. Phys. Lett.* **98** 013107
[20] Sobac B and Brutin D 2012 *Phys. Rev. E* **86** 021602
[21] Wang C, Lu H, Wang Z, Xiu P, Zhou B, Zuo G, Wan R, Hu J and Fang H 2009 *Phys. Rev. Lett.* **103** 137801
[22] Wang S, Tu Y, Wan R and Fang H 2012 *J. Phys. Chem. B* **116** 13863
[23] Yao X, Song Y and Jiang L 2011 *Adv. Mater.* **23** 719
[24] Parker A R and Lawrence C R 2001 *Nature* **414** 33
[25] Byrne M E, Barley R, Curtis M, Arroyo J M, Dunham M, Hudson A and Martienssen R A 2000 *Nature* **408** 967
[26] Wang H, Ngwenyama N, Liu Y, Walker J C and Zhang S 2007 *The Plant Cell* **19** 63
[27] Feng L, Li S H, Li H J, Zhai J, Song Y L, Jiang L and Zhu D B 2002 *Angew. Chem.-Int. Edit.* **41** 1221
[28] Martines E, Seunarine K, Morgan H, Gadegaard N, Wilkinson C D W and Riehle M O 2005 *Nano Lett.* **5** 2097
[29] Yang C, Tartaglino U and Persson B N J 2006 *Phys. Rev. Lett.* **97** 116103
[30] Zhao X D, Fan H M, Liu X Y, Pan H H and Xu H Y 2011 *Langmuir* **27** 3224
[31] Jung Y C and Bhushan B 2007 *Scr. Mater.* **57** 1057
[32] Wu J B, Zhang M Y, Wang X, Li S B and Wen W J 2011 *Langmuir* **27** 5705
[33] Wan R, Wang C, Lei X, Zhou G and Fang H 2015 *Phys. Rev. Lett.* **115** 195901
[34] Chen D, Feng H B and Li J H 2012 *Chem. Rev.* **112** 6027
[35] Park S and Ruoff R S 2009 *Nat. Nanotechnol.* **4** 217
[36] Geim A K and Novoselov K S 2007 *Nat. Mater.* **6** 183
[37] Mao H Y, Laurent S, Chen W, Akhavan O, Imani M, Ashkarran A A and Mahmoudi M 2013 *Chem. Rev.* **113** 3407
[38] Hong B J, Compton O C, An Z, Eryazici I and Nguyen S T 2012 *Acs Nano* **6** 63
[39] Krishnamoorthy K, Veerapandian M, Yun K and Kim S J 2013 *Carbon* **53** 38
[40] Yang J R, Shi G S, Tu Y S and Fang H P 2014 *Angew. Chem.-Int. Edit.* **53** 10190
[41] Lee M, Lee J, Park S Y, Min B, Kim B and In I 2015 *Scientific Reports* **5** 11707
[42] Morimoto N, Kubo T and Nishina Y 2016 *Scientific Reports* **6** 21715
[43] Tong W L, Ong W J, Chai S P, Tan M K and Hung Y M 2015 *Scientific Reports* **5** 11896
[44] Paredes J I, Villar-Rodil S, Martinez-Alonso A and Tascon J M D 2008 *Langmuir* **24** 10560
[45] Eda G and Chhowalla M 2010 *Adv. Mater.* **22** 2392
[46] Mattevi C, Eda G, Agnoli S, Miller S, Mkhoyan K A, Celik O, Mastrogiovanni D, Granozzi G, Garfunkel E and Chhowalla M 2009 *Adv. Funct. Mater.* **19** 2577
[47] Cai W W, Piner R D, Stadermann F J, Park S, Shaibat M A, Ishii Y, Yang D X, Velamakanni A, An S J, Stoller M, An J H, Chen D M and Ruoff R S 2008 *Science* **321** 1815
[48] Pacile D, Meyer J C, Rodriguez A F, Papagno M, Gomez-Navarro C, Sundaram R S, Burghard M, Kern K, Carbone C and Kaiser U 2011 *Carbon* **49** 966
[49] Gomez-Navarro C, Meyer J C, Sundaram R S, Chuvilin A, Kurasch S, Burghard M, Kern K and Kaiser U 2010 *Nano Lett.* **10** 1144
[50] Tu Y S, Lv M, Xiu P, Huynh T, Zhang M, Castelli M, Liu Z R, Huang Q, Fan C H, Fang H P and Zhou R H 2013 *Nat. Nanotechnol.* **8** 594
[51] Wan R Z and Shi G S 2017 *Phys. Chem. Chem. Phys.* **19** 8843
[52] Drisdell W S, Saykally R J and Cohen R C 2009 *Proc. Natl. Acad. Sci. USA* **106** 18897
[53] Duffey K C, Shih O, Wong N L, Drisdell W S, Saykally R J and Cohen R C 2013 *Phys. Chem. Chem. Phys.* **15** 11634
[54] Chuang P Y, Charlson R J and Seinfeld J H 1997 *Nature* **390** 594
[55] Drisdell W S, Saykally R J and Cohen R C 2010 *J. Phys. Chem. C* **114** 11880
[56] Rizzuto A M, Cheng E S, Lam R K and Saykally R J 2017 *J. Phys. Chem. C* **121** 4420
[57] Nan X, Guo Y W and Wan R Z 2019 *Nucl. Sci. Tech.* **30** 122
[58] Liu Y W and Zhang X R 2013 *Phys. Rev. E* **88** 012404
[59] Sumith Y D and Maroo S C 2015 *J. Phys. Chem. Lett.* **6** 3765
[60] Zhong X and Duan F 2016 *Phys. Chem. Chem. Phys.* **18** 20664
[61] Nagata Y, Hasegawa T, Backus E H G, Usui K, Yoshimune S, Ohto T and Bonn M 2015 *Phys. Chem. Chem. Phys.* **17** 23559
[62] Fukatani Y, Orejon D, Kita Y, Takata Y, Kim J and Sefiane K 2016 *Phys. Rev. E* **93** 043103
[63] Jackson R B, Carpenter S R, Dahm C N, McKnight D M, Naiman R J, Postel S L and Running S W 2001 *Ecol. Appl.* **11** 1027
[64] Guo Y W and Wan R Z 2018 *Phys. Chem. Chem. Phys.* **20** 12272