Electronic Supporting Information

Ferrocenyl Chalcones with Phenolic and Pyridyl Anchors as Potential Sensitizers in Dye-Sensitized Solar Cells

Ratna Chauhan,[‡a] Reena Yadav,[‡b] Ashish Kumar Singh,[c] Manoj Trivedi,[d] Gabriele Kociok-Köhn,[e] Abhinav Kumar,*[b] Suresh Gosavi[f] and Sunit Rane[a]

[a] Center for Materials for Electronic Technology, Pune-411008, India

[b] Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow 226 007, India

Email: abhinavmarshal@gmail.com

[c] School of Material Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India

[d] Department of Chemistry, University of Delhi, Delhi, India

[e] Chemical Characterisation and Analysis Facility (CCAF), University of Bath, Bath BA2 7AY, UK

[f] Department of Physics, University of Pune, Pune-411021, India

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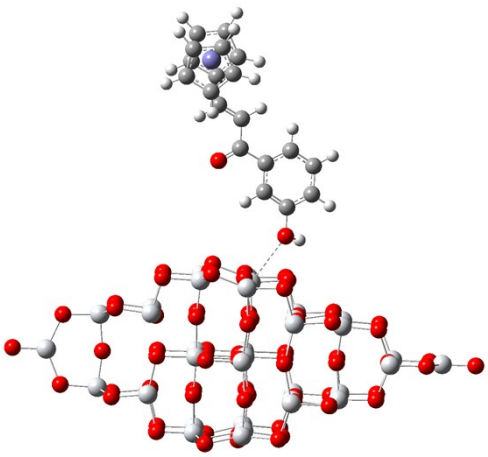
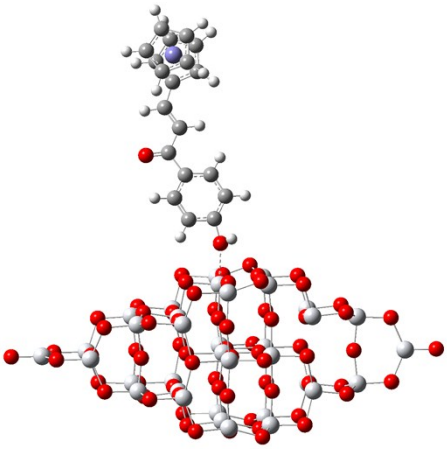


$(TiO_2)_{30}$+H-1



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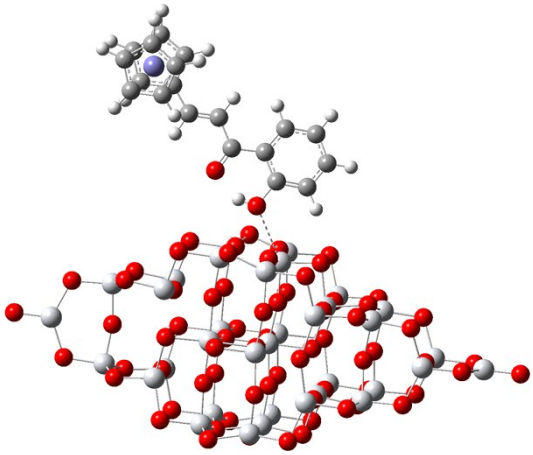

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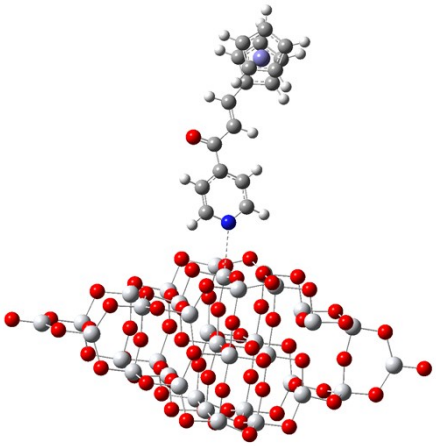

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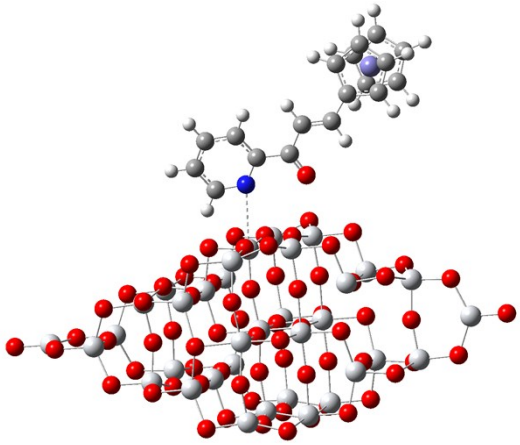

$(TiO_2)_{30}$+H-5

Fig. S1. Adsorption modes of **H1-H5** on $(TiO_2)_{30}$ cluster.

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Table S1. Incident photon to current conversion efficiencies of N719 and H-1 to H-5 dyes at different monochromatic wavelengths.

Wavelength (nm)	Intensity (mW/cm^2)	Current density ($\mu A/cm^2$)						% IPCE					
		N719	**H-1**	**H-2**	**H-3**	**H-4**	**H-5**	**N719**	**H-1**	**H-2**	**H-3**	**H-4**	**H-5**
400	12.3	1.904516	1.507742	1.785484	1.706129	1.349032	1.190323	48	38	45	43	34	30
410	12.8	1.904516	1.523613	1.692903	1.608258	1.354323	1.14271	45	36	40	38	32	27
420	13.1	1.907952	1.419871	1.641726	1.508613	1.286758	1.064903	43	32	37	34	29	24
430	13.7	1.947831	1.377734	1.567766	1.425242	1.282718	1.045177	41	29	33	30	27	22
440	14.2	1.965097	1.310065	1.511613	1.360452	1.20929	1.007742	39	26	30	27	24	20
450	14.6	2.013387	1.271613	1.430565	1.271613	1.165645	1.006694	38	24	27	24	22	19
460	14.4	1.976516	1.228645	1.335484	1.175226	1.121806	1.014968	37	23	25	22	21	19
470	13.8	1.935339	1.359968	1.359968	1.203048	1.150742	1.098435	37	26	26	23	22	21
480	13	1.912258	1.509677	1.409032	1.308387	1.258065	1.157419	38	30	28	26	25	23
490	12.4	2.058	1.666	1.666	1.519	1.372	1.176	42	34	34	31	28	24
500	12.2	2.262903	1.820161	1.869355	1.820161	1.475806	1.279032	46	37	38	37	30	26
510	11.7	2.406048	1.876718	2.021081	2.021081	1.587992	1.347387	50	39	42	42	33	28
520	11.3	2.558903	1.80071	2.227194	2.037645	1.611161	1.469	54	38	47	43	34	31
530	11.2	2.632903	1.723355	2.297806	2.010581	1.675484	1.531871	55	36	48	42	35	32
540	10.5	2.469194	1.554677	2.149113	1.783306	1.508952	1.371774	54	34	47	39	33	30
550	10.8	2.443065	1.437097	2.107742	1.676613	1.437097	1.293387	51	30	44	35	30	27
560	11.3	2.347484	1.377871	2.04129	1.633032	1.377871	1.224774	46	27	40	32	27	24
570	11.3	2.129685	1.194702	1.869968	1.506363	1.194702	1.038871	41	23	36	29	23	20
580	10.3	1.734387	0.963548	1.4935	1.252613	0.915371	0.770839	36	20	31	26	19	16
590	9.8	1.4455	0.839323	1.305613	1.072468	0.746065	0.606177	31	18	28	23	16	13
600	9.5	1.287097	0.735484	1.149194	0.965323	0.643548	0.505645	28	16	25	21	14	11
610	8.8	1.082258	0.606065	0.952387	0.779226	0.519484	0.389613	25	14	22	18	12	9

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Wavelength (nm)	Intensity (mW/cm^2)	Current density ($\mu A/cm^2$)						% IPCE					
		N719	**H-1**	**H-2**	**H-3**	**H-4**	**H-5**	**N719**	**H-1**	**H-2**	**H-3**	**H-4**	**H-5**
620	8.4	0.924	0.504	0.798	0.672	0.462	0.336	22	12	19	16	11	8
630	8	0.812903	0.406452	0.690968	0.569032	0.365806	0.284516	20	10	17	14	9	7
640	8.2	0.719484	0.380903	0.634839	0.507871	0.338581	0.253935	17	9	15	12	8	6
650	7.8	0.613306	0.327097	0.531532	0.408871	0.28621	0.204435	15	8	13	10	7	5
660	6	0.415161	0.191613	0.35129	0.255484	0.191613	0.127742	13	6	11	8	6	4
670	6.2	0.3685	0.201	0.3015	0.201	0.1675	0.1005	11	6	9	6	5	3
680	6.3	0.310935	0.138194	0.241839	0.172742	0.138194	0.069097	9	4	7	5	4	2
690	6	0.200323	0.100161	0.166935	0.133548	0.100161	0.066774	6	3	5	4	3	2
700	5.6	0.158065	0.094839	0.063226	0.063226	0.063226	0.063226	5	3	2	2	2	2

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Table S2 Comparison of photocurrent calculated at the maximum of IPCE measurement and *J-V* measurement

Dye	Current density obtained from IPCE at maxima (mA/cm^2) (monochromatic light)*	Current density obtained from *J-V* curve (mA/cm^2) (white light)**	% IPCE value
N719	2.63	13.62	55
H-1	1.90	10.44	39
H-2	2.30	11.99	48
H-3	2.05	11.22	43
H-4	1.65	9.13	35
H-5	1.50	8.70	32