

Electronic Supplementary Information for

**Molecular Insight into the Dynamical Adsorption Behavior
of Nanoscale Water Droplet on Heterogeneous Surface**

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Table S1 The number of water molecules included in each water droplet

Radius/Å	8	9	10	11	12	13	14	15
Number	74	106	151	191	246	311	389	479
Radius/Å	16	17	18	19	20	21	22	
Number	584	702	831	980	1125	1308	1506	

1. The**interaction energy between water droplet and -CH₃ or -NH₂ surface**

During the adsorption process of the water droplet on the -CH₃ or -NH₂ surface, it would release energy. Then the total energy of the system would decrease. The released energy is the interaction energy (E_{inter}). Therefore, we calculate the intrinsic energy of water droplet without surface, the intrinsic energy of surface without water droplet, and the total energy of the water droplet and surface, respectively. Then, the interaction energy can be calculated by the following equation ¹⁻²:

$$E_{inter}=E_{total}-(E_{water}+E_{surface}) \quad (1)$$

Where E_{total} refers to the energy of whole system containing water droplet and surface, E_{water} is the intrinsic energy of water droplet without surface, and $E_{surface}$ represent the intrinsic energy of surface without water droplet. Similarly, E_{vdw} and E_{ele} contributed from Van der Waals and electrostatic interactions are also calculated. These calculated interaction energies are shown in Table S2.

Table S2. Interaction Energies E_{total} , Van der Waals Potentials E_{vdw} and Electrostatic Potentials E_{elec} Between Water and -CH₃ or -NH₂ Surfaces

Surface	$E_{total}/\text{KJ}\cdot\text{mol}^{-1}$	$E_{coul}/\text{KJ}\cdot\text{mol}^{-1}$	$E_{vdw}/\text{KJ}\cdot\text{mol}^{-1}$
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-NH ₂	-3832.72	-4699.52	866.80
-CH ₃	-100.36	-81.94	-18.42

Reference:

- 1 Y. Li, H. Li, K. Zhang, K. M. Liewb, *Carbon*, 2012, **2**, 566–576.
- 2 X. Li, Y. Z. He, Y. Wang, J. C. Dong, Hui Li. *Scientific Reports*, 2013, **4**, 3938.