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

Lexuan Zhong1, James J. Brancho2, Stuart Batterman1\*, Bart M. Bartlett2, Christopher Godwin1

1 Environmental Health Sciences, University of Michigan, Ann Arbor, MI, USA

2 Chemistry, University of Michigan, Ann Arbor, MI, USA

Mar. 12, 2017

*\*Corresponding email:* [*stuartb@umich.edu*](mailto:stuartb@umich.edu)

M6075 SPH II, 1415Washington Heights, Ann Arbor, MI 48109-2029, USA

Tel: 734/763-2417 E-mail: stuartb@umich.edu

**Supplemental Materials**

|  |  |
| --- | --- |
| Supplemental Table S1 | ATD and GC/MS operating parameters. |
| Supplemental Table S2 | Experimental conditions |
| 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). |
| 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. |
| 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. |

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

|  |  |  |
| --- | --- | --- |
| 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 |

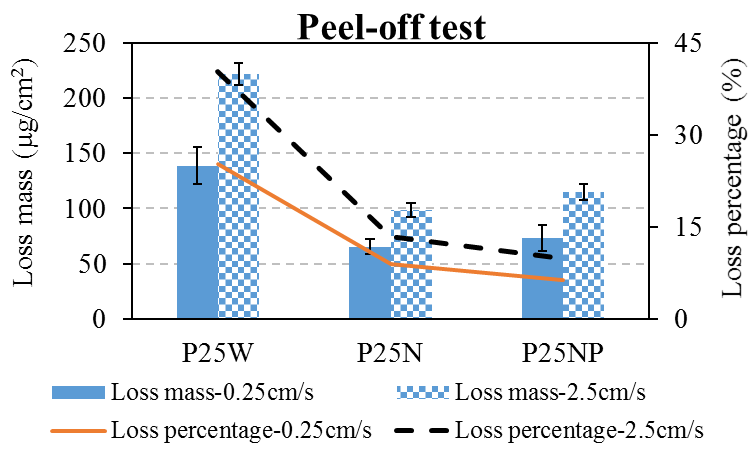
**Supplemental Table S2**. Experimental conditions.

|  |  |
| --- | --- |
| 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 |

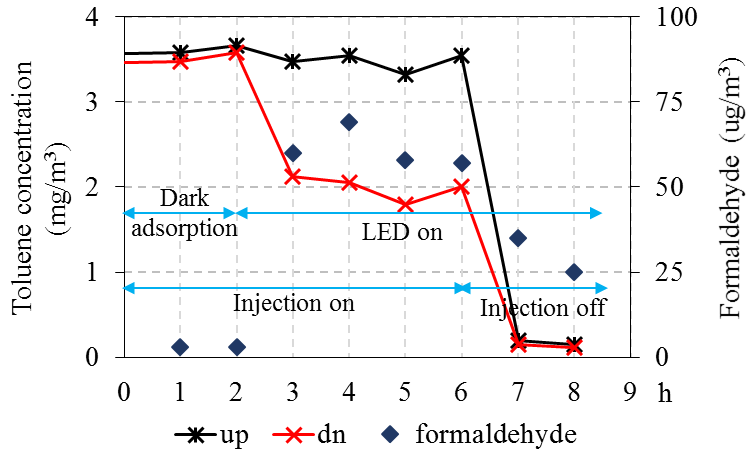


**Supplemental Figure S1**: Comparison of PCO and regeneration performance for three coatings challenged by 3.8 mg/m3 toluene at 25% RH and 0.2 L/min with BLB (7.5 W/m2). Note: P25W stands for P25 mixing with water containing 0.1 ml acetylacetone; P25N stands for P25 mixing with n-methyl pyrrolidone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

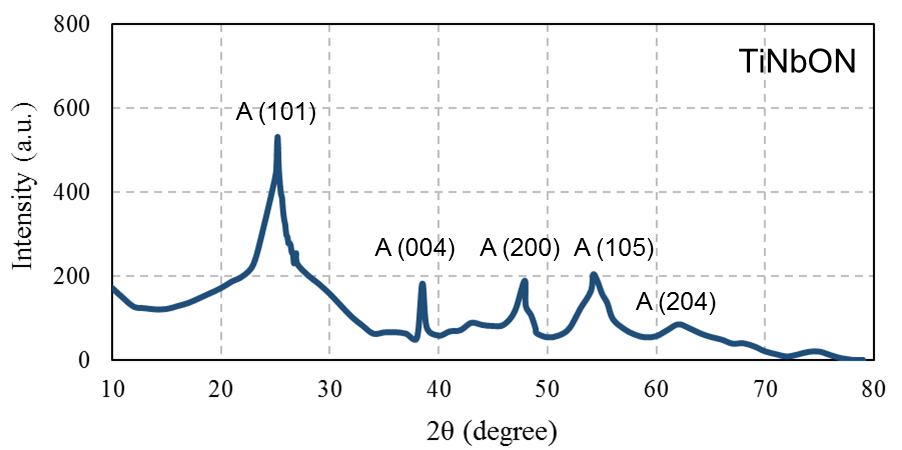
The adhesion strength of P25W, P25N, and P25NP on the aluminum pieces was carried out by peeling-off tests. The results indicate that P25W has poorest adhesions at two peeling speeds and P25NP has a slightly better bonding than P25N to the surfaces.



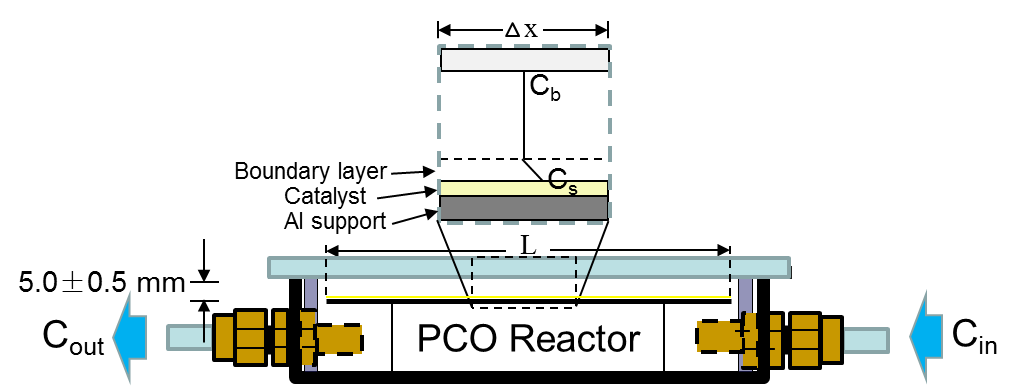
**Supplemental Figure S2**: Loss masses and loss percentages for three coatings at peeling-off speeds of 2.5 cm/s and 0.25 cm/s.



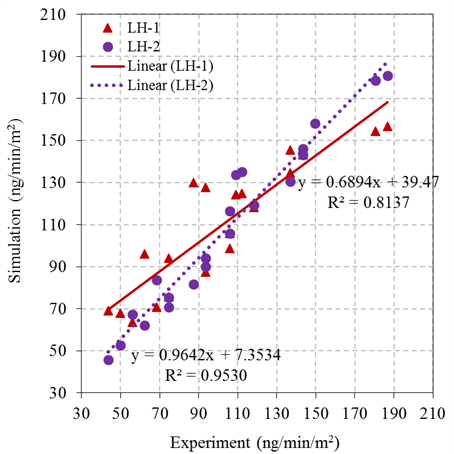
**Supplemental Figure S3**. Toluene concentrations at upstream and downstream and formaldehyde generation during adsorption and PCO of toluene (inlet toluene=3.8 mg/m3, 25%RH, I=95W/m2).



**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.