Supporting Information for

Titanium Dioxide Nanoparticle Surface Reactivity with Atmospheric Gases, CO_2, SO_2 and NO_2: Roles of Surface Hydroxyl Groups and Adsorbed Water in the Formation and Stability of Adsorbed Products

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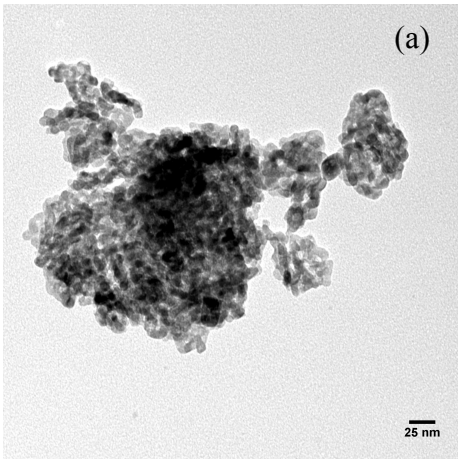
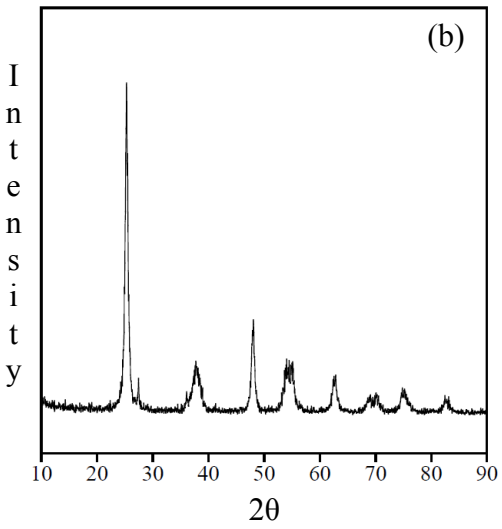
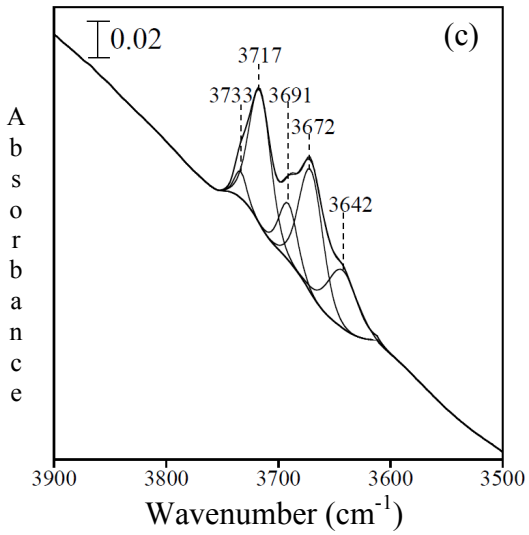
Supporting Figure 1. (a) Transmission electron microscopy (TEM) image, (b) X-ray Diffraction (XRD) pattern and (c) a curve fit FTIR spectrum of the hydroxyl group region for the hydroxylated TiO_2 nanoparticles used for this study.







Supporting Table 1. Assignment of vibrational frequencies of adsorbed surface products following the adsorption of CO_2, SO_2 and NO_2 on hydroxylated TiO_2 nanoparticles.

Surface species description		Vibrational mode assignment	Frequency (cm^{-1})	Refs[a]
CO_2	Carbonate	Monodentate		
		ν_3 (low)	1375	1
		ν_3 (high)	1511	1
		ν_1	1055	1
		Bidentate		1
		ν_3 (low)	1336	1
		ν_3 (high)	1580	1
		ν_1	n.o.[b]	1
		Carboxylate		1
		ν_3 (low)	1269	1
		ν_3 (high)	1675	1
	Bicarbonate	ν_1 (OH)	3606	1
		ν_2 (O-C-O)	1623	1
		ν_3 ((O-C-O))	1433	1
		δ_4 (COH)	1222	1
SO_2	Molecular SO_2	ν_1	1139	2
		ν_3	1325	2
	Sulfite	Monodentate		
		ν_1	923	2
		ν_1	971	2
		ν_3	1033	2
		Bidentate		
		ν_1	886	2
		ν_3	1006	2
	bisulfite	ν (SO)	1077	2,3
		ν_1 (OH)	3648	2,4
	Solvated sulfite		1050	2,4
NO_2	Nitrate	Monodentate		
		ν_3 (low)	1280	5
		ν_3 (high)	1507	5
		ν_1	925	6
		Bidentate		
		ν_3 (low)	1240	5
		ν_3 (high)	1582	5
		ν_1	998	6
		Bridged		
		ν_3 (low)	1216	5
		ν_3 (high)	1631	5
		ν_1	1029	5
	Nitrite	ν_3	1178	5
	NO^+		2218	7,8
	N_2O_3	ν (N=O)	1911	7
	Solvated Nitrate	ν_3 (low)	1336	5
		ν_3 (high)	1409	5
		ν_1	1044	6

[a] Literature references on TiO_2 and Al_2O_3 surfaces and references therein

[b] n.o.: not observed

References

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