Supporting Information:

Surface and structural dependent reactivity of titanium oxide nanostructures with 2-chloroethyl ethyl sulfide under ambient conditions

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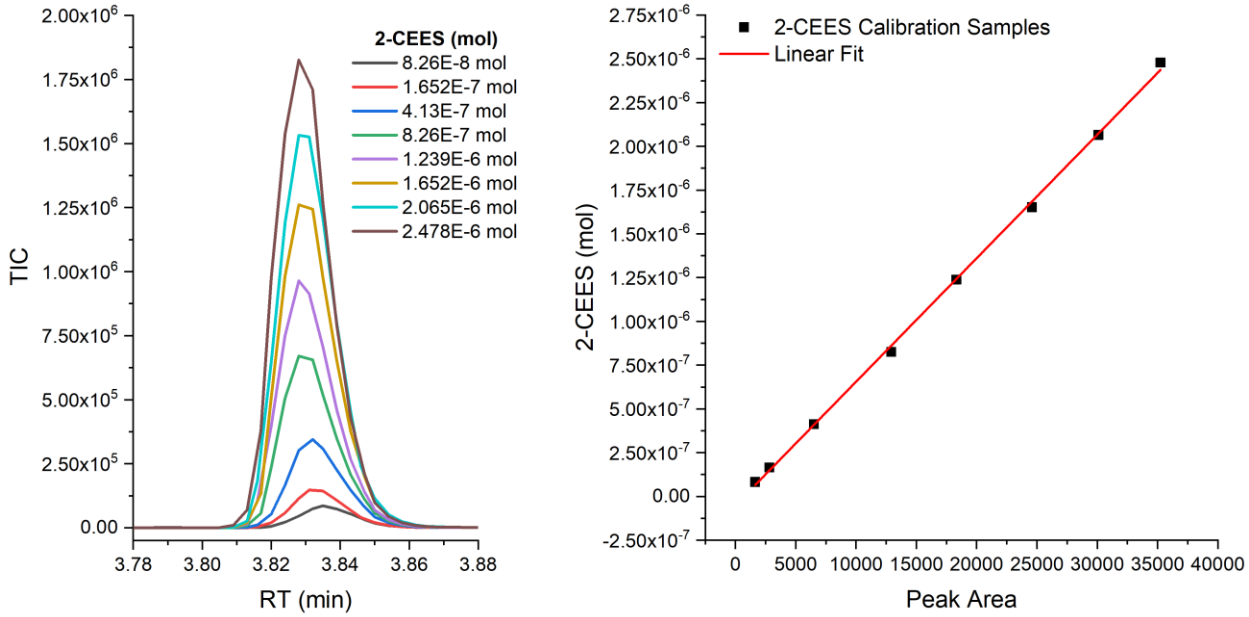

Figure S1. GC-MS concentration analysis of 2-CEES and corresponding peak area-concentration calibration curve.

Table S1. 2-CEES calibration curve data.

Intercept	-4.99984E-8	± 1.68335E-8
Slope	7.05485E-11	± 8.27843E-13
Reduced Chi-Squared	7.71603E-16	
Pearson's r	0.99959	
R-Square	0.99917	

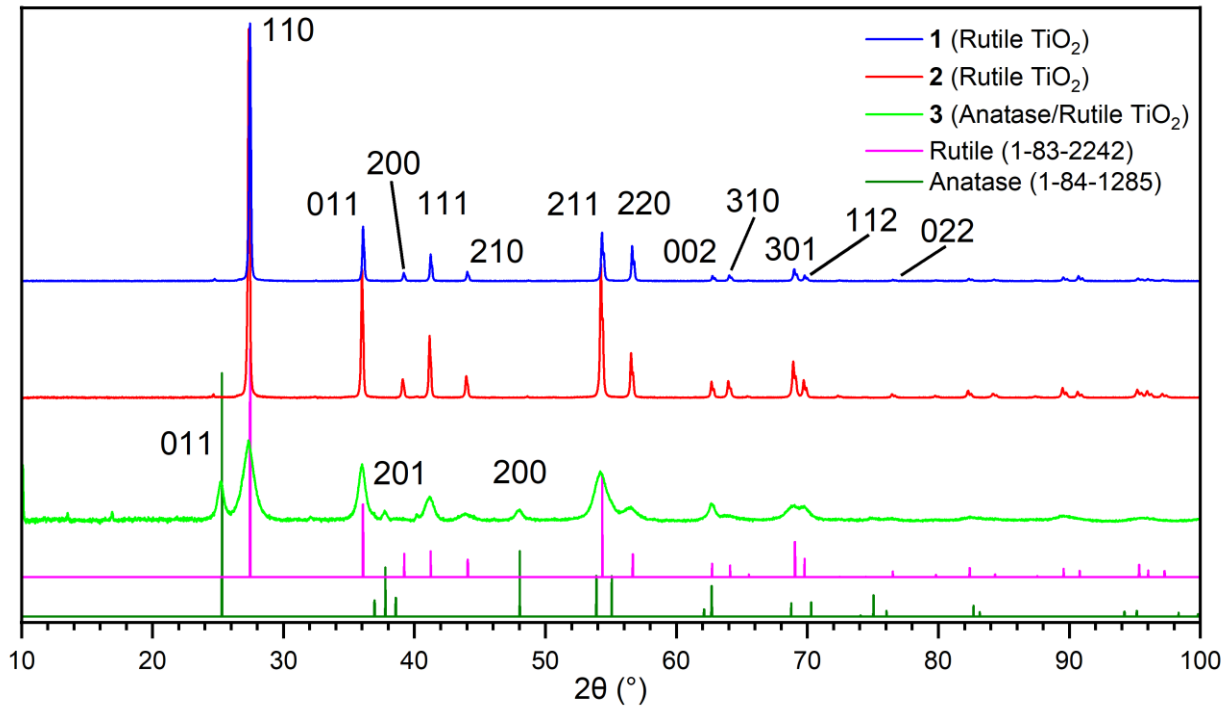

Figure S2. PXRD patterns of materials **1-3** with comparative standard data for Rutile and Anatase TiO_2 phases.

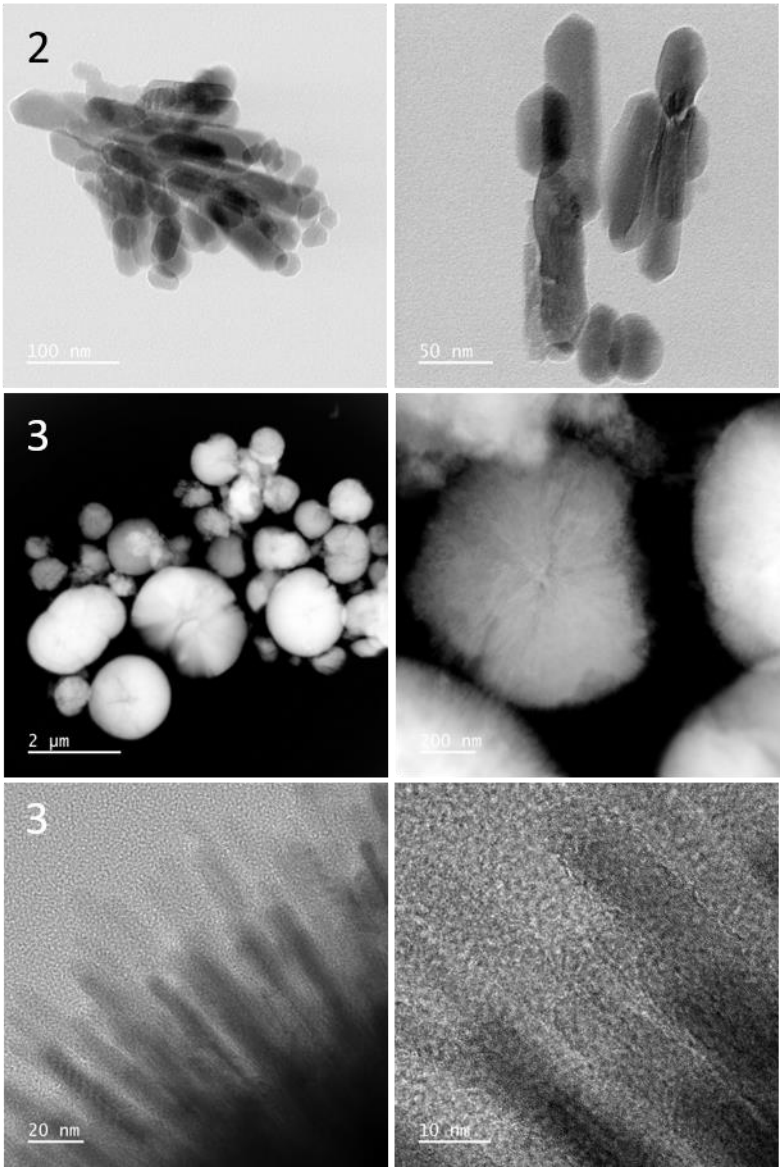

Figure S3. STEM-BF images of material **2**, STEM-HAADF images of material **3**, and HRTEM images of material **3.**

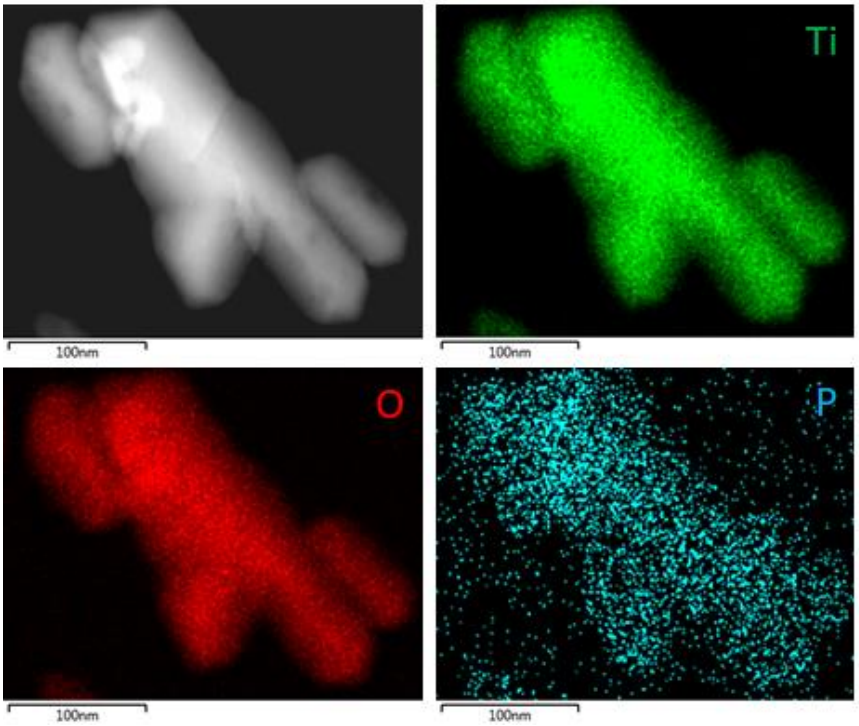

Figure S4. EDS mapping of Ti, O, and P for material **2**.

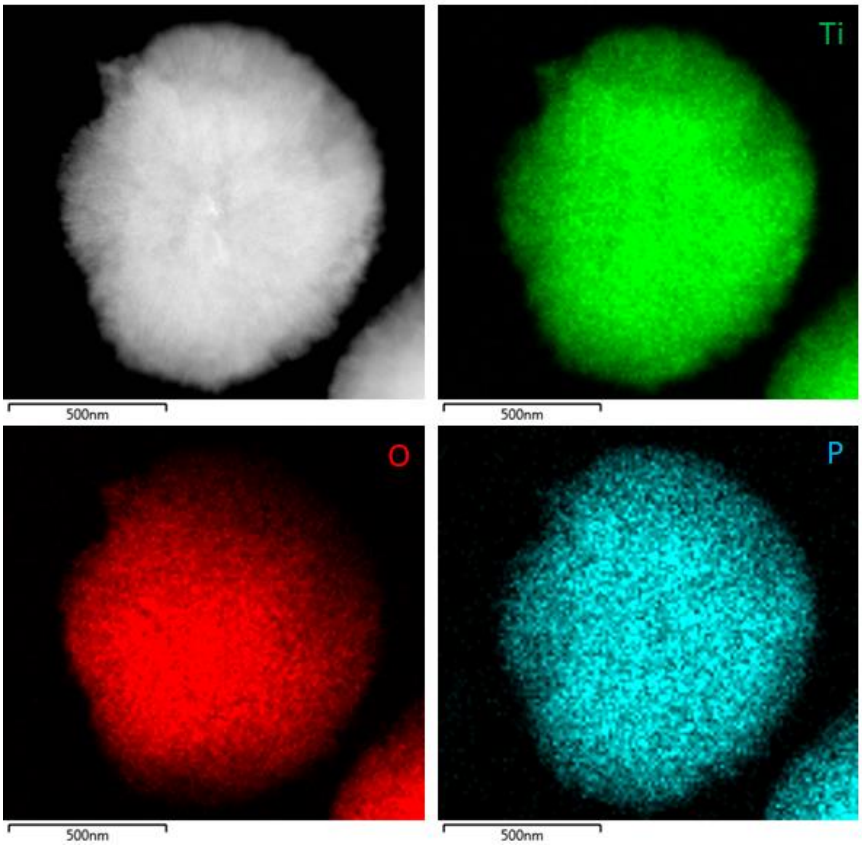

Figure S5. EDS mapping of Ti, O, and P for material **3**.

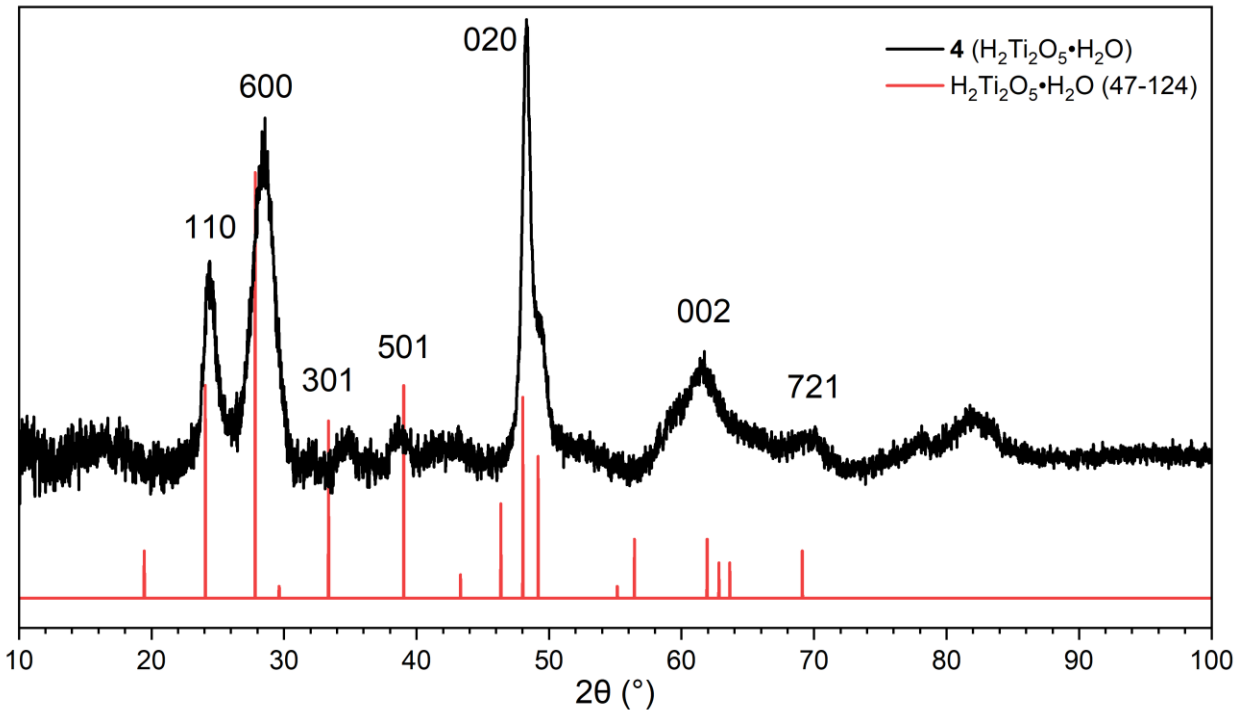

Figure S6. PXRD patterns of materials **4** with comparative standard data for $H_2Ti_2O_5 \cdot H_2O$.

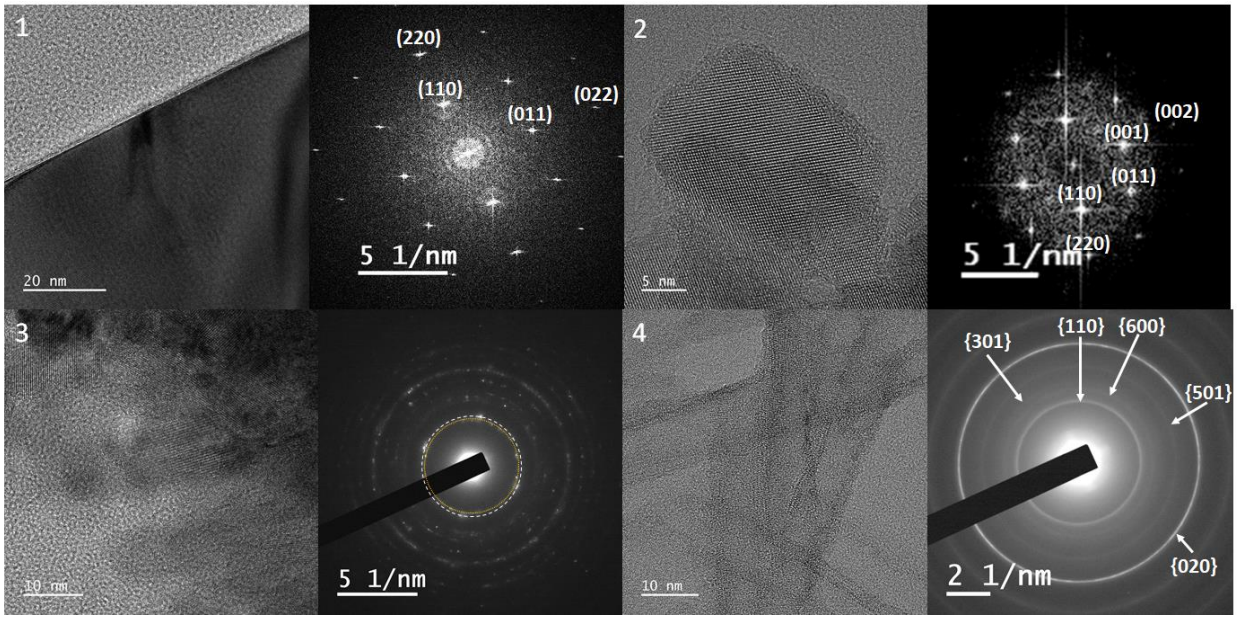

Figure S7. High-resolution TEM images and FFT/SAED analysis of the materials **1-4**. For materials 1 and 2, the corresponding FFT reflections are labeled with matching crystal planes for the rutile structure. Note that the 001 plane reflection observed for material **2** is forbidden due to the laws of diffraction so it is not observed in XRD. For material **3** the SAED pattern is annotated with an orange dotted circle over the reflections for the anatase {011} planes and a white dashed circle over the reflections for the rutile {110} planes. For material **4**, the rings in the SAED pattern are labeled with the corresponding families of planes in the $H_2Ti_2O_5 \cdot H_2O$ structure.

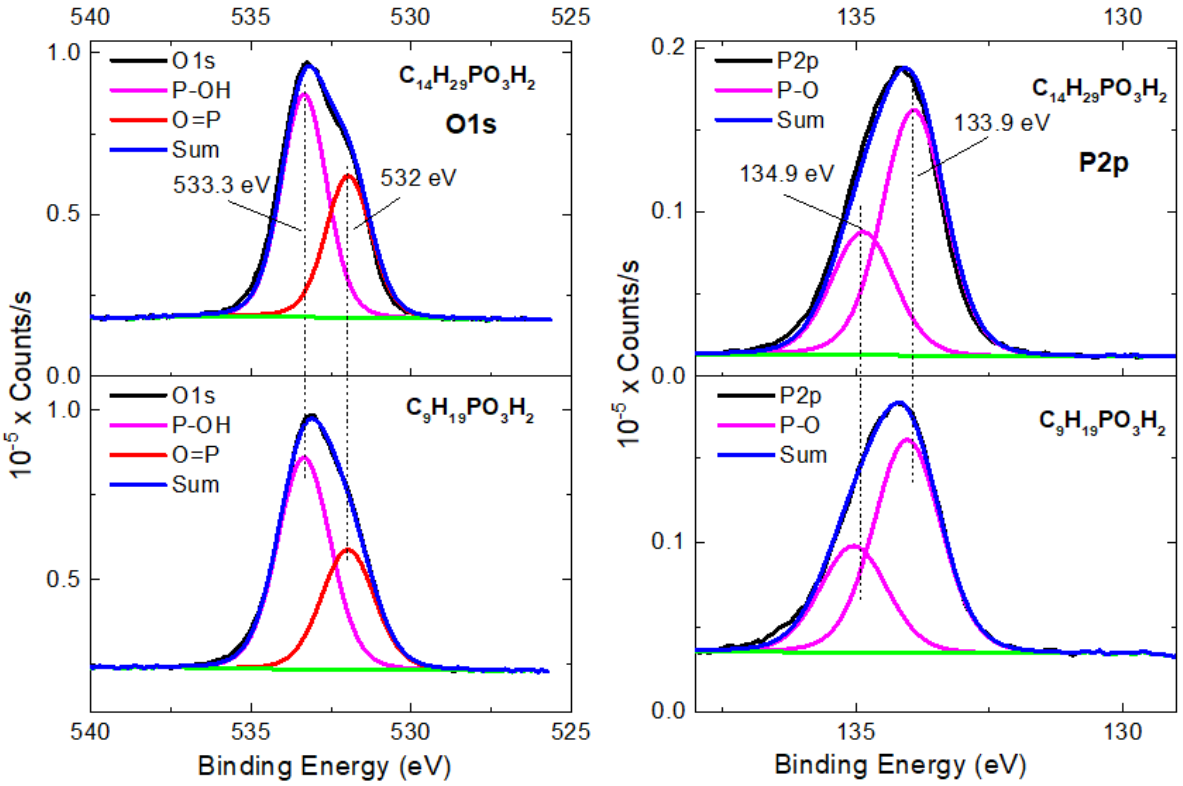

Figure S8. O1s and P2p core level spectra of neat $C_{14}H_{29}CO_3H_2$ and $C_9H_{19}CO_3H_2$ phosphonic acids.

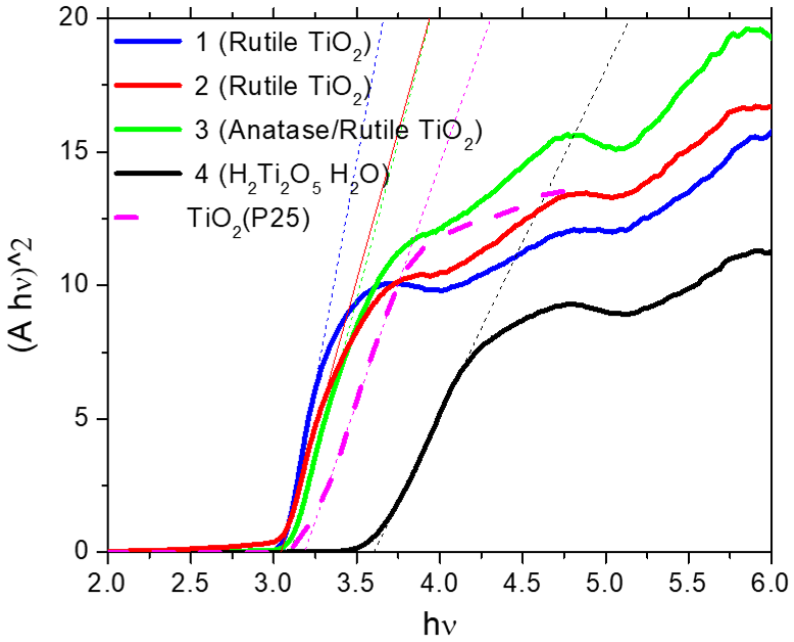

Figure S9. Tauc plots for band gap determinations of materials **1**-**4**. The plot for P25 TiO_2 is shown as a reference.

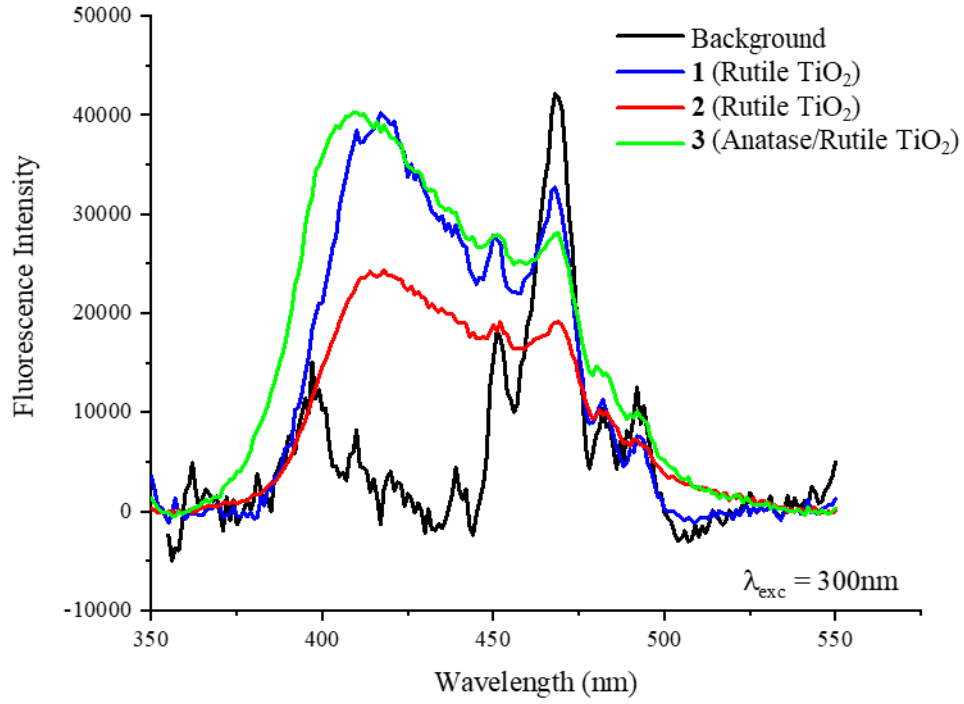

Figure S10. Photoluminescence spectra of materials **1**-**3** with corresponding background spectra to illustrate features attributed to background scattering from the glass slide substrate.

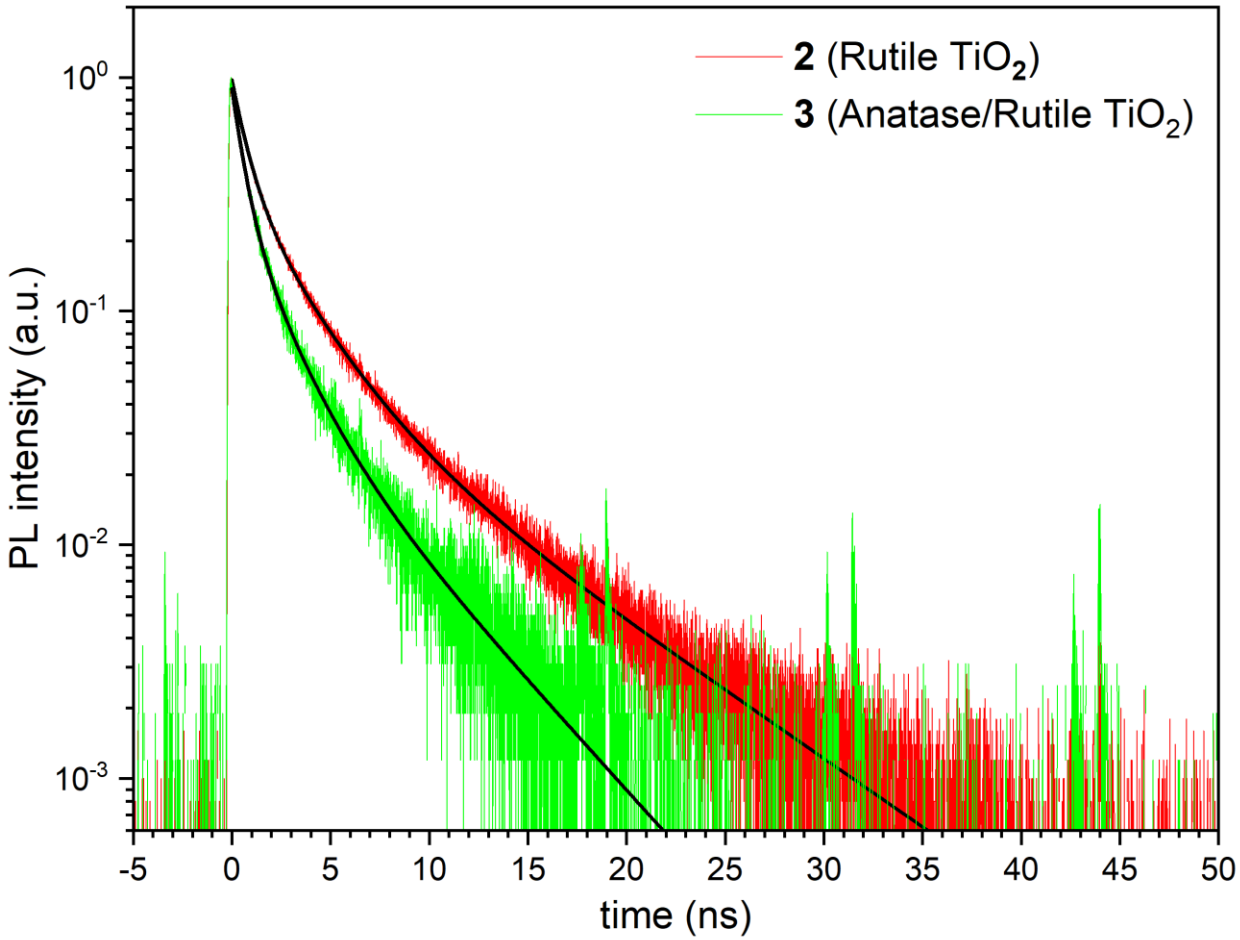

Figure S11. Photoluminescence lifetimes of materials **2** and **3** obtained using the time-correlated single photon counting method. Excitations were performed using ~120 fs pulses at a wavelength of 370 nm, and the time-resolved total integrated emission intensity > 480 nm was obtained with a long pass filter and a fast photodiode detector.

Table S2. Results of the fit of the photoluminescence lifetime decays.

Material	f_1	τ_1 (ns)	f_2	τ_2 (ns)	f_3	τ_3 (ns)	τ_{avg} (ns)
1	--	--	--	--	--	--	--
2	0.59	0.720	0.32	2.58	0.07	7.44	3.54
3	0.58	0.555	0.25	1.75	0.06	4.67	2.22

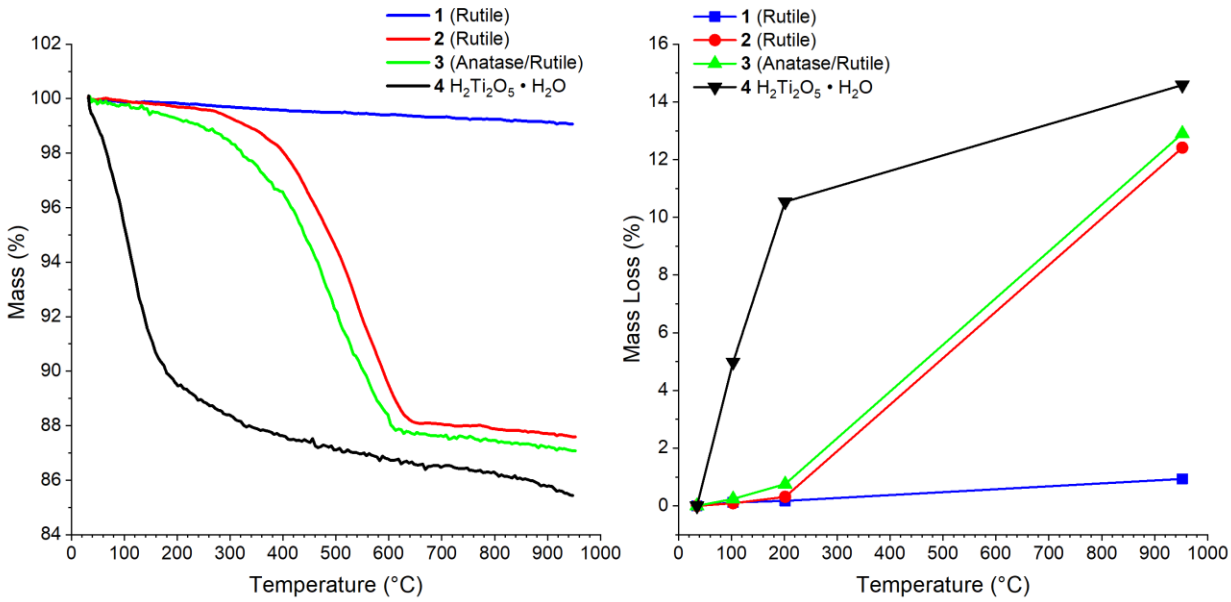

Figure S12. Thermal gravimetric analysis thermal grams of synthesized materials **1-4** and corresponding mass loss plot.

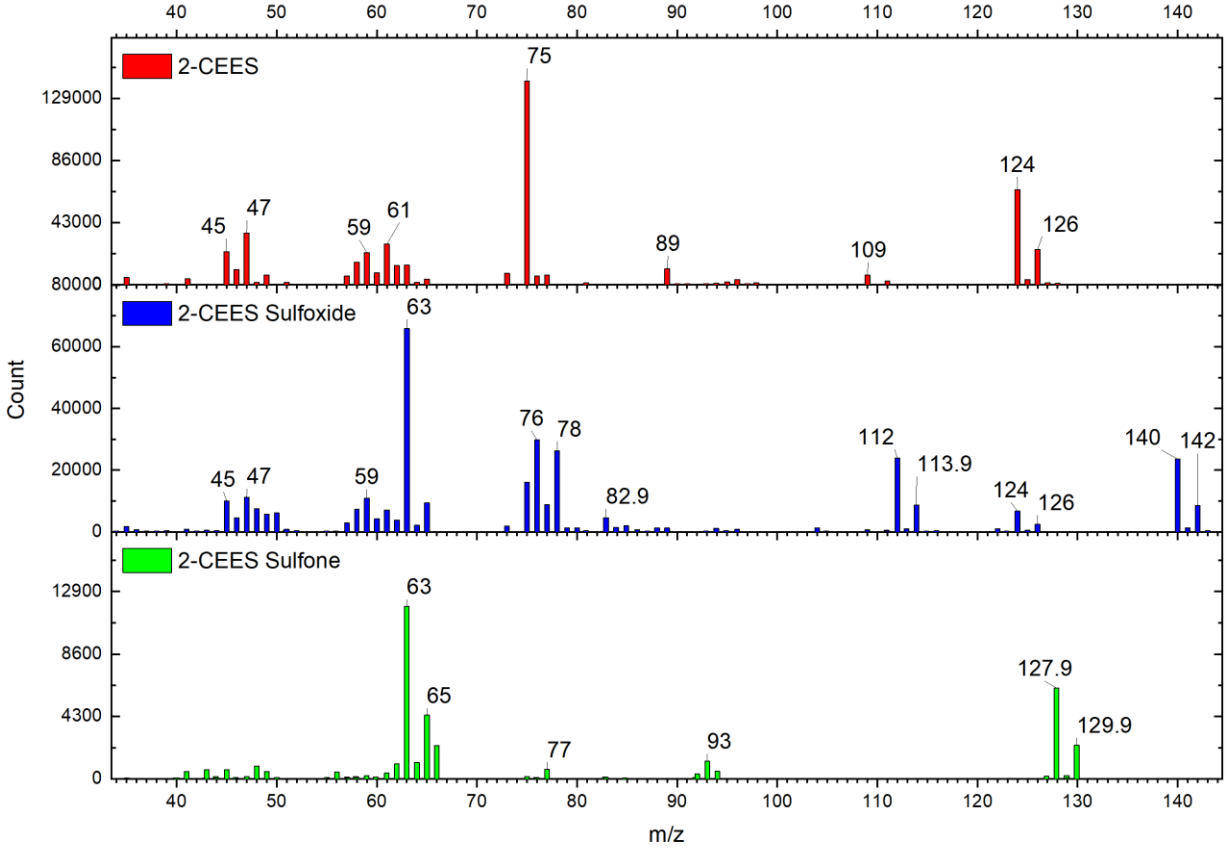

Figure S13. Mass fragmentation pattern comparisons 2-CEES and the oxidation products from challenges with TiO_2 material **2**.

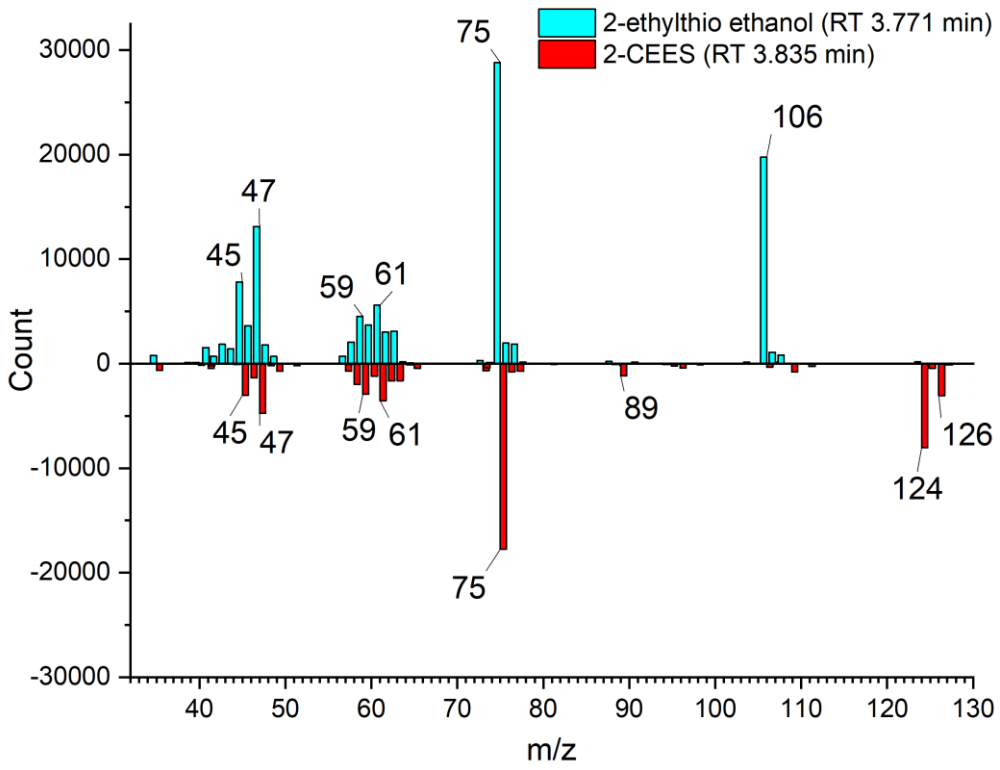

Figure S14. Head to tail comparison of mass spectrum fragmentation patterns from peaks in the gas chromatography trace in the one-hour material **4** ($H_2Ti_2O_5 \cdot H_2O$) challenges (Figure 7). Products are identified as 2-ethylthio ethanol (RT 3.771 min) and 2-CEES (RT 3.835 min).

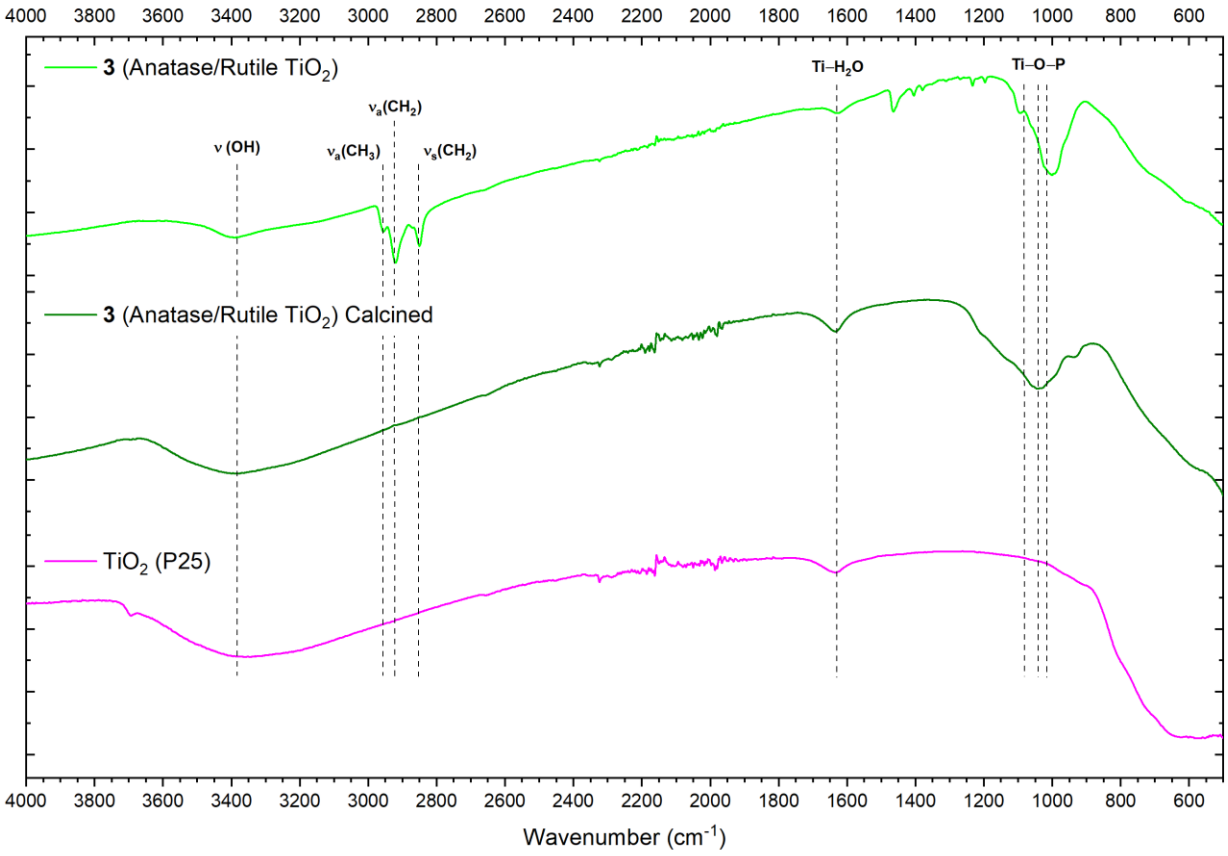

Figure S15. Infrared spectra of the material **3**-pre and post calcination in comparison with P25 TiO_2 to show surface bound phosphates post calcination. Infrared spectra were collected by ATR on a diamond window and are displayed as % transmission.

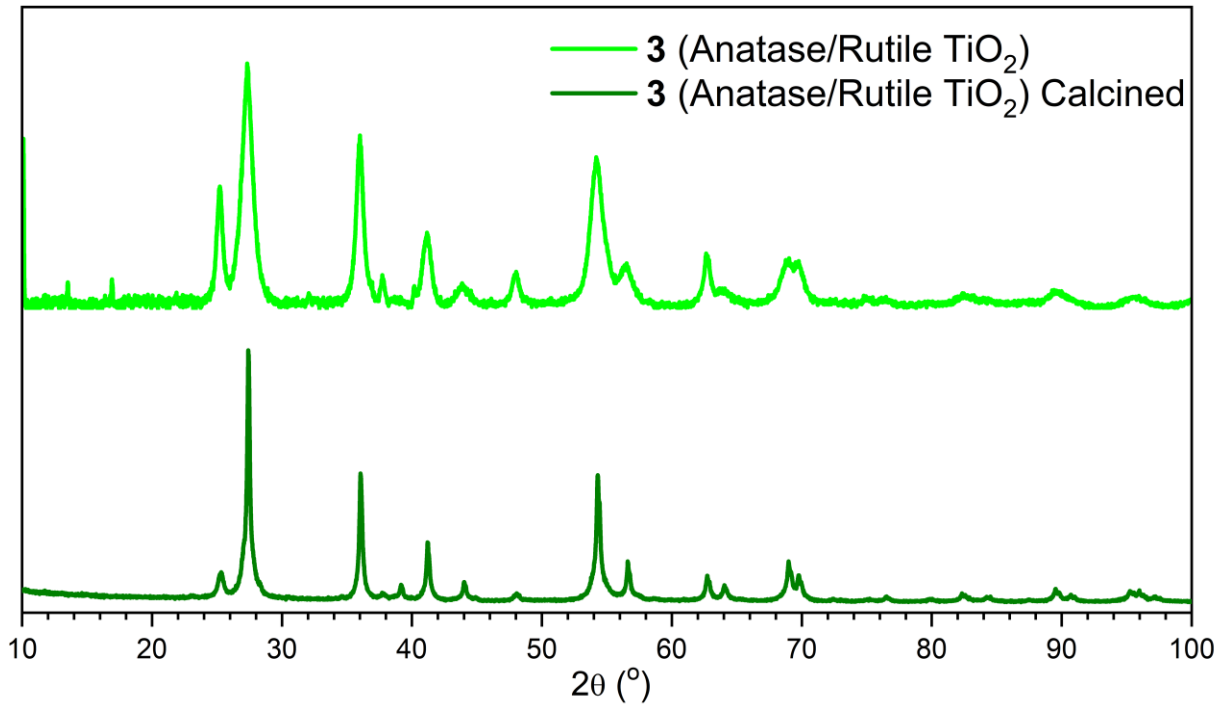

Figure S16. PXRD patterns of material **3** before and after calcination