Supplementary Information

Contact Between Water Vapor and Silicate Surface Causes Abiotic Formation of Reactive Oxygen Species in an Anoxic Atmosphere

Yu Xia,[a,b,c] Juan Li,[b,d] Yuanzheng Zhang,[d] Yongguang Yin,[e] Bolei Chen,[a,b,e,*] Yong Liang,[a,b,*] Guibin Jiang[e], and Richard N. Zare[c,*]

[a]State Key Laboratory of Precision Blasting, Jianghan University, Wuhan, 430056, China.
[b]Hubei Key Laboratory of Environmental and Health Effects of Persistent Toxic Substances, Jianghan University, Wuhan, 430056, China.
[c]Department of Chemistry, Stanford University, Stanford, CA 94305, USA.
[d]School of Physics and Technology, Wuhan University, Wuhan, 430072, China.
[e]State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, P. O. Box 2871, Beijing 10085, China.

*Bolei Chen https://orcid.org/ **0000-0001-8552-3334**;
Yong Liang https://orcid.org/ **0000-0002-3718-0987**;
Richard N. Zare https://orcid.org/ **0000-0001-5266-4253**
Email: bl_chen@jhun.edu.cn; ly76@263.net; zare@stanford.edu

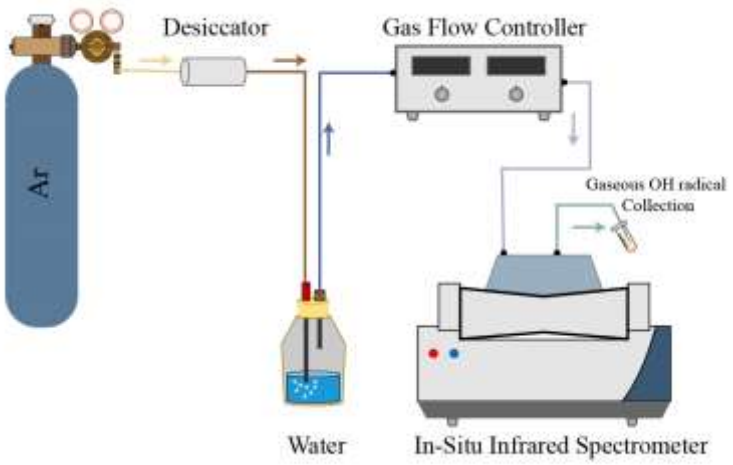

Figure S1 | The schematic of the experimental setup.

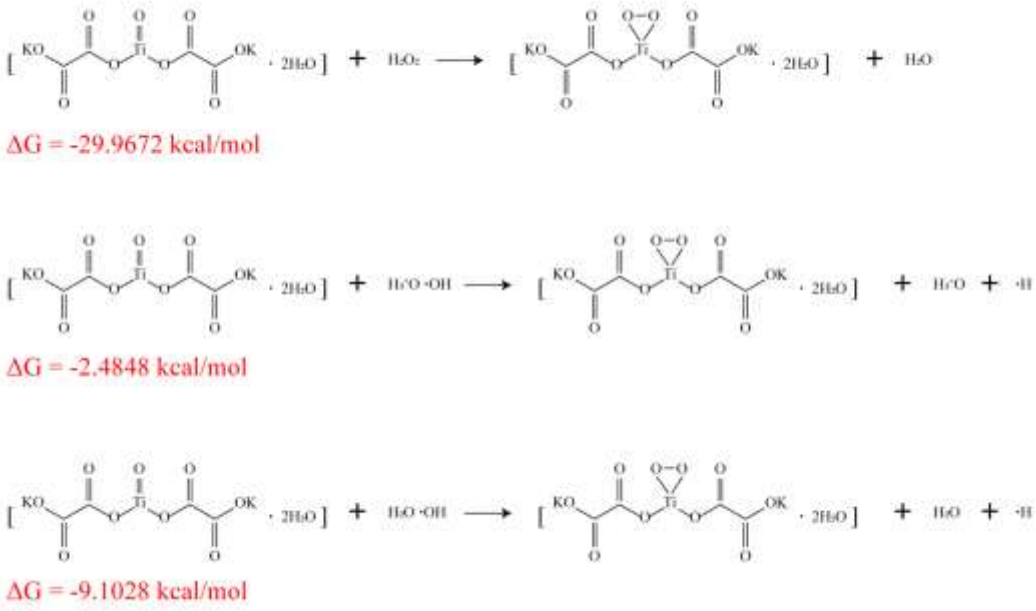

Figure S2 | DFT calculation of Gibbs Free Energy (ΔG) about the reaction of H_2O_2, $H_3^+O{\cdot}OH$ and $H_2O{\cdot}OH$ with titanium potassium oxalate.

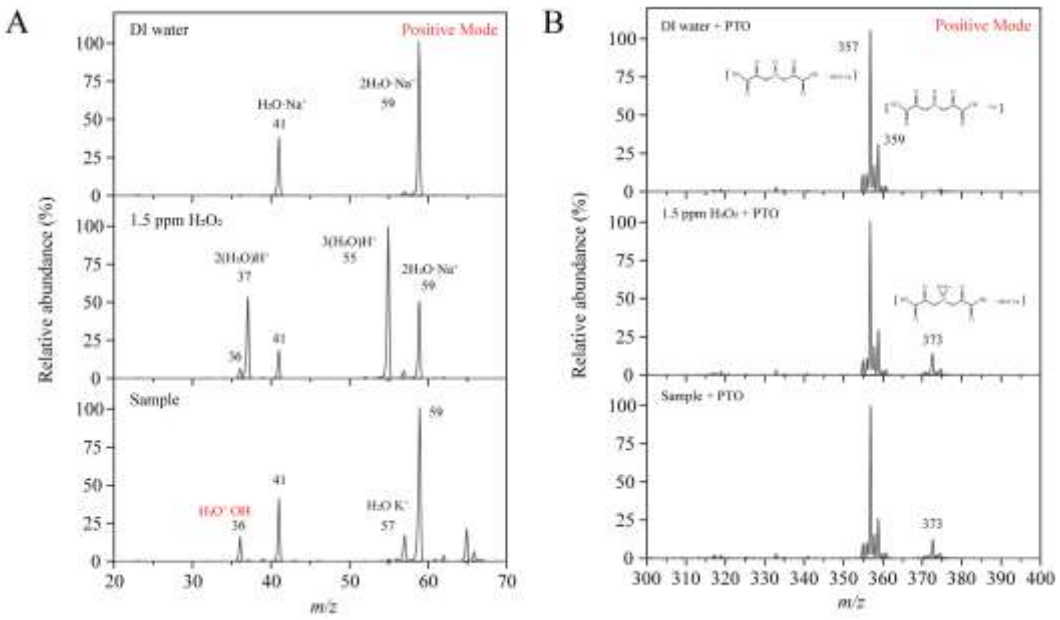

Figure S3 | (A) Mass spectral results of DI water, 1.5 ppm H_2O_2 and sample in positive ion mode, (B) Mass spectral results of DI water, 1.5 ppm H_2O_2 and sample reacted with PTO solution in equal volume.

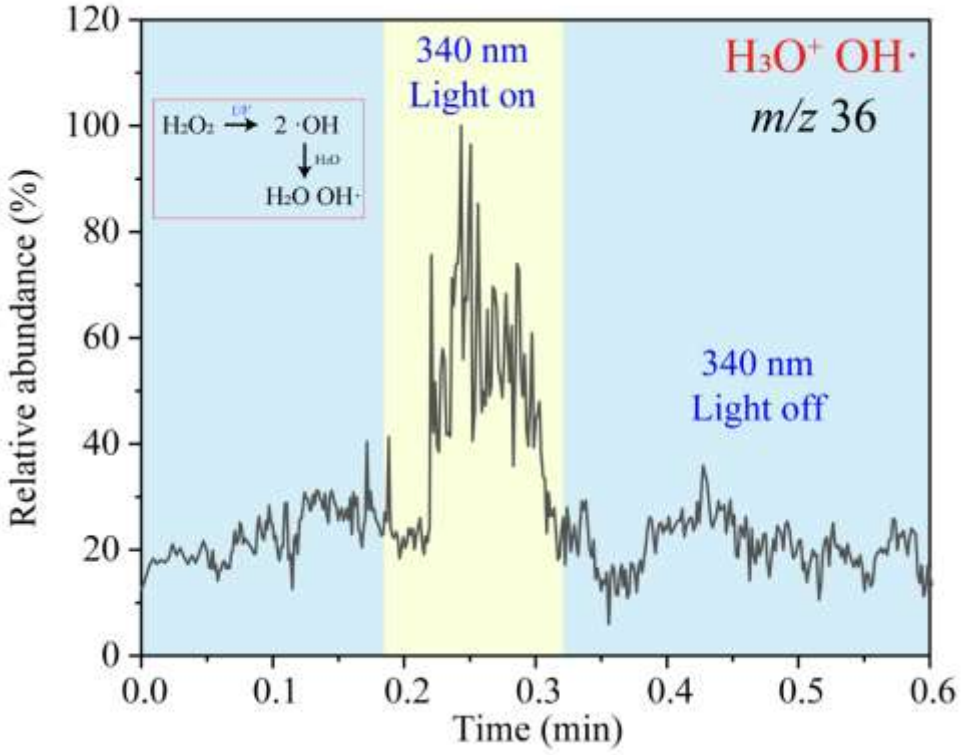

Figure S4 | Signal intensity at *m/z* 36 versus time for 1.5 ppm H_2O_2 solution. (positive ion mode of mass spectrometry) exposed to 340 nm UV radiation, which is turned off, on, and off.

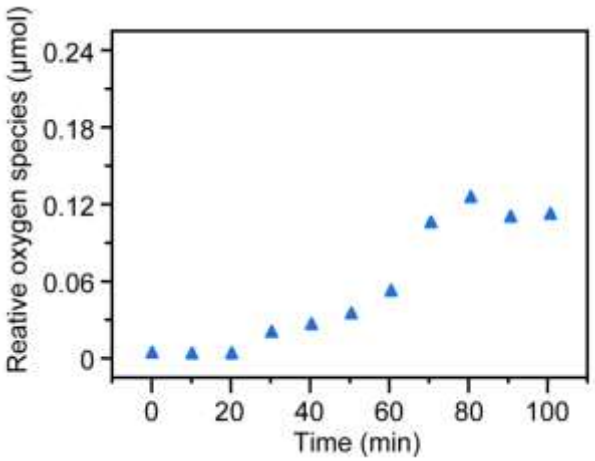

Figure S5 | The relationship between the amount of reactive oxygen species in the leaving gas and reaction time during the contact process.

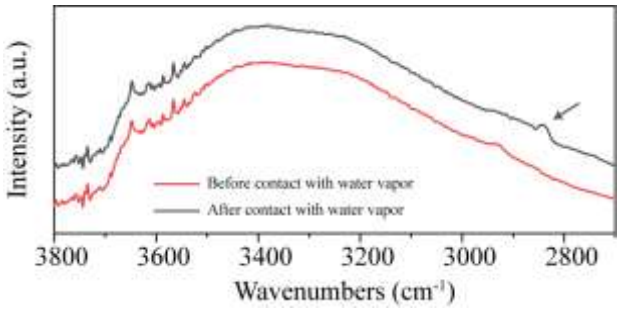

Figure S6 | The FT-IR spectra of a flat SiO_2 substrate before and after contact with water vapor. The arrow points to the H_2O_2 absorption feature.

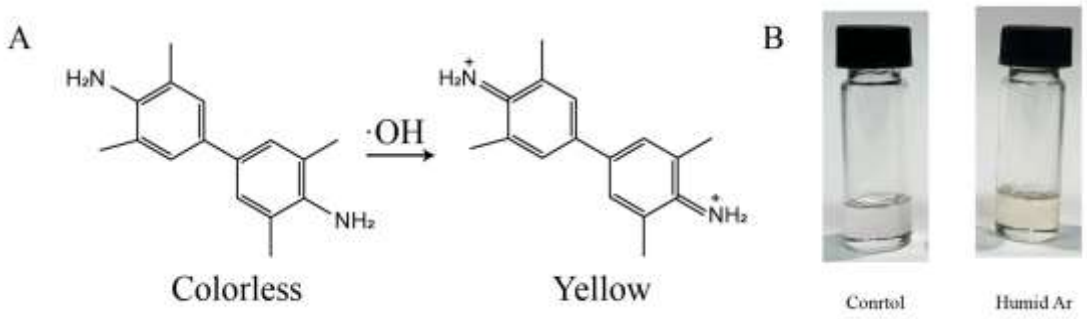

Figure S7 | (A) The reaction mechanism of TMB oxidization. (B) The digital images of the end-product of TMB oxidized by hydroxyl radicals.

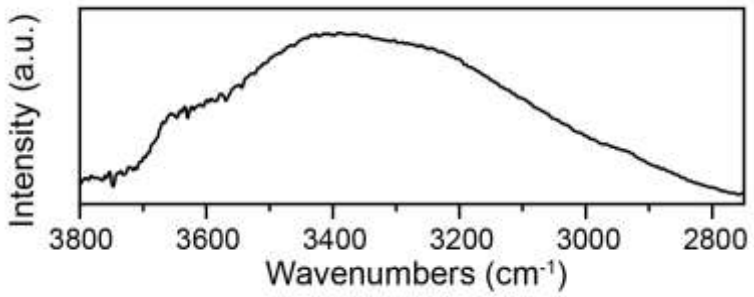

Figure S8 | A typical FT-IR spectrum of commercial SiO_2 nanoparticles.

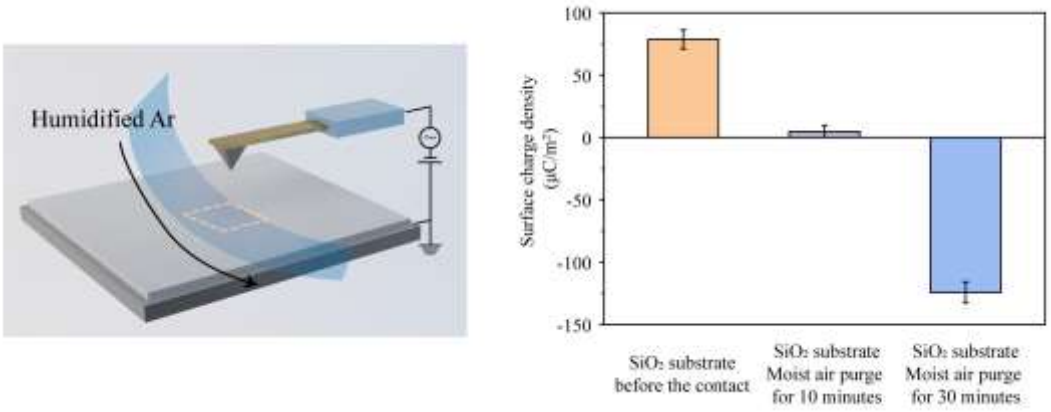

Figure S9 | The surface charge density of the SiO_2 substrate before and after contact with water vapor.

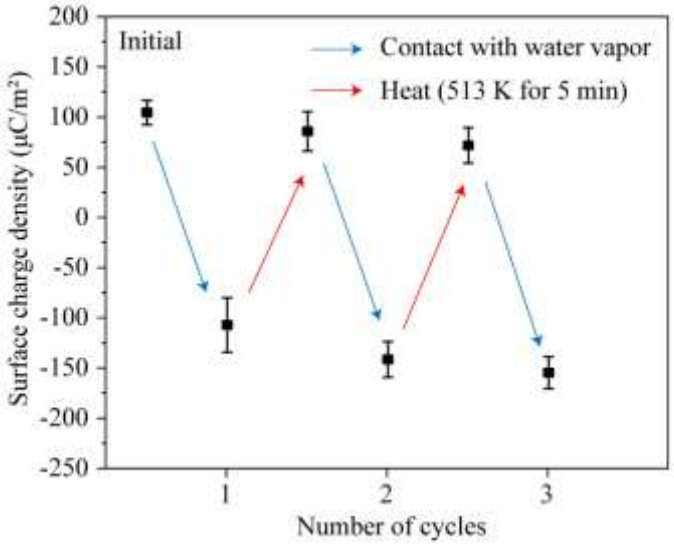

Figure S10 | The surface charge density of the SiO_2 substrate following contact with water vapor and then heating, which is repeated three times.