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Supporting Information

Selective Anthracene Photooxidation over Titania-supported Single Atom Catalysts

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Here we show other variations of the formula include multiplying by $(hv)^n$ where n is the corresponding electronic transition (see Figure S1). The parameter n corresponds to a direct allowed transition for n = ½. For n = 2, this corresponds to an indirect allowed transition. [1]

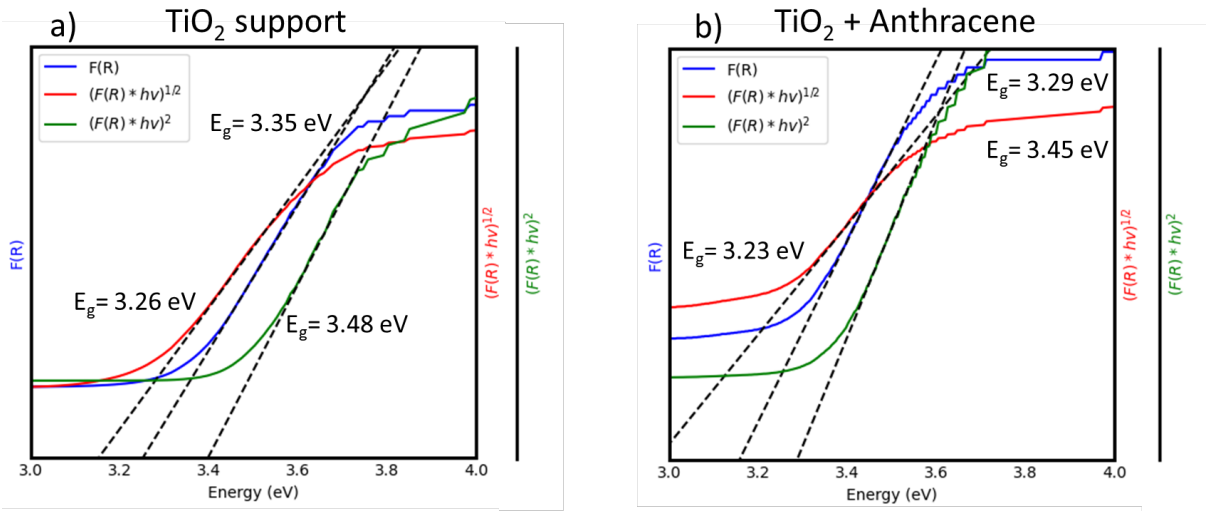

Figure S1 – Other fitting variations of the DRS results. The differences in the bandgap between the TiO_2 support and anthracene dried over the surface are highlighted.

We also recorded the photochemical conversions for different supports with different bandgaps as reference material. We see a unique behavior of anthracene oxidation possible on TiO_2, irrespective of the bandgap.

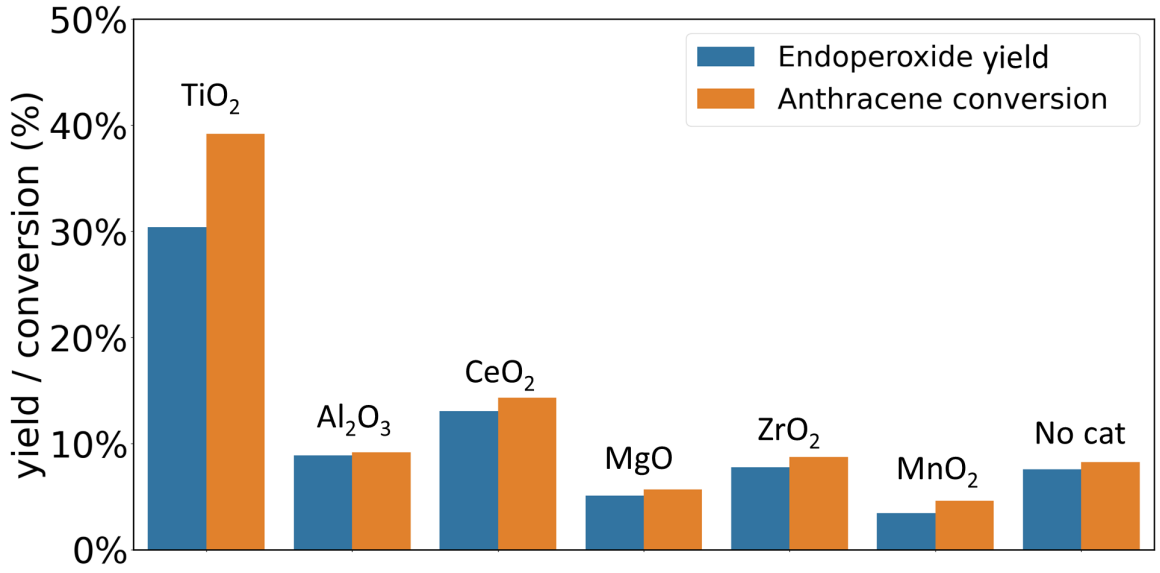

Figure S2 – Endoperoxide selectivity and anthracene conversion for different supports for a 30 min reaction. It shows that anthracene conversion is not limited to the metal oxide. Nevertheless, TiO_2 showed the highest conversion. Bandgap literature; TiO_2 = 3.0 eV [2], Al_2O_3 = 8.7 eV [2], CeO_2 = 3-4 e V[3], MgO = , ZrO_2 = 5.8 eV [4], MnO = 2.5 [5].

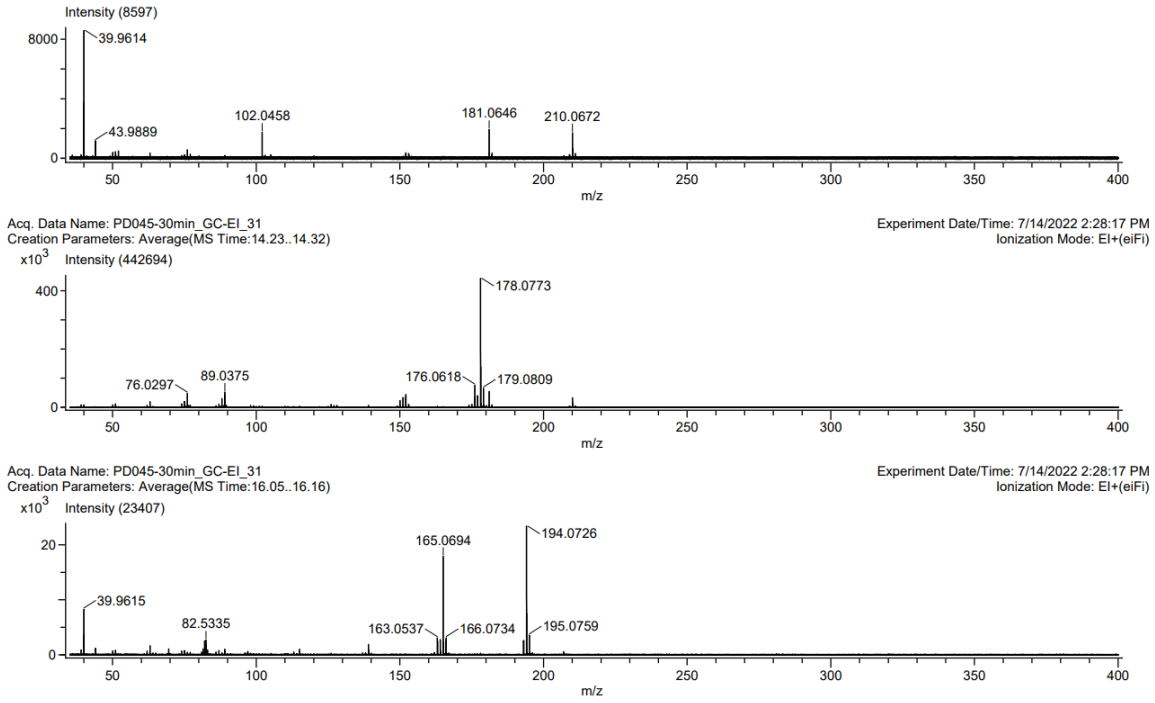

Figure S3 – GC-MS spectrum of the anthracene endoperoxide. 210.0672 matches the exact m/z ratio for EPO.

We also recorded anthracene conversions to quantify the role of oxygen from the TiO_2 support. We noticed that there was a small contribution (<10%) of the remaining oxygen from the TiO_2 support. This could be replenished with gaseous O_2 and would lead to a Mars van Krevelen type of mechanism for the SAC.

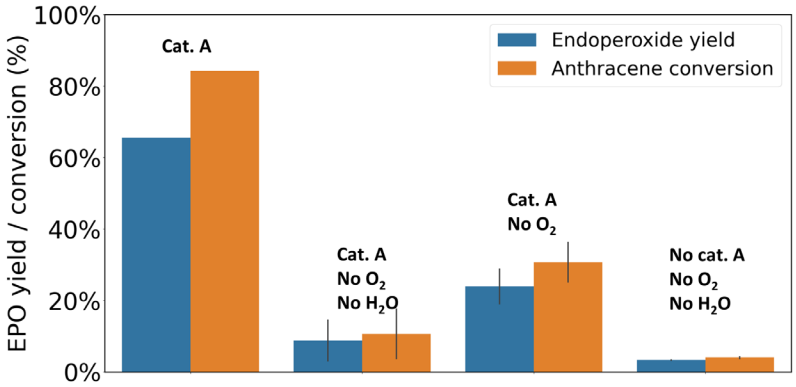

Figure S4 – Conversions when studying the relevance of oxygen. The total conversion decreased completely removing oxygen from the system (duplo measurements). There was a small increase of the conversion when adding a SAC compared to not adding a SAC. These were experiments of 30 minutes.

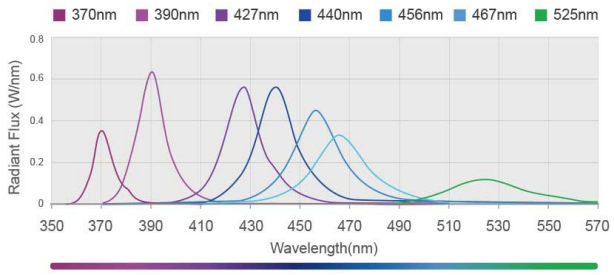

Figure S5 – Emission profile of the lamps available at https://kessil.com/products/science_PR160L.php. Observe the emission profile for the lamp that has a peak maximum of 456 nm.

References

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