Deciphering the hydrophilic behavior and vibrational characteristics of θ-Al_2O_3 (010) surface

Wanxiang Yang[a], Mei Zheng[a,b*], Wei Lin[a,c*]

[a]*State Key Laboratory of Photocatalysis on Energy and Environment, College of Chemistry, Fuzhou University, Fuzhou 350108, China*

[b]*School of Materials Science & Engineering, Nanyang Technological University, Singapore 639798, Singapore*

[c]*Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Xiamen University, Xiamen, 361005, China*

Email: mei.zheng@ntu.edu.sg; wlin@fzu.edu.cn

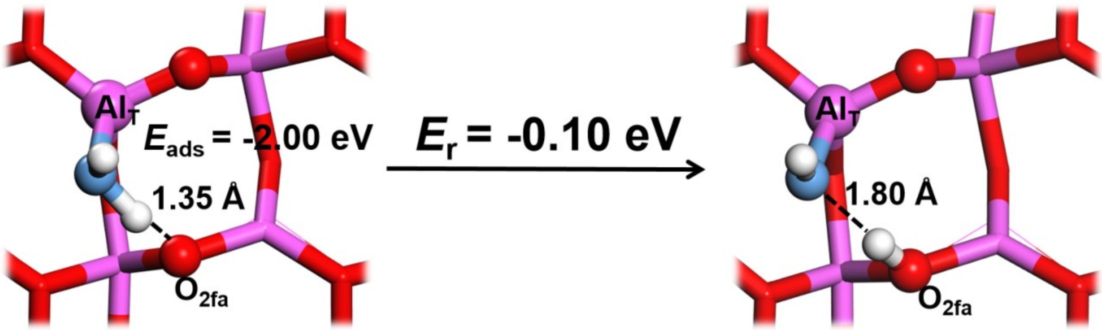


Fig. S1. Potential energy diagram for H_2O decomposition on Al_T site by pure θ-Al_2O_3(010) ($^*H_2O \rightarrow ^*OH + ^*H$).

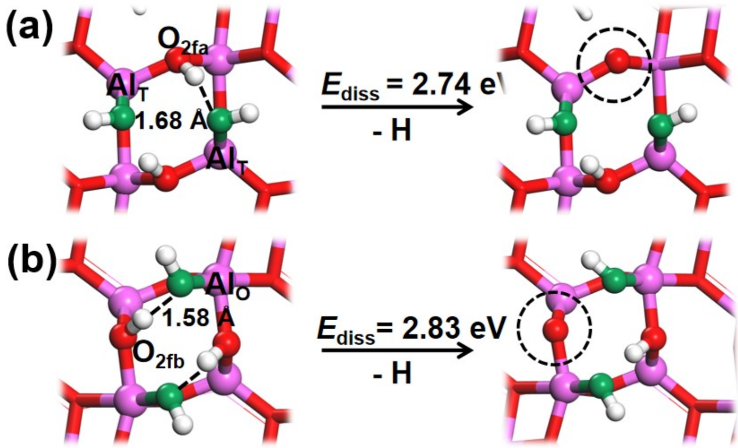


Fig. S2. The bridged H is dissociated from (a) O_{2fa} and (b) O_{2fb} atom.

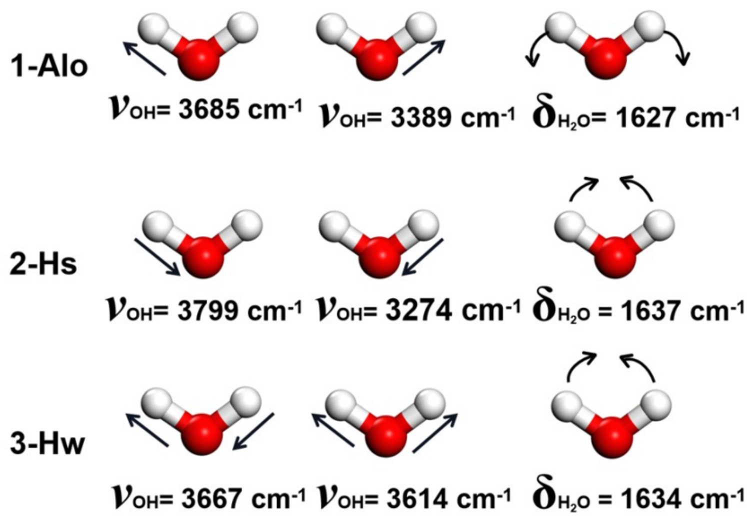


Fig. S3. (a) H_2O possible adsorption sites on hydroxylated θ-Al_2O_3 (010). (b) Vibrational frequencies of H_2O adsorption on the hydroxylated θ-Al_2O_3 (010).

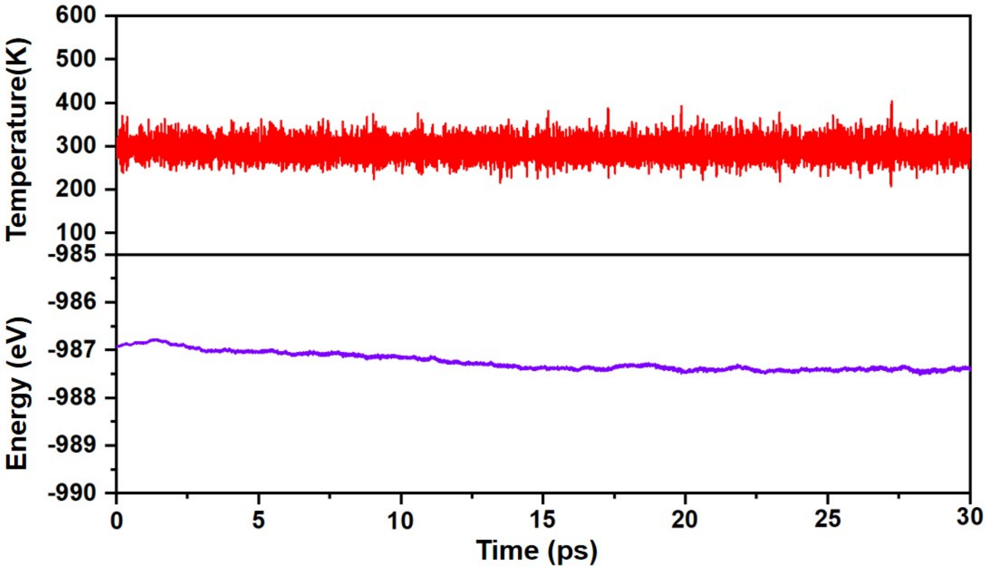


Fig. S4. The relationship between temperature and energy with time for 30 ps simulations in the microcanonical (NVT) ensemble at 300 K.

Table S1. Comparison of Vibrational Frequencies of OHs on the $H_2O/\theta\text{-}Al_2O_3(010)$.

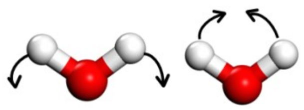
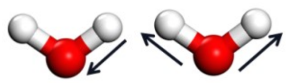
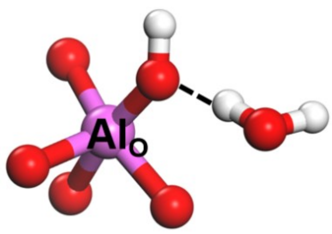
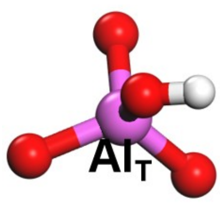
<table>
<tr><th colspan="3">H-O-H
bending vibration
(OHs of water)</th><th colspan="2">H-O-H
stretching vibration
(OHs of water)</th></tr>
<tr><th colspan="2">Harmonic vibration</th><th>MD-VDOS</th><th>Harmonic vibration</th><th>MD-VDOS</th></tr>
<tr><td>1620 cm^{-1}</td><td>1636 cm^{-1}</td><td>1628 cm^{-1}</td><td>3177 cm^{-1}
3284 cm^{-1}
3472 cm^{-1}
3520 cm^{-1}</td><td>3160 cm^{-1}
3261 cm^{-1}
3446 cm^{-1}
3510 cm^{-1}</td></tr>
<tr><td colspan="3"></td><td colspan="2"></td></tr>
<tr><th colspan="3">H-O-H…O
stretching vibration</th><th colspan="2">Free (dangling) OHs
stretching vibration</th></tr>
<tr><th colspan="3">H bonded OHs</th><th colspan="2"></th></tr>
<tr><th colspan="2">Harmonic vibration</th><th>MD-VDOS</th><th>Harmonic vibration</th><th>MD-VDOS</th></tr>
<tr><td colspan="2">3624 cm^{-1}</td><td>3610 cm^{-1}</td><td>3719 cm^{-1}</td><td>3742 cm^{-1}</td></tr>
<tr><td colspan="3"></td><td colspan="2"></td></tr>
</table>

Table S2 Comparison of calculated and experimental vibrational frequencies.

	Cal. (cm^{-1})	Exp. (cm^{-1})*
H-O-H bending vibration (OHs of water)	1628	1648 [1] 1642 [2] 1637 [3,4]
O-H stretching vibration	3322	3319 [2]
	3350	3500 [5] 3499 [1]

* The experimental vibrational frequencies are obtained from Refs. 1-5.

References

1 W. Lin, W. Wu, E. Weitz and G. C. Schatz, *J. Phys. Chem. C*, 2019, **123**, 27704–27711.

2 H. A. Al-Abadleh and V. H. Grassian, *Langmuir*, 2003, **19**, 341–347.

3 M. Takeuchi, R. Kurosawa and J. Ryu, *J. Raman Spectrosc.*, 2022, **53**, 1793–1804.

4 M. Takeuchi, L. Bertinetti, G. Martra, S. Coluccia and M. Anpo, *Appl. Catal. Gen.*, 2006, **307**, 13–20.

5 C. Dyer, P. J. Hendra, W. Forsling and M. Ranheimer, *Spectrochim. Acta Part Mol. Spectrosc.*, 1993, **49**, 691–705.