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APPENDICES

Appendix A. Calculation of Crystallite Size of TiO_2 Catalysts and Reaction Pathway.

A.1 Calculation of crystallite sizes

The crystallite sizes of TiO_2 were determined from the broadening of the anatase and rutile main peak by Debye-Scherrer equation:

$$d = k\lambda/b\cos\theta \qquad (3.1)$$

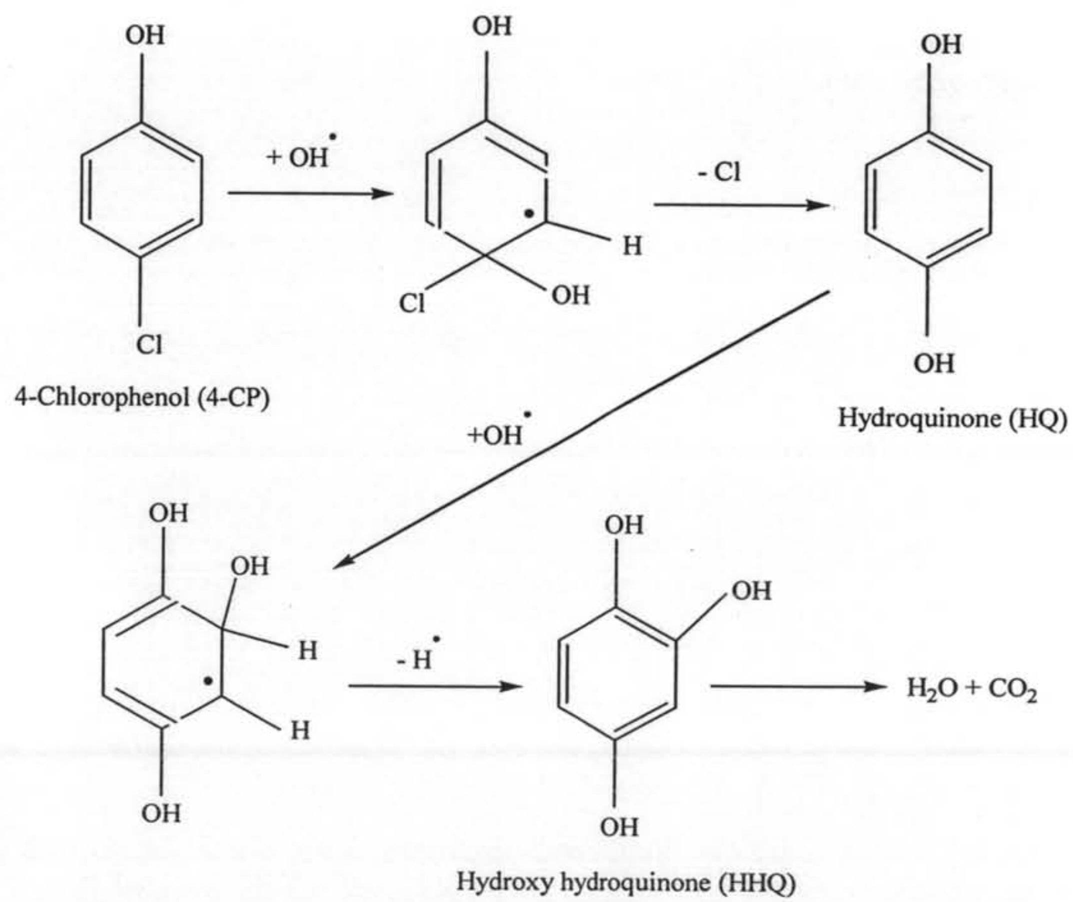
Anatase phase

Catalyst	FWHM	b	2θ (deg)	cosθ	d (nm)
TiO_2 (Degussa P25)	0.353	0.0062	25.26	0.976	25.62
TiO_2 (TTIP, 500°C)	0.329	0.0057	25.30	0.976	32.08
TiO_2 (TBT, 500°C)	0.329	0.0057	25.28	0.976	27.50
TiO_2 (TEOT, 500°C)	0.329	0.0057	25.32	0.976	27.50
TiO_2 (TTIP, 600°C)	0.329	0.0057	25.34	0.976	32.08
TiO_2 (TBT, 600°C)	0.306	0.0053	25.28	0.997	28.92
TiO_2 (TEOT, 600°C)	0.329	0.0057	25.34	0.995	26.97
TiO_2 (TTIP, 700°C)	0.235	0.0041	25.28	0.997	37.66
TiO_2 (TBT, 700°C)	0.235	0.0041	25.32	0.996	37.73
TiO_2 (TEOT, 700°C)	0.235	0.0041	25.30	0.996	37.69
1%Ag/TiO_2	0.282	0.0049	25.36	0.994	31.50
2%Ag/TiO_2	0.282	0.0049	25.38	0.992	31.54
3%Ag/TiO_2	0.282	0.0049	25.36	0.994	31.50
4%Ag/TiO_2	0.306	0.0053	25.48	0.985	29.28

Rutile phase

Catalyst	FWHM	b	2θ (deg)	cosθ	d (nm)
TiO_2 (Degussa P25)	0.282	0.0049	27.40	0.972	32.22
TiO_2 (TTIP, 500°C)	-	-	-	-	-
TiO_2 (TBT, 500°C)	-	-	-	-	-
TiO_2 (TEOT, 500°C)	-	-	-	-	-
TiO_2 (TTIP, 600°C)	-	-	-	-	-
TiO_2 (TBT, 600°C)	-	-	-	-	-
TiO_2 (TEOT, 600°C)	0.118	0.0021	27.42	0.972	76.95
TiO_2 (TTIP, 700°C)	0.165	0.0029	27.42	0.972	55.04
TiO_2 (TBT, 700°C)	0.165	0.0029	27.44	0.971	55.04
TiO_2 (TEOT, 700°C)	0.165	0.0029	27.42	0.971	55.04
1%Ag/TiO_2	0.118	0.0021	27.36	0.972	76.94
2%Ag/TiO_2	0.172	0.0030	27.33	0.972	52.83
3%Ag/TiO_2	0.141	0.0025	27.46	0.971	64.44
4%Ag/TiO_2	0.141	0.0025	27.46	0.971	64.44

A.2 Reaction pathway for the photocatalytic degradation of 4-CP



Appendix B. Experimental Data from Photocatalytic Degradation of 4-CP in Batch System.

B.1 Photocatalytic degradation of 4-CP using visible light without TiO_2

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.39	-	-	1.00	1.00
20	0.38	-	-	0.99	1.00
40	0.41	-	-	1.04	1.00
60	0.46	-	-	1.17	0.99
120	0.46	-	-	1.17	0.99
180	0.36	-	-	0.93	1.00
240	0.41	-	-	1.04	1.00
300	0.45	-	-	1.16	1.00
360	0.0.42	-	-	1.08	0.99

B.2 Photocatalytic degradation of 4-CP using UV light without TiO_2

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.31	-	-	1.00	1.00
20	0.08	-	-	0.27	0.94
40	0.02	-	-	0.06	0.89
60	0	-	-	0	0.84
120	0	-	-	0	0.80
180	0	-	-	0	0.72
240	0	-	-	0	-
300	0	-	-	0	0.66
360	0	-	-	0	0.55

B.3 Photocatalytic degradation of 4-CP using UV light with TiO_2 (Degussa P25)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.55	0	0	1.00	1.00
20	0.30	0.09	0.04	0.55	0.97
40	0.07	0.08	0.10	0.12	0.89
60	0.02	0.05	0.15	0.04	0.79
120	0	0.04	0.02	0	0.57
180	0	0	0.003	0	0.24
240	0	0	0.0009	0	0.08
300	0	0	0	0	0.03
360	0	0	0	0	0.03

B.4 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TTIP, 500°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.40	0	0	1.00	1.00
20	0.18	0.09	0.02	0.44	-
40	0.06	0.12	0.15	0.14	0.93
60	0	0.11	0.11	0	-
120	0	0.07	0.09	0	0.75
180	0	0.02	0.08	0	0.57
240	0	0	0.05	0	-
300	0	0	0.02	0	0.29
360	0	0	0.007	0	0.22

B.5 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TBT, 500°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.48	0	0	1.00	1.00
20	0.21	0.16	0.04	0.43	-
40	0.03	0.13	0.11	0.07	0.96
60	0	0.09	0.05	0	0.80
120	0	0.05	0.03	0	0.68
180	0	0	0.02	0	0.59
240	0	0	0.01	0	0.33
300	0	0	0.009	0	0.17
360	0		0.004	0	0.11

B.6 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TEOT, 500°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.41	0	0	1.00	1.00
20	0.15	0.14	0.02	0.37	0.95
40	0.05	0.16	0.02	0.12	0.84
60	0	0.11	0.07	0	0.82
120	0	0.02	0.05	0	-
180	0	0	0.03	0	0.55
240	0	0	0.005	0	0.34
300	0	0	0.002	0	0.19
360	0	0	0.001	0	0.12

B.7 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TTIP, 600°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.39	0	0	1.00	1.00
20	0.23	0.11	0.07	0.58	-
40	0.05	0.00	0.14	0.12	0.91
60	0.02	0.15	0.19	0.06	0.82
120	0	0.07	0.09	0	0.66
180	0	0.04	0.04	0	0.41
240	0	0	0.02	0	-
300	0	0	0.01	0	0.20
360	0	0	0.006	0	0.11

B.8 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TBT, 600°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.44	0	0	1.00	1.00
20	0.17	0.09	0.03	0.38	-
40	0.06	0.12	0.13	0.15	0.83
60	0	0.09	0.09	0	-
120	0	0.03	0.09	0	0.65
180	0	0	0.07	0	0.50
240	0	0	0.02	0	0.37
300	0	0	0.01	0	0.27
360	0	0	0.008	0	0.23

B.9 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TEOT, 600°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.49	0	0	1.00	1.00
20	0.16	0.09	0.05	0.32	-
40	0.05	0.11	0.13	0.10	0.87
60	0.02	0.11	0.09	0.04	-
120	0	0.03	0.12	0	0.67
180	0	0	0.05	0	0.49
240	0	0	0.02	0	0.38
300	0	0	0.01	0	0.25
360	0	0	0.008	0	0.15

B.10 Photo catalytic degradation of 4-CP using UV light with TiO_2 (TTIP, 700°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.49	0	0	1.00	1.00
20	0.23	0.15	0.05	0.47	-
40	0.05	0.16	0.14	0.10	0.96
60	0.02	0.15	0.15	0.04	-
120	0	0.08	0.21	0	0.82
180	0	0.03	0.15	0	0.76
240	0	0.02	0.09	0	-
300	0	0	0.06	0	0.56
360	0	0	0.03	0	0.46

B.11 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TBT, 700°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.42	0	0	1.00	1.00
20	0.20	0.12	0.07	0.49	-
40	0.04	0.12	0.16	0.09	0.95
60	0	0.07	0.09	0	-
120	0	0.04	0.08	0	0.82
180	0	0	0.02	0	0.67
240	0	0	0.01	0	-
300	0	0	0.006	0	0.46
360	0	0	0.005	0	0.33

B.12 Photocatalytic degradation of 4-CP using UV light with TiO_2 (TEOT, 700°C)

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.41	0	0	1.00	1.00
20	0.15	0.11	0.10	0.38	-
40	0.03	0.09	0.15	0.07	0.95
60	0	0.08	0.14	0	0.91
120	0	0.07	0.11	0	-
180	0	0	0.08	0	0.65
240	0	0	0.03	0	0.49
300	0	0	0.01	0	-
360	0	0	0.003	0	0.29

B.13 Photocatalytic degradation of 4-CP using UV light with 1%Ag/TiO_2

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.45	0	0	1.00	1.00
20	0.15	0.13	0.05	0.34	-
40	0	0.05	0.14	0	0.98
60	0	0.02	0.13	0	0.68
120	0	0	0.05	0	0.47
180	0	0	0.02	0	-
240	0	0	0.006	0	0.11
300	0	0	0.002	0	-
360	0	0	0.002	0	0.06

B.14 Photocatalytic degradation of 4-CP using UV light with 2%Ag/TiO_2

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.41	0	0	1.00	1.00
20	0.11	0.13	0.01	0.28	-
40	0	0.16	0.03	0	0.76
60	0	0.06	0.02	0	-
120	0	0.02	0.01	0	0.47
180	0	0	0.004	0	0.27
240	0	0	0.003	0	-
300	0	0	0.002	0	0.08
360	0	0	0.001	0	0.05

B.15 Photocatalytic degradation of 4-CP using UV light with 3%Ag/TiO_2

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.44	0	0	1.00	1.00
20	0.16	0.10	0.004	0.36	-
40	0.01	0.06	0.04	0.04	0.81
60	0	0.05	0.02	0	0.73
120	0	0.04	0.008	0	-
180	0	0	0.007	0	0.30
240	0	0	0.001	0	0.12
300	0	0	0.001	0	0.07
360	0	0	0.0007	0	0.04

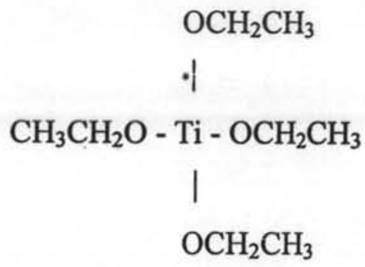
B.16 Photocatalytic degradation of 4-CP using UV light with 4%Ag/TiO_2

Time (min)	Concentration (mM)			Remaining fraction	
	4-CP	HQ	HHQ	4-CP	TOC
0	0.41	0	0	1.00	1.00
20	0.17	0.14	0.03	0.44	-
40	0.02	0.13	0.07	0.06	0.87
60	0	0.09	0.08	0	-
120	0	0	0.05	0	0.59
180	0	0	0.01	0	0.29
240	0	0	0.003	0	0.10
300	0	0	0.003	0	0.06
360	0	0	0.002	0	0.05

Appendix C. Molecular Structure of Ti-alkoxides.

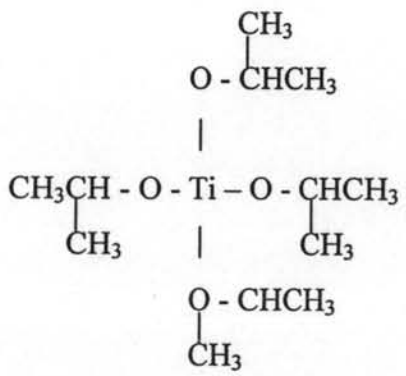
C.1 Molecular structure of titanium ethoxide (TEOT, MW 228.1)

Ti $(OC_2H_5)_4$



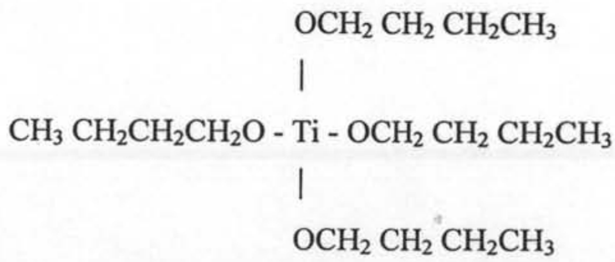
C.2 Molecular structure of titanium tetraisopropoxide (TTIP, MW 284.2)

Ti $(OCH(CH_3)_2)_4$



C.3 Molecular structure of titanium butoxide (TBT, MW 340.3)

Ti $(OCH(CH_3)_2)_4$



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