

Supporting Information

Nano TiO₂ and Molybdenum/Tungsten Iodide Octahedral Clusters: Synergism in UV/Visible-Light Driven Degradation of Organic Pollutants

Margarita V. Marchuk ¹, Igor P. Asanov ¹, Maxim A. Panafidin ², Yuri A. Vorotnikov ^{1,*}
and Michael A. Shestopalov ¹

¹ Nikolaev Institute of Inorganic Chemistry SB RAS, 3 Academician Lavrentiev Avenue,
630090 Novosibirsk, Russia

² Boreskov Institute of Catalysis SB RAS, 5 Academician Lavrentiev Avenue, 630090
Novosibirsk, Russia

* Correspondence: vorotnikov@niic.nsc.ru.

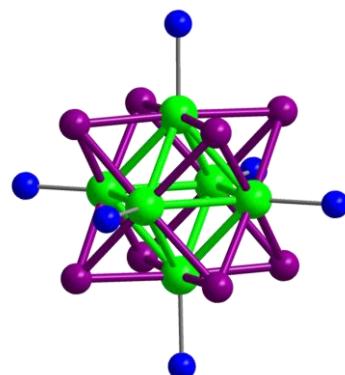


Figure S1. Representative structure of $\{[M_6I_8]_n\}$ ($M = Mo$ or W ; green octahedron is M_6 , violet spheres are inner iodine ligands, blue spheres are apical ligands (L) of any nature, n – charge) units.

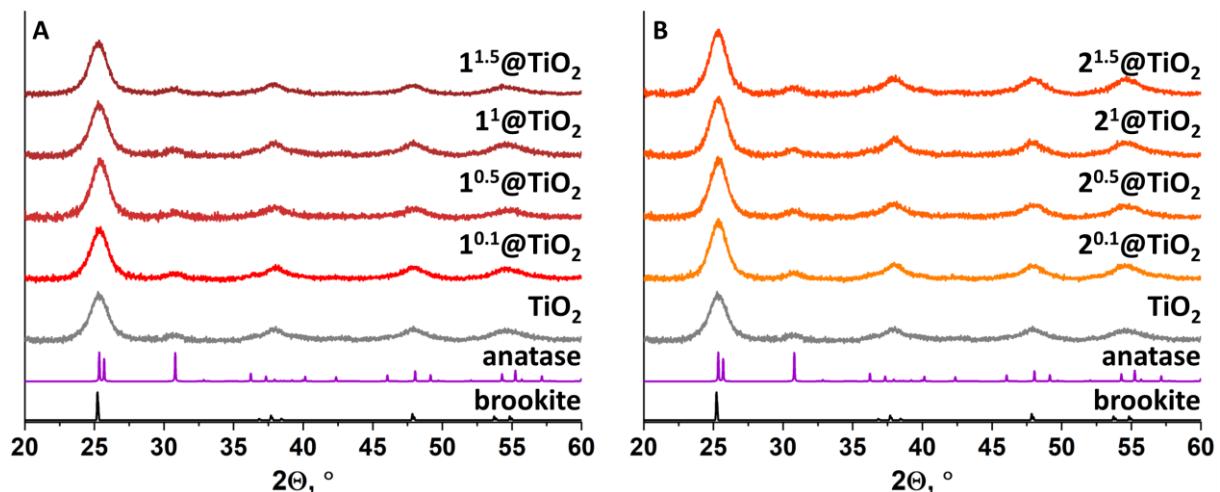


Figure S2. XRD patterns of $n^x@TiO_2$, $n = 1$ (A) or 2 (B) in comparison with pure TiO_2 and calculated anatase and brookite diffractograms.

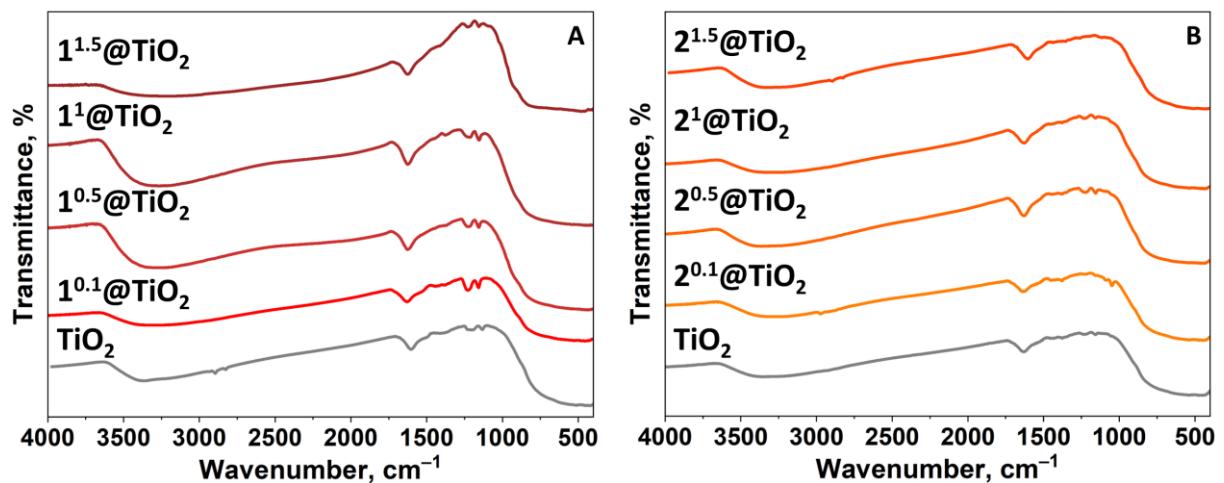


Figure S3. FTIR spectra of pure TiO_2 and $n^\times@\text{TiO}_2$, $n = 1$ (A) or 2 (B).

Table S1. Determination of the amount of $\{\text{M}_6\text{I}_8\}$ units anchored on TiO_2 using ICP-AES.

Material	n	M content, w%	$\{\text{M}_6\text{I}_8\}$ content, mmole($\{\text{M}_6\text{I}_8\}$) g(TiO_2) $^{-1}$
$1^n@\text{TiO}_2$	0.1	0.16 % wt.	0.0031
	0.5	0.27 % wt.	0.0046
	1	0.26 % wt.	0.0044
	1.5	0.29 % wt.	0.0050
$2^n@\text{TiO}_2$	0.1	1.3 % wt.	0.012
	0.5	3.2 % wt.	0.03
	1	5.2 % wt.	0.05
	1.5	8.0 % wt.	0.079

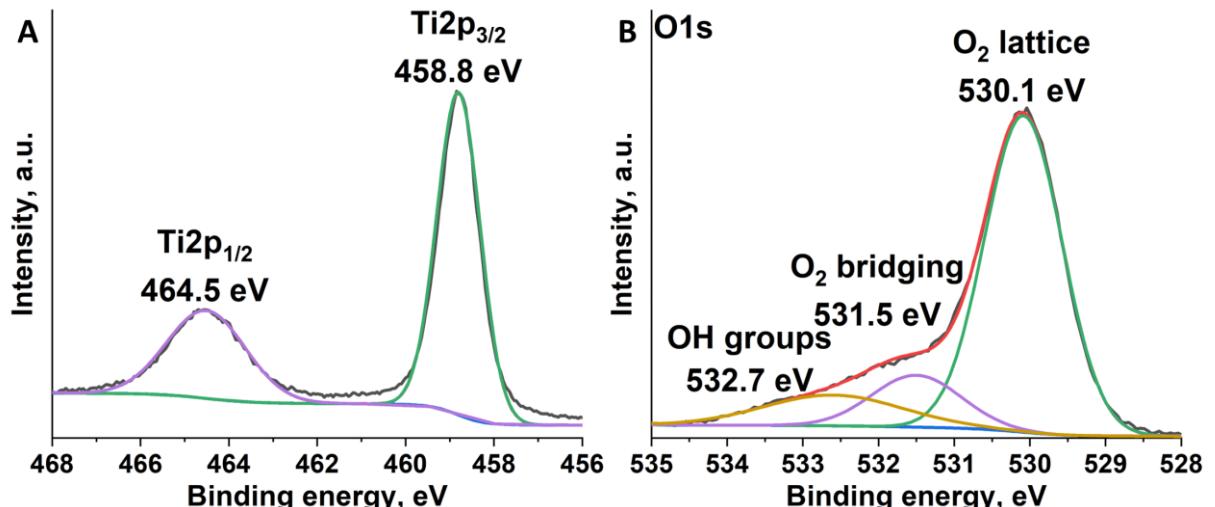


Figure S4. High-resolution XPS spectra of $\text{Ti}2\text{p}$ (A) and $\text{O}1\text{s}$ (B) core levels in $2^{0.1}@\text{TiO}_2$.

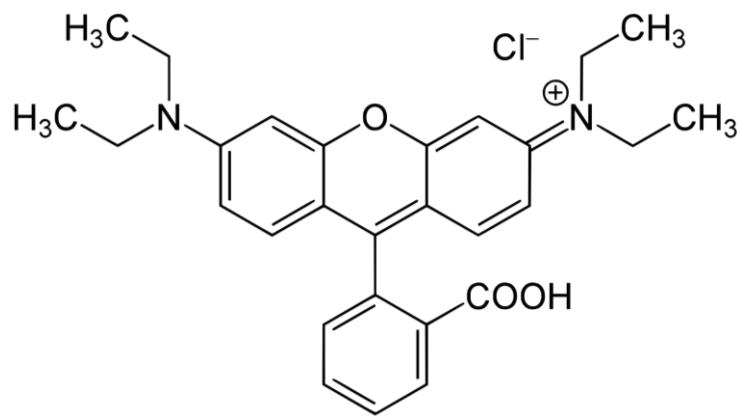


Figure S5. Structure of RhB molecule.

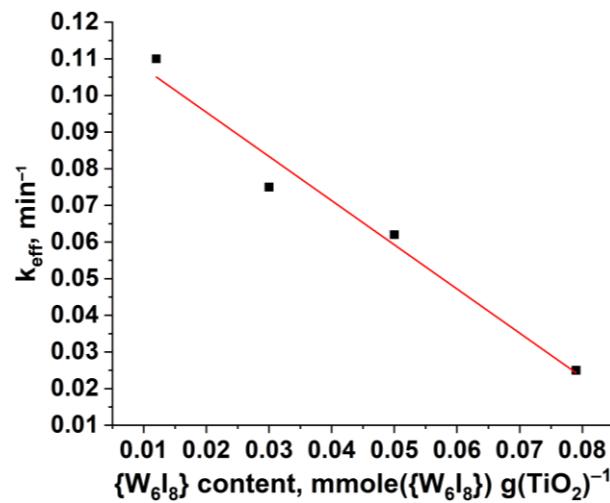


Figure S6. The dependency of k_{eff} of $2^x@\text{TiO}_2$ on real content of $\{\text{W}_6\text{I}_8\}$ determined using ICP-AES.

Table S2. Effective rate constants (k_{eff}) and R^2 values of RhB decomposition by $n^x@\text{TiO}_2$ in the presence of different scavengers.

Scavenger	$1^x@\text{TiO}_2$			$2^x@\text{TiO}_2$		
	$k_{\text{eff}}, \text{min}^{-1}$	R^2	RA [#] , %	$k_{\text{eff}}, \text{min}^{-1}$	R^2	RA [#] , %
No scavengers	0.099	0.99019	100	0.11	0.97244	100
iPrOH	0.088	0.99728	89	0.096	0.98827	87
AgNO ₃	0.019	0.99198	19	0.036	0.97546	33
Na ₂ C ₂ O ₄	0.028	0.9793	28	0.047	0.99003	43
Ar	0.015	0.97798	15	0.01	0.97153	9

[#]Relative activity (RA) was calculated according to the following formula: $RA = \frac{k_{\text{eff}}(\text{scav})}{k_{\text{eff}}(\text{NS})} \times 100\%$, where $k_{\text{eff}}(\text{scav})$ is effective rate constant in the presence of a certain scavenger, $k_{\text{eff}}(\text{NS})$ is effective rate constant in scavenger free experiment.