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APPENDICES

Appendix A Calculations of Ti:Si Molar Ratio

Table A1 X-Ray Fluorescence analysis of CTAB modified Na-bentonite

Analyte	Compound	Concentration (%)
Mg	MgO	1.675
Al	Al_2O_3	16.41
Si	SiO_2	78.48
K	K_2O	0.549
Ca	CaO	0.111
Ti	TiO_2	0.307
Mn	MnO_2	0.034
Fe	Fe_2O_3	2.403
Zn	ZnO	0.03

%LOI = 30%

Factor = 0.702

M.W. of SiO_2 = 60.09

1 g of CTAB modified Na-bentonite

= 0.702 g of Na-bentonite

= 0.702 g of Na-bentonite×0.7848 g of SiO_2

= 0.551 g of SiO_2

And 1 g of Na-bentonite

= 0.7848 g of SiO_2

P25/CTAB modified Na-bentonite

15 mole%Si

1 g basis of mixture

Assume P25 has 100%TiO_2

M.W. TiO_2 = 79.87

85 mole Ti: 15 mole Si

Assume X is TiO_2 weight, and then 1-X is CTAB modified bentonite weight.

$$\frac{Ti}{Si} = \frac{85 \text{ mole Ti}}{15 \text{ mole Si}} = \frac{X/79.87 \text{ mole Ti}}{(1-X) \times 0.5509/60.09 \text{ mole Si}}$$

X = 0.81 g P25

Thus, CTAB modified Na-bentonite = 0.19 g

P25/purified Na-bentonite

10 mole%Si

1 g basis of mixture

90 mole Ti: 10 mole Si

Assume X is TiO_2 weight, and then 1-X is CTAB modified bentonite weight.

$$\frac{Ti}{Si} = \frac{90 \text{ mole Ti}}{10 \text{ mole Si}} = \frac{X/79.87 \text{ mole Ti}}{(1-X) \times 0.7848/60.09 \text{ mole Si}}$$

X = 0.90 g P25

Thus, purified Na-bentonite = 0.10g

Sol-gel TiO_2/purified Na-bentonite

10 mole%Si

M.W. of $Ti(acac)_2OiPr_2$ = 364.27

M.W. of TiO_2 = 79.87

$Ti(acac)_2OiPr_2$ in ispropanol solution= 75 wt.%

Starting with 2.5 g $Ti(acac)_2OiPr_2$ = 2.5 g×0.75/364.27 = 5.15×10^{-3} mol Ti

Assume X = SiO_2 weight

$$\text{Thus, } 0.10 \text{ mole Si} = \frac{X/60.09 \text{ mole Si}}{5.15\times10^{-3} \text{ mole Ti} + X/60.09 \text{ mole Si}}$$

$X = 0.034$ g SiO_2

Thus, purified Na-bentonite = 0.034 g SiO_2/0.7848 = 0.044 g

And TiO_2 weight = 5.15×10^{-3} mol Ti×79.87 = 0.41 g

Appendix B Supplementary Results of Chapter IV

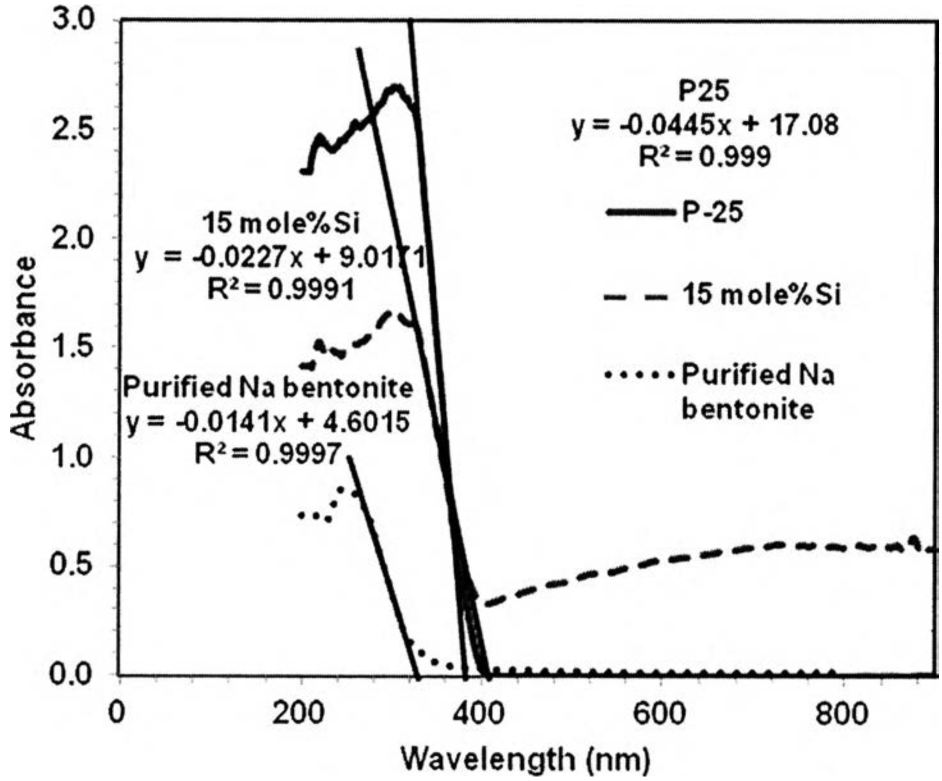


Figure B1 The energy band gap (Eg) of P25 and 15 mole%Si.

Eg = 1239.8/λ

λ of P25 = 388 nm

Eg of P25 = 3.20 eV

λ of 15 mole%Si = 409.7 nm

Eg of 15 mole%Si = 3.02 eV

λ of purified Na bentonite = 326.4 nm

Eg of purified Na bentonite = 3.80 eV

Appendix C Supplementary Results of Chapter V

Table C1 Textural properties of the semiconductor electrodes obtained from N_2 adsorption-desorption analysis

Semiconductor	Specific surface area (m^2/g)	Pore size (nm)	Total pore volume (ml/g)
Sol-gel TiO_2	120	3.61	0.163
5 mole% Si purified Na-bentonite	165	3.63	0.215
10 mole% Si purified Na-bentonite	198	3.64	0.246
20 mole% Si purified Na-bentonite	243	3.64	0.269
40 mole% Si purified Na-bentonite	267	3.63	0.292
60 mole% Si Na-bentonite	263	3.63	0.293
80 mole% Si purified Na-bentonite	184	3.62	0.265
Purified clay	62	-	-

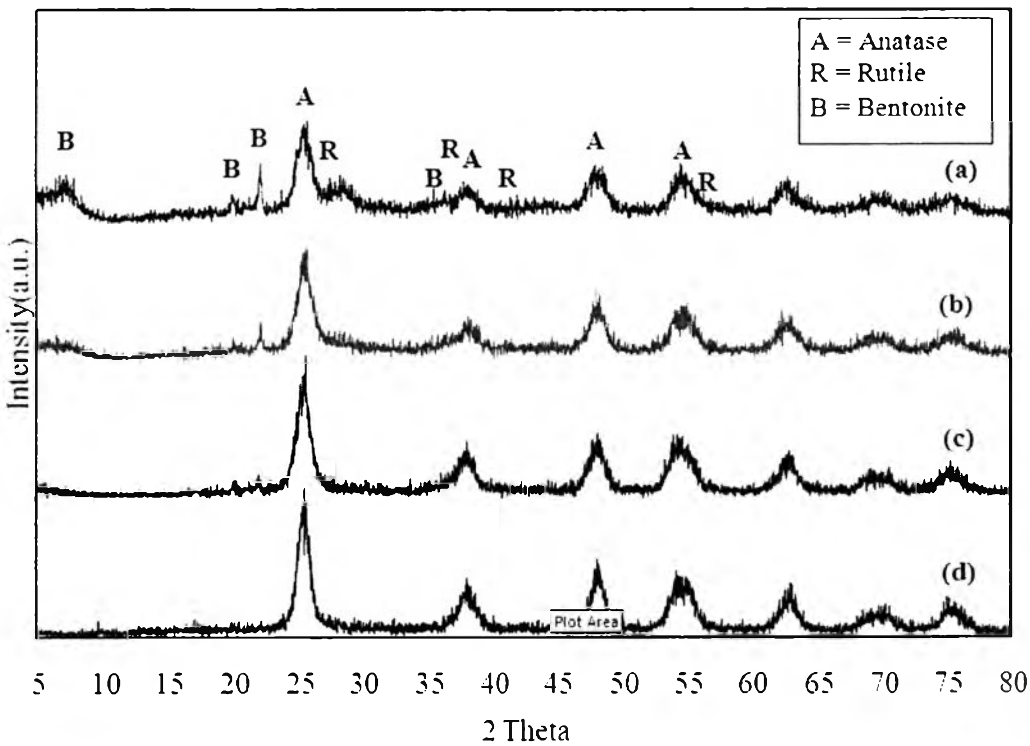
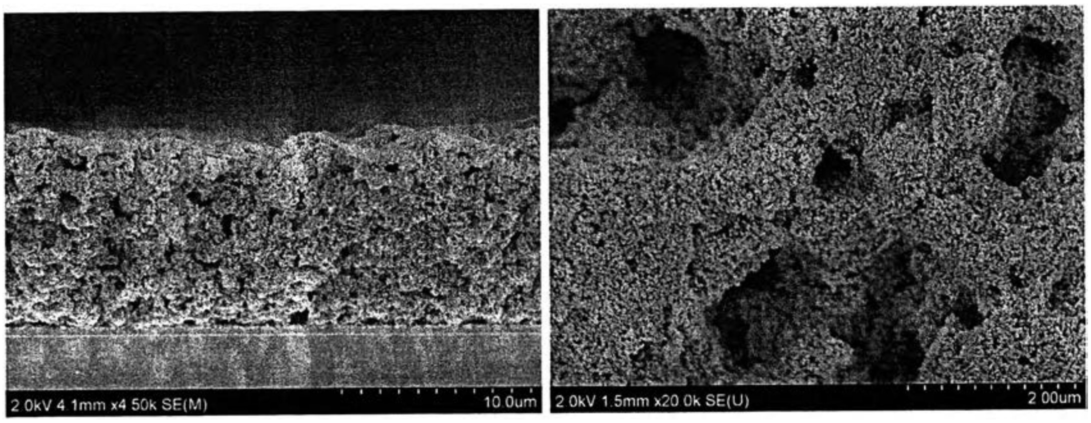
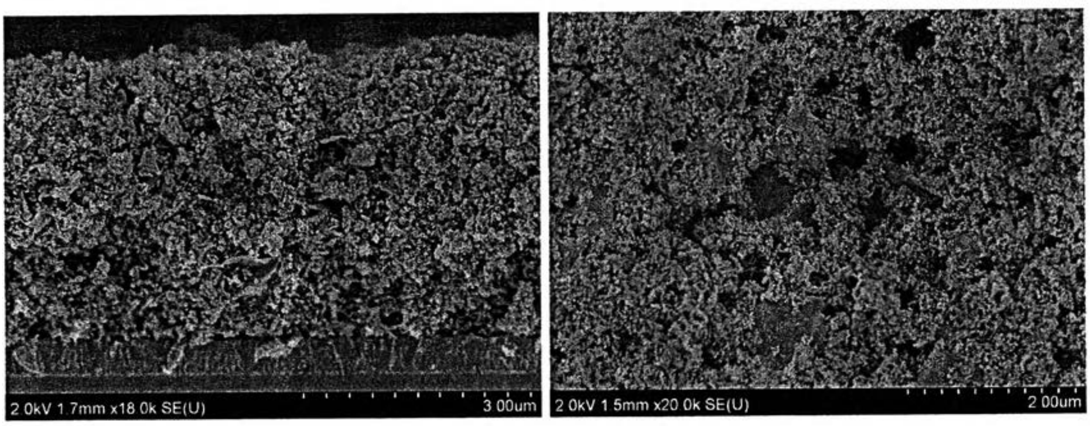


Figure C1 XRD patterns of (a) TiO_2/60 wt.% purified Na-bentonite, (b) TiO_2/40 wt.% purified Na-bentonite, (c) TiO_2/20 wt.% purified Na-bentonite, and, (d) TiO_2 electrodes.

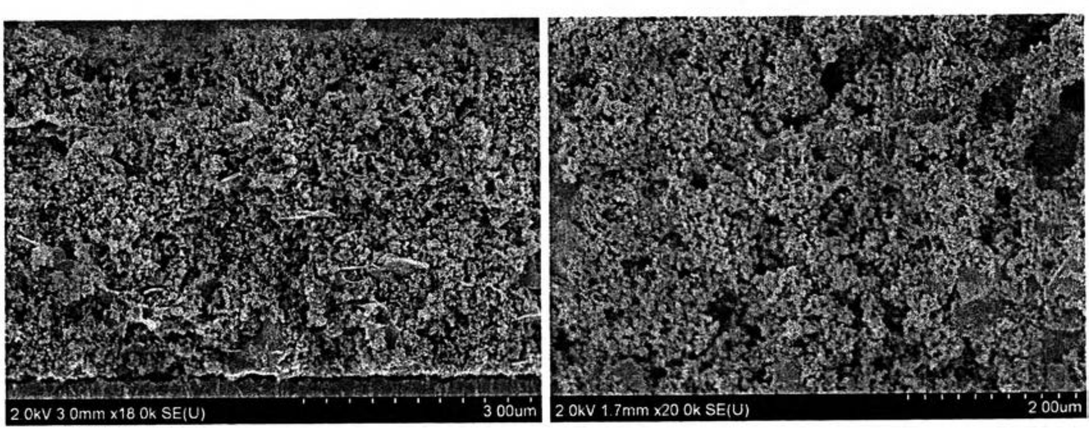
Appendix D Supplementary Results of Chapter VI



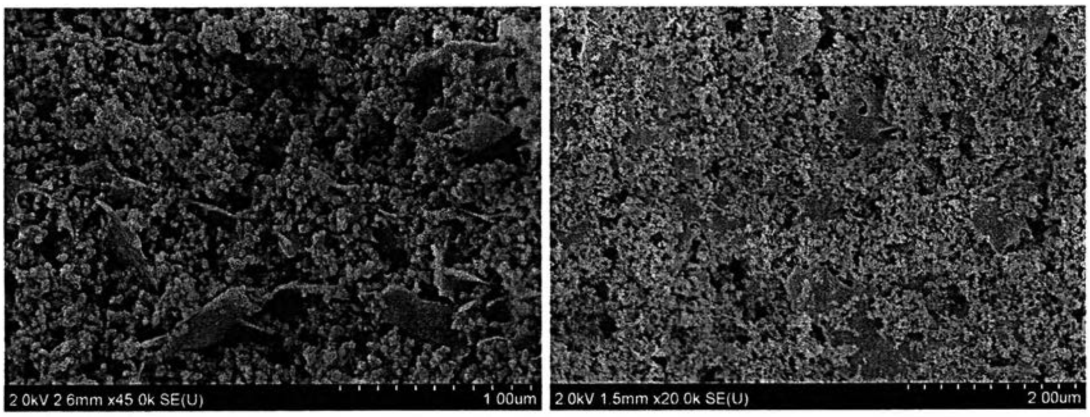
a.



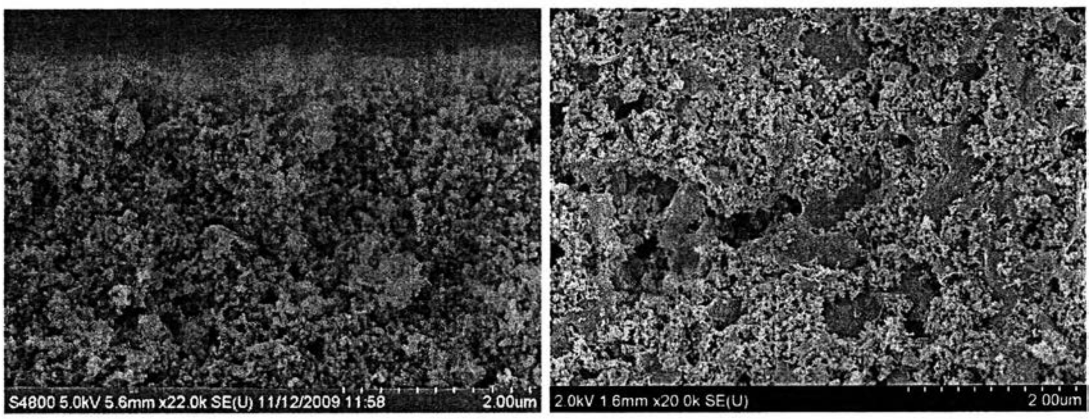
b.



c.



d.



e.

Figure D1 Top-viewed SEM micrographs on the left hand side and cross-sectional FE-SEM micrographs on the right hand side of (a) P25 TiO_2, (b) P25 TiO_2/5 mol% modified-bentonite, (c) P25 TiO_2/10 mol% modified-bentonite, (d) P25 TiO_2/5 mol% purified Na-bentonite, and (e) P25 TiO_2/10 mol% purified Na-bentonite.

Table D1 Photovoltaic properties of DSSC sensitized by red cabbage dye

Semiconductor-based film	Thickness (μm)	J_{sc} (mA/cm^2)	V(V)	FF	η (%)
P25	7.5	2.07	0.60	0.33	0.40
	10.0	2.12	0.59	0.31	0.39
5 mol% Si modified-bentonite	5.0	1.65	0.63	0.25	0.26
	8.0	1.84	0.59	0.27	0.29
	12.0	1.92	0.59	0.25	0.28
10 mol% Si modified-bentonite	4.0	1.58	0.61	0.21	0.20
	7.0	1.71	0.59	0.22	0.22
	11.5	2.00	0.58	0.19	0.22
5 mol% Si purified Na-bentonite	5.0	1.38	0.59	0.25	0.20
	8.5	1.76	0.59	0.25	0.26
	11.5	1.93	0.58	0.24	0.27
10 mol% Si purified Na-bentonite	4.5	1.23	0.62	0.16	0.12
	7.0	1.45	0.59	0.17	0.15
	11.5	1.49	0.58	0.18	0.15

Appendix E Supplementary Results of Chapter VII

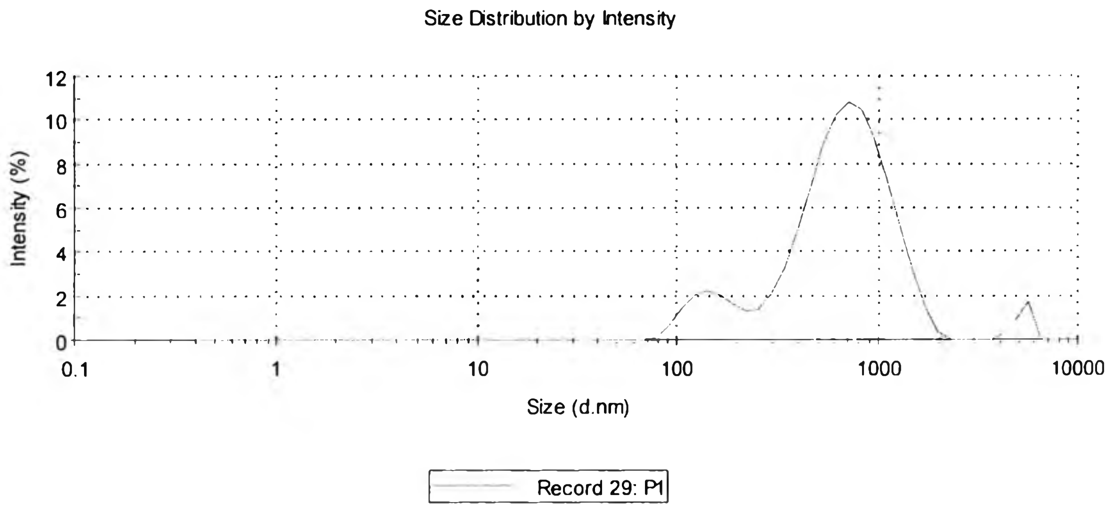


Figure E1 Size distribution of purified Na-bentonite collected from the top of settling raw Na bentonite swollen in deionized water.

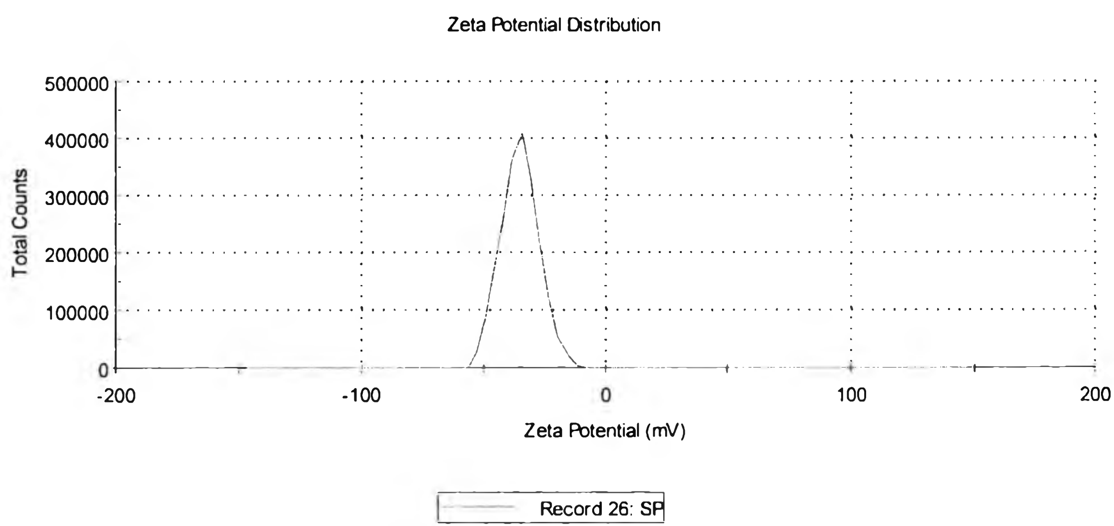


Figure E2 Zeta potential distribution of purified Na-bentonite collected from the top of settling raw Na bentonite swollen in deionized water.

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	Company name:	Swiss Federal Institute of Technology in Lausanne (EPFL)

Publications:

1. Saelim, N.-o., Magaraphan, R., and Sreethawong, T. (2011). TiO_2/modified natural clay semiconductor as a potential electrode for natural dye-sensitized solar cell. <u>Ceramic International</u>, 37(2), 659-663.
2. Saelim, N.-o., Magaraphan, R., and Sreethawong, T. (2011). Preparation of sol–gel TiO_2/purified Na-bentonite composites and their photovoltaic application for natural dye-sensitized solar cells. <u>Energy conversion Management</u>, 52(8-9), 2815-2818.
3. Saelim, N.-o., and Magaraphan, R. Fabrication of TiO_2/purified Na-bentonite and TiO_2/CTAB-modified Na-bentonite composites for DSSC electrodes.
4. Saelim, N.-o., and Magaraphan, R. Electrophoretic deposition of TiO_2/purified Na-bentonite composites for DSSC electrodes.
5. Saelim, N.-o., and Magaraphan, R. Gel electrolyte of polymethyl acrylate and clay aerogel for dye-sensitized solar cells.

Proceedings:

1. Saelim, N.; Magaraphan, R.; and Sreethawong, T. (2008, August 19-20) Nanoparticle titanate-clay semiconductor for dye-sensitized solar cell with natural dyes. Proceedings of Thai-Japan Joint Symposium on Advances in Materials Science and Environmental Technology, Bangkok, Thailand.

Presentations:

1. Saelim, N.; Magaraphan, R.; and Sreethawong, T. (2009, February 25-27) Nanoparticle titanate-clay semiconductor for dye-sensitized solar cell by using natural dyes. Global Plastics Environmental Conference 2009, Plastics: The wonderful World of Sustainability and Recycling, Orlando, Florida.
2. Saelim, N.; Magaraphan, R.; and Sreethawong, T. (2009, April 3-5) Nanoparticle TiO_2-clay semiconductor for dye-sensitized solar cell with red cabbage extracted dye as sensitizer. RGJ-Ph.D. Congress X "Climate Change and Its Impacts", Chonburi, Thailand.
3. Saelim, N.; Magaraphan, R.; and Sreethawong, T. (2009, August 7) Use of natural dyes in dye-sensitized solar cell fabricated with TiO_2 nanoparticle-clay semiconductor. RGJ Seminar Series LX II: Advanced Materials, Bangkok, Thailand.
4. Saelim, N.; Magaraphan, R.; and Sreethawong, T. (2010, April 1-3) Use of TiO_2/Purified Natural Clay as a Potential Electrode for Dye-Sensitized Solar Cell. RGJ-Ph.D. Congress XI "Research Towards Sustainability", Chonburi, Thailand.