**Experimental and modeling study of visible light responsive photocatalytic oxidation (PCO) materials for toluene degradation**

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**Supplemental Materials**

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**Supplemental Table S1**. ATD and GC/MS operating parameters.

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| Step | Parameter | Value |
| Auto-thermal desorption | ATD purge time | 1.0 min |
| ATD inject time | 1.0 min |
| ATD desorption temperature | 200.0°C |
| ATD desorb time | 5.0 min |
| Cryo-Trap cool temperature | -140°C |
| Cryo-Trap cool time | 7.3 min |
| Cryo-Trap heat temperature | 250°C |
| Cryo-Trap heat time | 5.0 min |
| GC separation | Carrier gas | Helium, 1 mL/min, velocity at 25 cm/sec |
| Injector | Split, temperature at 230°C, split ratio:8:1 |
| Column | DB-VRX (J&W Scientific)60 m x 0.25 mm, 1.4 um film thickness |
| Oven temperature program | 45°C hold for 10 min; 8°C /min to 140°C, hold for 10 min; 30°C /min to 225°C hold for 13 min.  |
| MS | Mass type | Scan |
| Low mass | 29 AMU |
| High mass | 270 AMU |
| MS quad temp | 150°C |
| MS source | 230°C |
| Scan rate | 3 scan/sec |
| Step size | 0.1 AMU |

**Supplemental Table S2**. Experimental conditions.

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| --- | --- |
| Parameter | Experimental conditions |
| VOC | Toluene |
| Inlet concentration (mg/m3) | 3.8, 7.5, 18.8 |
| Air flow rate (L/min) | 0.2, 1.0, 2.0 |
| Air velocity (mm/s) | 7.8, 39.2, 78.4 |
| Resident time (s) | 1.3, 6.5, 13 |
| RH (%) | 25, 50, 65 |
| Irradiance (W/m2) | 42, 64, 95 |
| Temperature (°C) | 21-22 |



**Supplemental Figure S1**: Comparison of PCO and regeneration performance for three coatings challenged by 3.8 mg/m3 toluene at 25% RH and 0.2 L/min with BLB (7.5 W/m2). Note: P25W stands for P25 mixing with water containing 0.1 ml acetylacetone; P25N stands for P25 mixing with n-methyl pyrrolidone (NMP); P25NP stands for P25 mixing with NMP and additional polyvinylidine fluoride (PVDF; 25 mg for 5%).

The adhesion strength of P25W, P25N, and P25NP on the aluminum pieces was carried out by peeling-off tests. The results indicate that P25W has poorest adhesions at two peeling speeds and P25NP has a slightly better bonding than P25N to the surfaces.



**Supplemental Figure S2**: Loss masses and loss percentages for three coatings at peeling-off speeds of 2.5 cm/s and 0.25 cm/s.



**Supplemental Figure S3**. Toluene concentrations at upstream and downstream and formaldehyde generation during adsorption and PCO of toluene (inlet toluene=3.8 mg/m3, 25%RH, I=95W/m2).



**Supplemental Figure S4**. PXRD pattern of TiNbON catalysts



**Supplemental Figure S5**. Schematic diagram of the control volume in the cross-section of the PCO reactor



**Supplemental Figure S6**. Overall model predictions vs. experimental results for the models of LH-1 and LH-2.