Noble Metal-Free Deoxygenation of Epoxides: Titanium Dioxide as a Photocatalytically-Regenerable Electron-Transfer Catalyst

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SUPPORTING INFORMATION

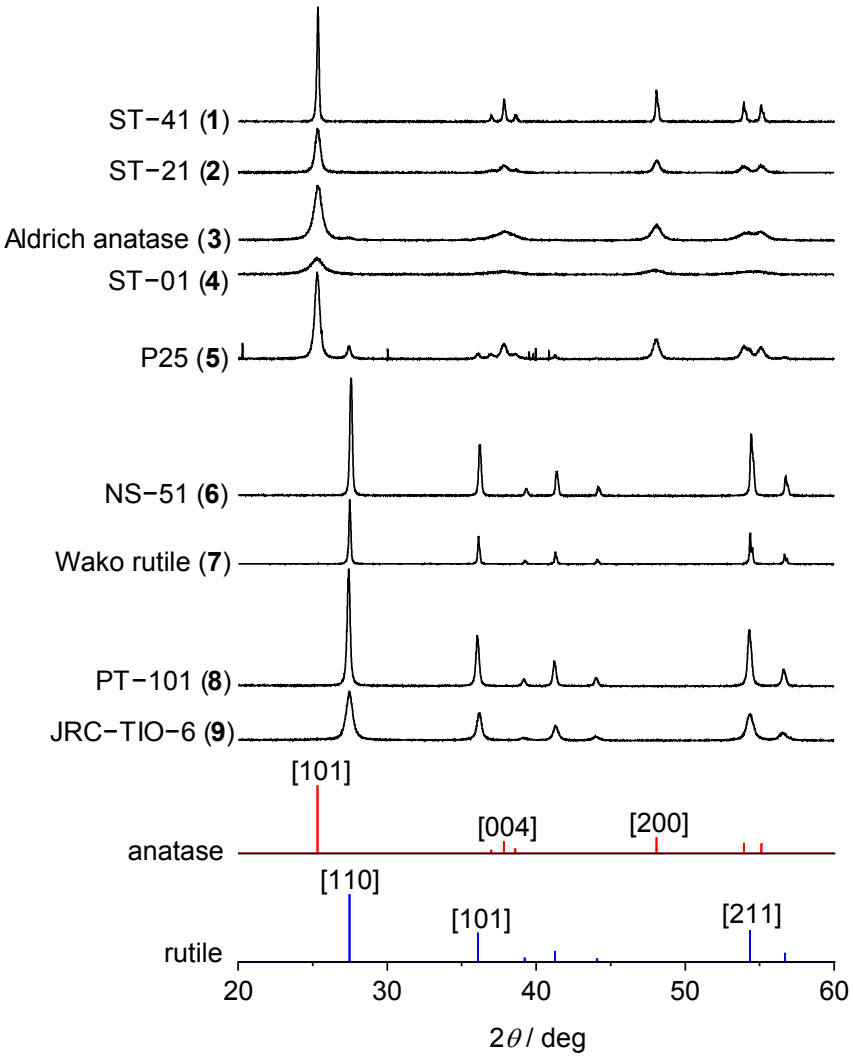


Figure S1. XRD patterns of respective TiO_2 particles and standard patterns for anatase (JCPDS 21-1272) and rutile (JCPDS 21-1276). The number in parenthesis denotes the sample number listed in Table 1 (manuscript).

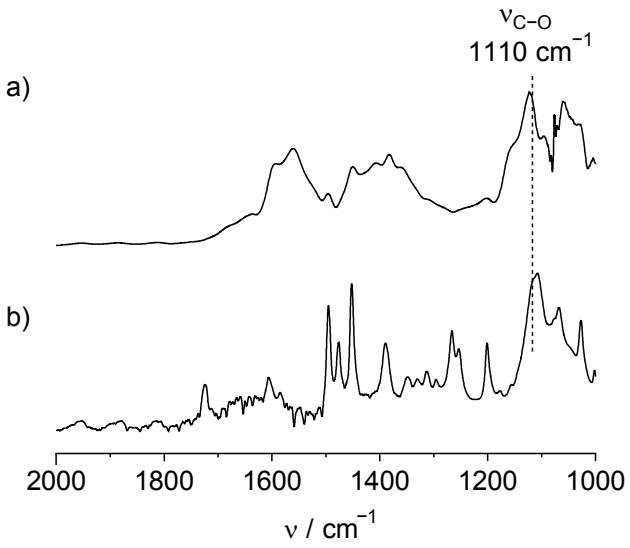


Figure S2. a) IR spectra of the nonvolatile product recovered after photoreaction (sample **4**). The solution obtained after photoreaction was concentrated by evaporation and subjected to analysis with KBr disk. b) IR (ATR) spectrum of poly(styrene oxide) synthesized by the iodine method (S. L. N. Seung, R. N. Young, *J. Polym. Sci. Polym. Lett. Ed.* **1980**, *18*, 89–96).

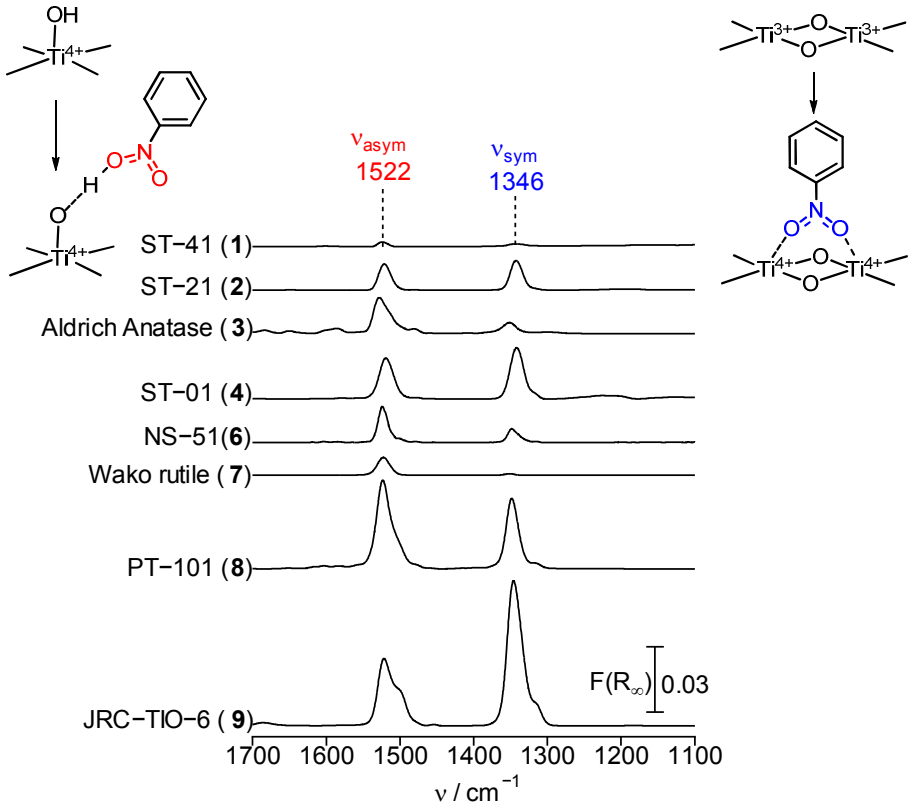


Figure S3. DRIFT spectra of nitrobenzene adsorbed onto the respective TiO_2 particles in the gas phase at 303 K. The spectra were measured as follows: respective TiO_2 (50 mg) were placed in a DR cell and evacuated (0.9 Pa) at 423 K for 3 h. Nitrobenzene (16.5 μ mol) was introduced to the cell at 303 K and left for 1 h. The cell was then evacuated (0.9 Pa) for 1 h to remove the physically adsorbed nitrobenzene.

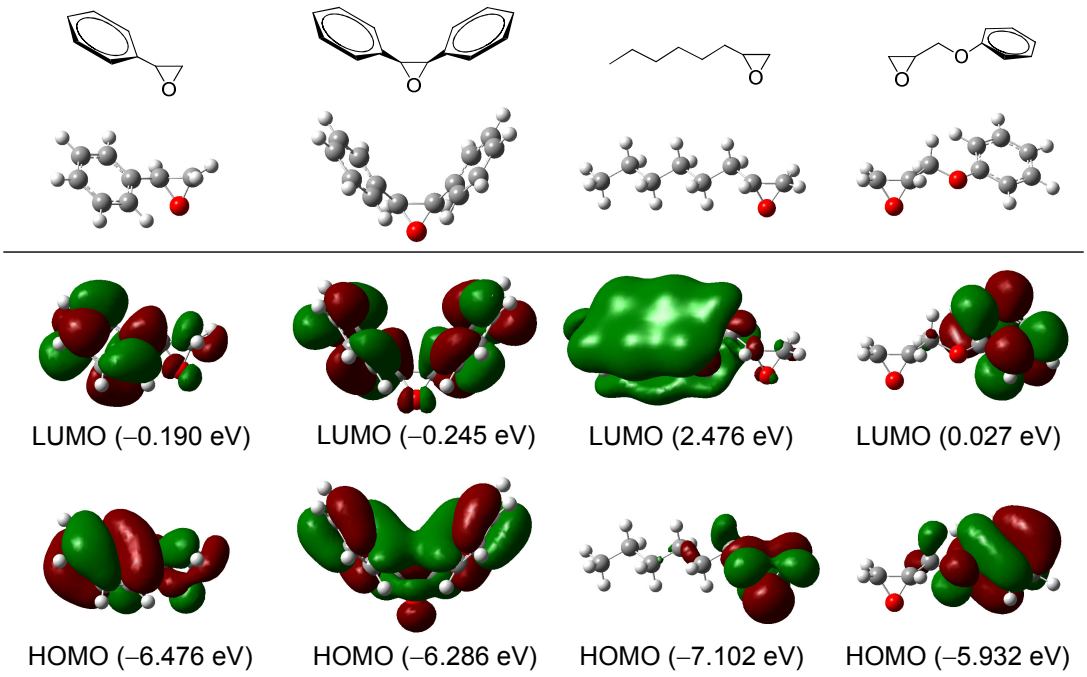


Figure S4. Optimized structures and interface plots of HOMO and LUMO for respective epoxides (B3LYP/6-31G (d)). Green and deep red parts on the molecular orbitals refer to the different phases of the molecular wave functions, where the isovalue is 0.02 au.

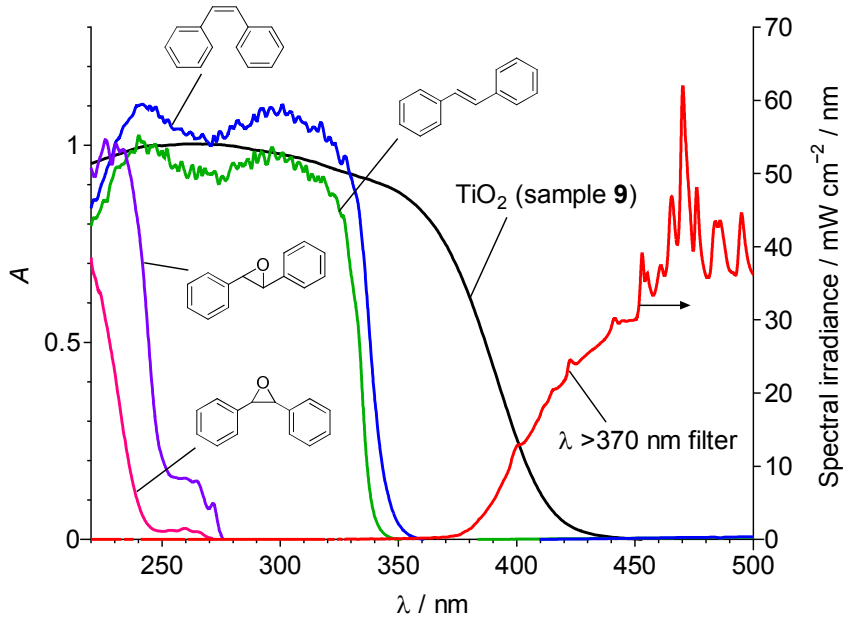
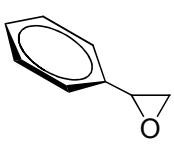
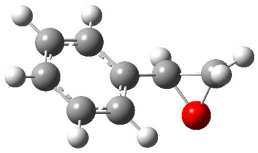


Figure S5. Absorption spectra of respective epoxides and TiO_2 (sample **9**), and light emission spectrum for Xe lamp with a cut-off filter (λ >370 nm).

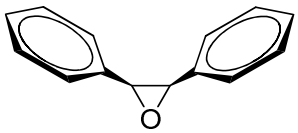
Cartesian Coordinates (in Å) of styrene oxide

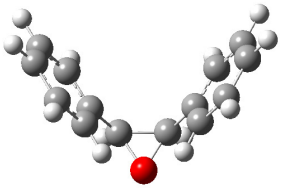




C	-1.665276	-1.339705	0.030443	H	-2.866141	1.842569	0.101044
C	-0.303203	-1.062537	-0.078755	H	-3.654143	-0.515425	0.184792
C	0.146563	0.263200	-0.116933	C	1.602561	0.578076	-0.205063
C	-0.788135	1.303874	-0.058328	H	1.840848	1.543023	-0.657268
C	-2.150573	1.025838	0.055132	C	2.590379	0.021084	0.742549
C	-2.592795	-0.297474	0.101446	H	3.501268	0.577174	0.968233
H	-2.004577	-2.372072	0.053492	H	2.245958	-0.656008	1.524474
H	0.422727	-1.866222	-0.157532	O	2.490550	-0.480442	-0.592357
H	-0.447468	2.336361	-0.101326				

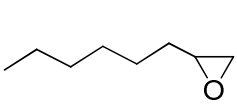
Cartesian Coordinates (in Å) of cis-stilbene oxide

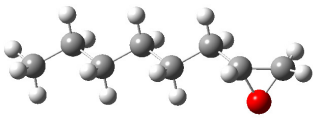




C	0.746532	1.855866	0.123431	C	-1.756474	-0.115377	-1.092467
C	-0.746550	1.855859	0.123413	C	-2.281147	0.236143	1.238411
C	1.597293	0.630551	0.080141	C	-2.573572	-1.246900	-1.101487
C	1.756641	-0.115261	-1.092470	H	-1.250015	0.207787	-1.995389
C	2.280973	0.236066	1.238514	C	-3.092659	-0.896868	1.230272
C	2.573750	-1.246775	-1.101467	H	-2.174169	0.819001	2.151017
H	1.250307	0.207973	-1.995439	C	-3.240050	-1.643351	0.058561
C	3.092497	-0.896936	1.230397	H	-2.692610	-1.816942	-2.019222
H	2.173856	0.818846	2.151154	H	-3.613056	-1.195075	2.136614
C	3.240065	-1.643318	0.058644	H	-3.875731	-2.524722	0.049826
H	2.692925	-1.816739	-2.019232	O	0.000003	2.220126	-1.042516
H	3.612764	-1.195217	2.136791	H	1.212196	2.708686	0.625077
H	3.875753	-2.524685	0.049926	H	-1.212241	2.708676	0.625036
C	-1.597301	0.630535	0.080103				

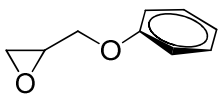
Cartesian Coordinates (in Å) of 1-epoxyoctane

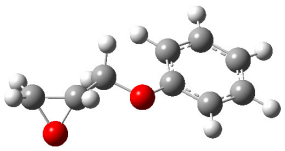




C	0.216901	-0.024683	-0.034744	C	-0.355119	5.067053	0.055654
H	0.112572	-0.104041	1.054462	H	0.709351	5.205356	-0.175713
H	1.288100	0.053581	-0.258262	H	-0.431103	5.035913	1.152779
H	-0.146799	-0.961132	-0.473008	C	-1.134602	6.280334	-0.472844
C	-0.551835	1.184148	-0.577870	H	-2.202823	6.171354	-0.233297
H	-0.459856	1.214853	-1.672945	H	-1.055807	6.324882	-1.567043
H	-1.623805	1.061526	-0.366736	C	-0.638124	7.585339	0.103957
C	-0.071613	2.518877	0.006577	H	-0.722019	7.677707	1.190537
H	0.999664	2.644718	-0.209714	C	-0.584960	8.828898	-0.677351
H	-0.157242	2.485766	1.103103	H	-0.653251	9.794384	-0.174497
C	-0.842257	3.733893	-0.525278	H	-0.918840	8.824783	-1.715865
H	-1.913264	3.609661	-0.304895	O	0.608333	8.080115	-0.413643
H	-0.759900	3.764642	-1.621938				

Cartesian Coordinates (in Å) of glycidyl phenyl ether





C	3.139996	-1.041330	-0.061005	O	-0.447139	-0.565019	0.203711
C	1.776860	-1.288125	0.053761	C	-1.420133	0.468996	0.271329
C	0.871250	-0.217577	0.087980	H	-1.410784	1.076446	-0.644146
C	1.342343	1.097566	0.004769	H	-1.216075	1.126424	1.130738
C	2.717410	1.328873	-0.109863	C	-2.766957	-0.181450	0.432281
C	3.621393	0.270212	-0.143169	H	-2.833920	-0.897012	1.253392
H	3.832483	-1.878668	-0.086838	C	-3.990692	0.496258	-0.017643
H	1.385796	-2.298814	0.117396	H	-3.925406	1.474053	-0.497023
H	0.659376	1.939222	0.025144	H	-4.934647	0.291774	0.487560
H	3.075297	2.353253	-0.174247	O	-3.436354	-0.590867	-0.764935
H	4.686993	0.459880	-0.232832				