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 $n = \frac{1}{2}$. For $n = 2$, this corresponds to an indirect allowed transition.\footnote{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\footnote{2}, Al$_2$O$_3$ = 8.7 eV\footnote{2}, CeO$_2$ = 3.4 eV\footnote{3}, MgO = , ZrO$_2$ = 5.8 eV\footnote{4}, MnO = 2.5\footnote{5}.}.
We also recorded anthracene conversions to quantify the role of oxygen from the TiO₂ support. We noticed that there was a small contribution (<10%) of the remaining oxygen from the TiO₂ support. This could be replenished with gaseous O₂ and would lead to a Mars van Krevelen type of mechanism for the SAC.
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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