Supporting Information for

Molecular-level Insights on the Facet-dependent Degradation of Perfluorooctanoic Acid

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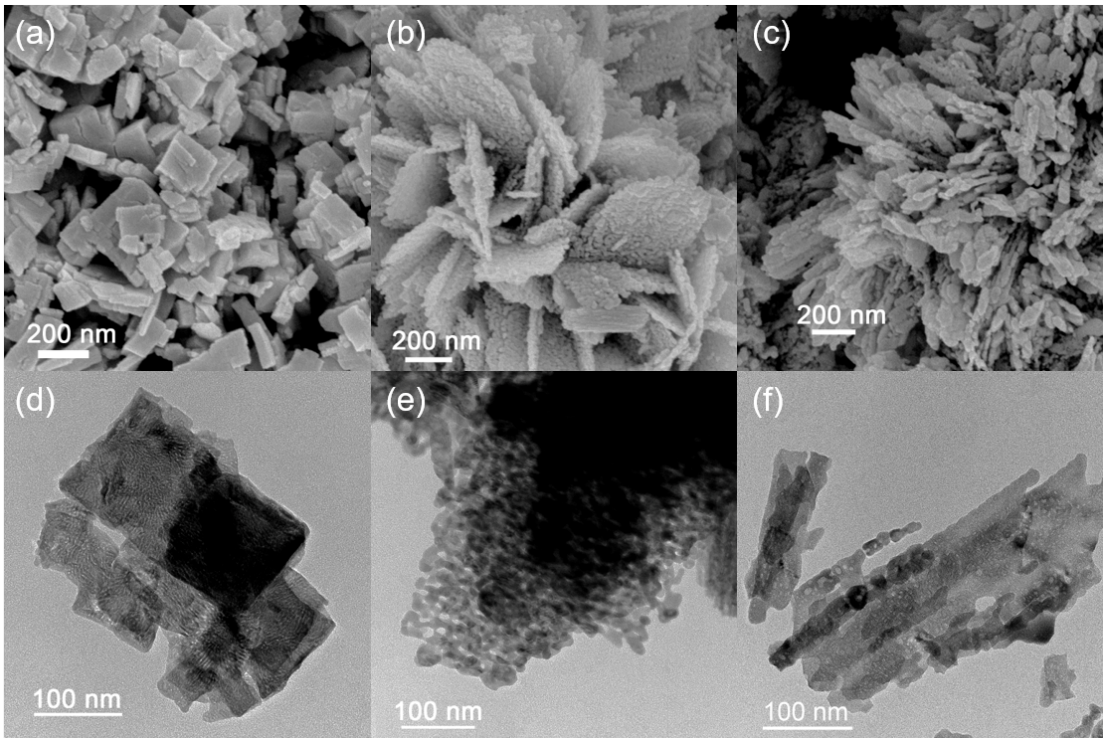

Figure S1 TEM (a-c) and SEM (d-f) images of catalysts, (a), (d): In_2O_3-P, (b), (e): In_2O_3-L, (c), (f): In_2O_3-R

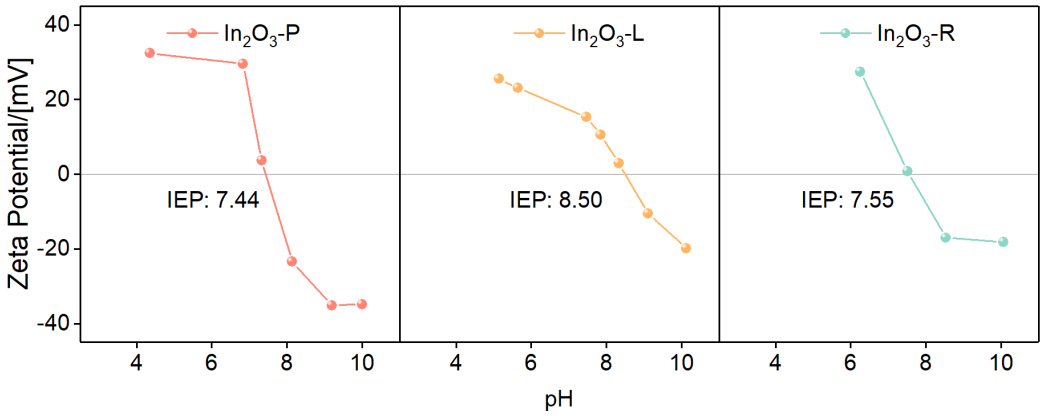

Figure S2 pH-dependent zeta potential of catalysts, the isoelectric points (IEP) were pointed out in images.

Table S1 Synthesis recipe for In_2O_3

Catalysts	$In(NO_3)_3$ solution			Urea solution		
	$In(NO_3)_3 \cdot 4, 5H_2O$ (g)	DI water (mL)	Ethanol (mL)	Urea (g)	DI water (mL)	Ethanol (mL)
In2O3-P	4.07	32	0	4	20	0
In2O3-L	4.07	5	32	4	5	20
In2O3-R	4.07	12	20	4	5	20

Table S2 Optimized structure parameters of In_2O_3 unit cells

Phase	a [Å]	b [Å]	c [Å]	α [degrees]	β [degrees]	γ [degrees]	Number of Indium	Number of Oxygen
$Ia\bar{3}$	10.30	10.30	10.30	90	90	90	32	48
$R\bar{3}c$	5.58	5.58	14.75	90	90	120	12	18

Table S3 Structure parameters of In_2O_3 surface slabs for adsorption energy calculation

Phase	Facet	a [Å]	b [Å]	Thickness [Å]	Surface area [Å^2]	Number of Indium	Number of Oxygen
$Ia\bar{3}$	{111}	14.57	14.57	8.92	123.17	48	72
	{110}	20.60	14.57	15.21	268.22	144	216
$R\bar{3}c$	{012}	16.75	17.64	12.13	264.05	108	162
	{110}	14.75	19.34	8.37	254.98	72	108

Table S4 BET-surface area and pore volume of In_2O_3 catalysts

Catalysts	$a_{s,BET}$/[m^2g^{-1}]	Pore volume/[cm^3/g]
In_2O_3-P	61.536	0.1946
In_2O_3-L	60.265	0.2657
In2O3-R	49.599	0.2248

Table S5 Energy band properties of In_2O_3 surface slabs

Phase	Facet	E_{VBM} [vs. vacuum eV]	E_{CBM} [vs. vacuum eV]	Work function [eV]	Bandgap [eV]
$Ia\bar{3}$	{111}	-6.02	-5.62	5.81	0.41
	{110}	-5.38	-4.88	5.12	0.50
$R\bar{3}c$	{012}	-6.11	-5.15	5.80	0.95
	{110}	-6.50	-5.87	6.20	0.63

Table S6 Bond length of C-O in adsorbed PFOA and In-O formed by adsorption

Phase	Facet	C-O bond length [Å]	Averaged C-O bond length [Å]	In-O bond length [Å]	Averaged In-O bond length [Å]
$Ia\bar{3}$	{111}	1.258/1.259	1.259	2.244/2.382	2.313
	{110}	1.247/1.265	1.256	2.281/2.325	2.303
$R\bar{3}c$	{012}	1.253/1.267	1.260	2.192/2.313	2.253
	{110}	1.251/1.259	1.255	2.211/2.342	2.277

Table S7 Charge transferred to atoms of PFOA through four exposed facets.

Phase	Facet	O in -COO^- [e/molecule]	C in -COO^- [e/molecule]	-COO^- [e/molecule]	PFOA [e/molecule]
$Ia\bar{3}$	{111}	0.50	-0.03	0.48	0.60
	{110}	0.35	0.11	0.46	0.67
$R\bar{3}c$	{012}	0.44	-0.05	0.39	0.60
	{110}	0.48	-0.02	0.46	0.59

Table S8 Adsorption energy calculation results

Phase	Facet	ΔE_{ad} [eV]
$Ia\bar{3}$	{111}	-4.52
	{110}	-1.15
$R\bar{3}c$	{012}	-2.35
	{110}	-4.95

Table S9 Surface energy of In_2O_3 surface slabs

Phase	Facet	Surface cleavage energy [J/m^2]	Surface reconstruction energy [J/m^2]	γ_s [J/m^2]
$Ia\bar{3}$	{111}	1.592	-0.396	1.20
	{110}	1.377	-0.144	1.23
$R\bar{3}c$	{012}	1.425	-0.230	1.19
	{110}	1.645	-0.258	1.39

Table S10 First-order reaction rate constants of defluorination and PFOA degradation processes

Catalysts	Defluorination rate constant [h^{-1}]	R^2 (defluorination)	PFOA degradation rate constant [h^{-1}]	R^2 (degradation)
In_2O_3-P	0.35	0.995	3.43	0.988
In_2O_3-L	0.34	0.992	3.38	0.970
In_2O_3-R	0.23	0.975	2.49	0.979

Table S11 Energy change in the first step of PFOA degradation

Phase	Facet	$E(C_8F_{15}O_2H^*)$ [eV]	$E(CO_2+\cdot C_7F_{15})$ [eV]	$E(H^{+*})$ [eV]	E_{VBM} [vs. vacuum eV]	ΔE [eV]
$Ia\bar{3}$	{111}	-151.45	-143.81	-3.99	-6.02	-0.21
	{110}	-154.05	-143.81	-3.00	-5.38	-1.94
$R\bar{3}c$	{012}	-153.62	-143.81	-2.55	-6.11	-1.02
	{110}	-150.25	-143.81	-4.71	-6.50	-0.98

$C_8F_{15}O_2H^*$ and H^{+*}refer to adsorbed $C_8F_{15}O_2H$ and adsorbed H^+, respectively.