Supporting Information

for

Enhanced Trapping Efficiency in Acid-treated Silica Nanostructures

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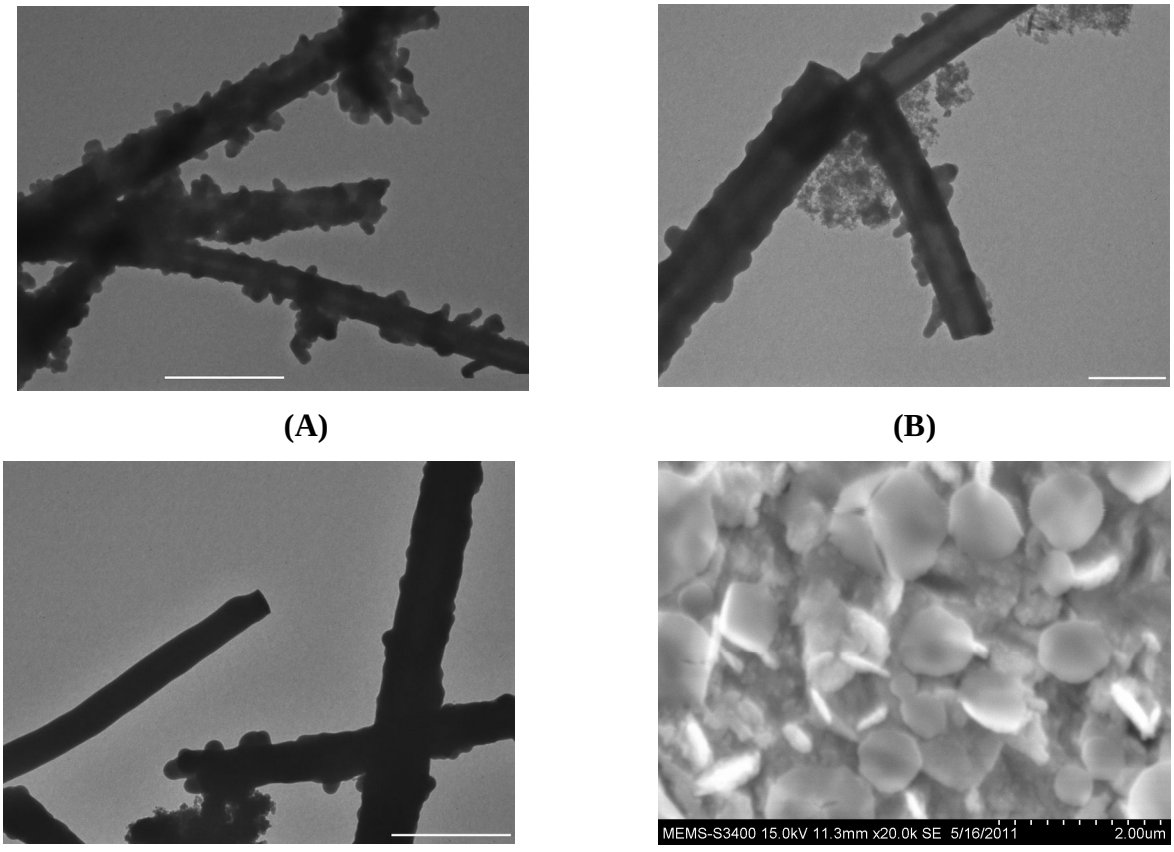

Figure S1. Transmission electron micrographs (TEM) of SNT (A) before the addition of acid, (B) after the addition of $HClO_4$ and (C) after the addition of HCl; (D) Scanning electron micrograph (SEM) of silica nanodisk prepared by RMSG method at w_0=22. Scale bar is 2 μm.

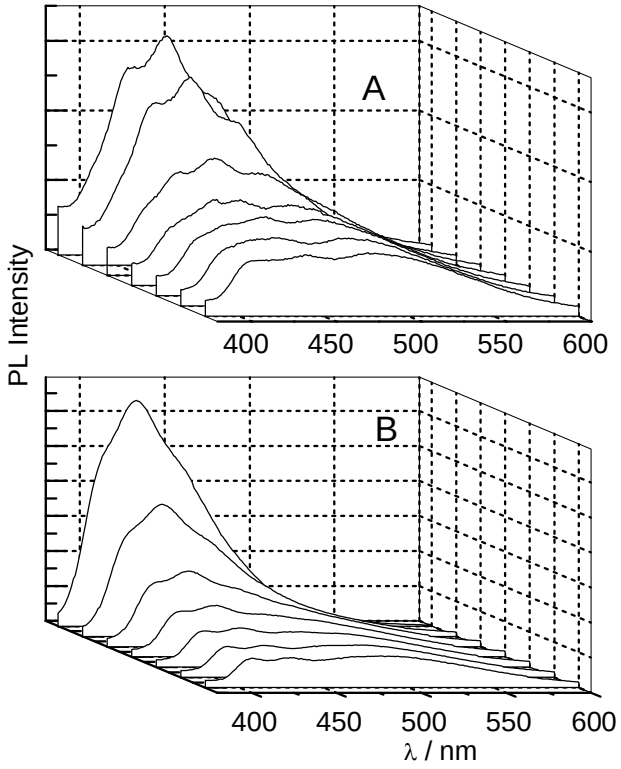

Figure S2. Effect of addition of (A) HCl and (B) H_2SO_4, on the blue PL of SNT dispersed in ethanol, λ_{ex} = 360 nm. The concentration of acids used are 0, 0.36, 0.72, 1.07, 1.45, 1.75, 2.00 N. λ_{ex} = 360 nm.

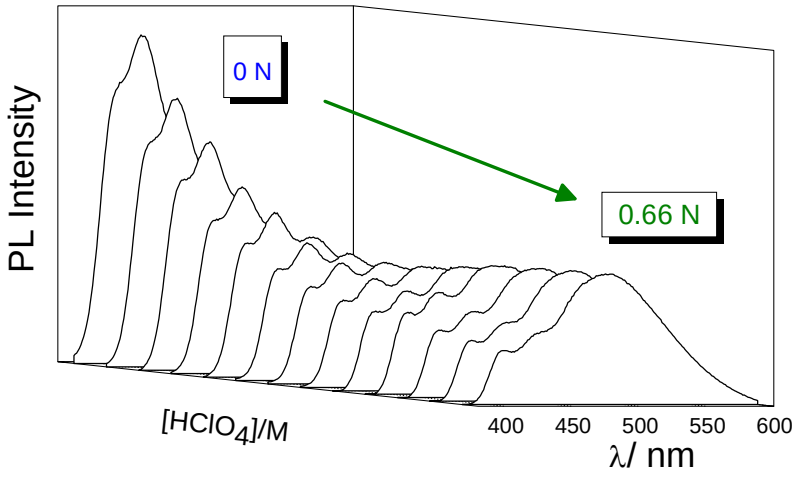

Figure S3. Red shift and loss in structure of the PL of SND dispersed in ethanol, upon the addition of $HClO_4$ .The concentration of $HClO_4$ used are 0, 0.06, 0.12, 0.17, 0.23, 0.28, 0.34, 0.39, 0.45, 0.50, 0.55, 0.60, 0.66 N. λ_{ex} = 360 nm.

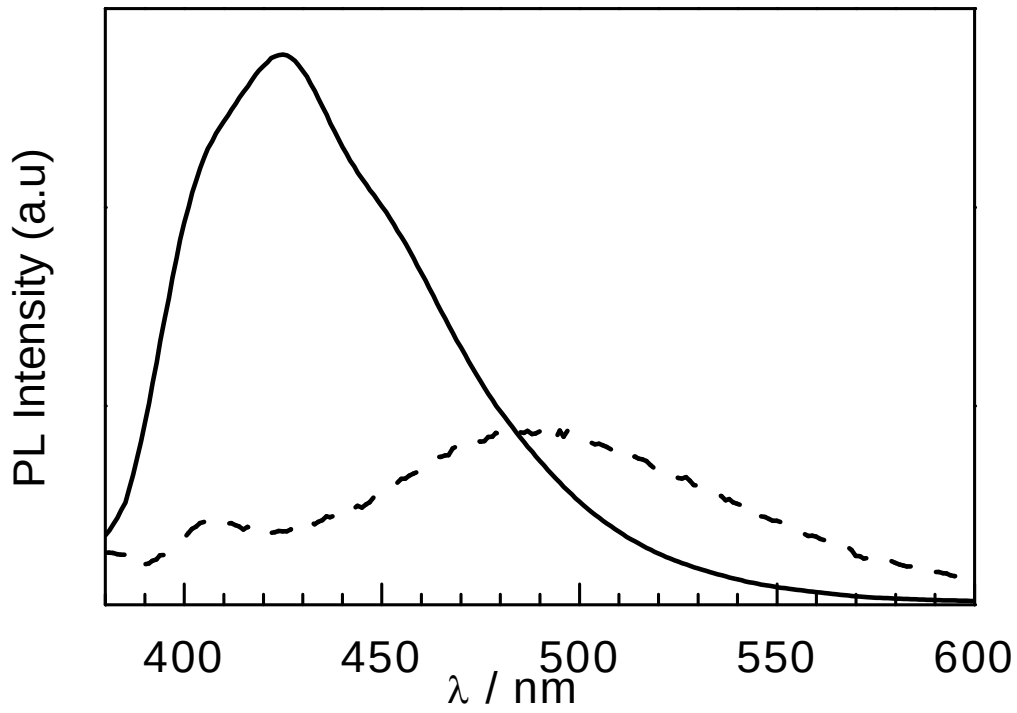

Figure S4. Regeneration of the bluish green peak from the washed nanotube by readdition of $HClO_4$. The solid line represents the blue PL from SNT without $HClO_4$. The dashed line represents the bluish –green PL peak after the $HClO_4$ addition.

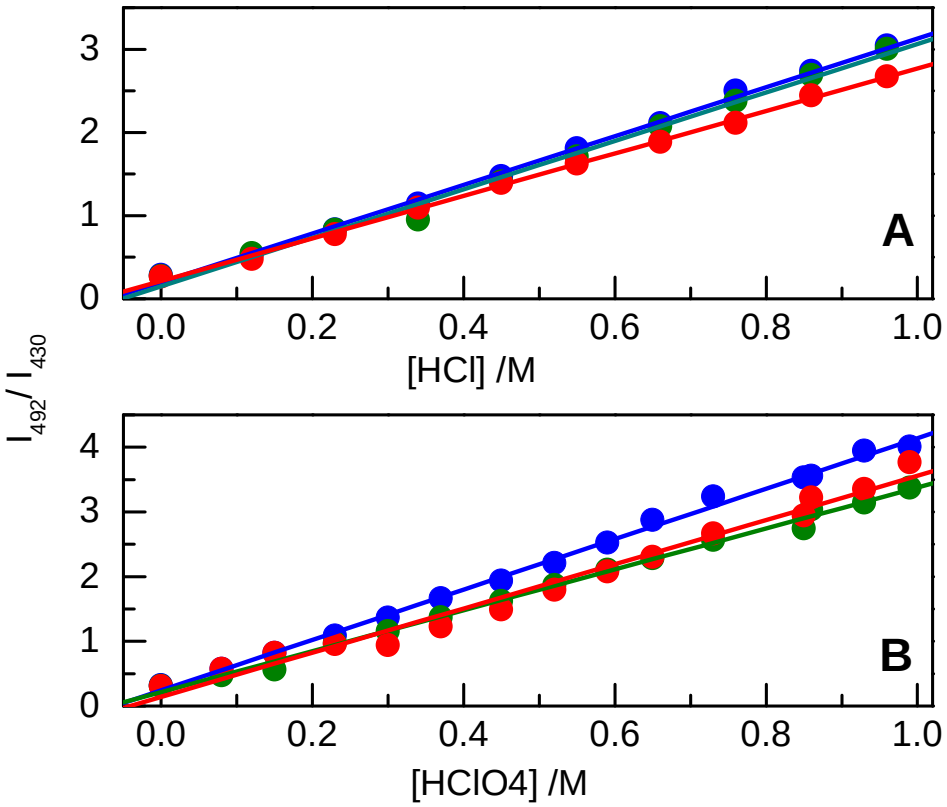

Figure S5. Variation of the ratio of the PL intensity of SNT at 492 nm to 430 nm with the increase of concentration of (A) HCl and (B) $HClO_4$. SNT is dried at three temperature: room temperature (blue), 300^{o}C (red), 600^{o}C (green).

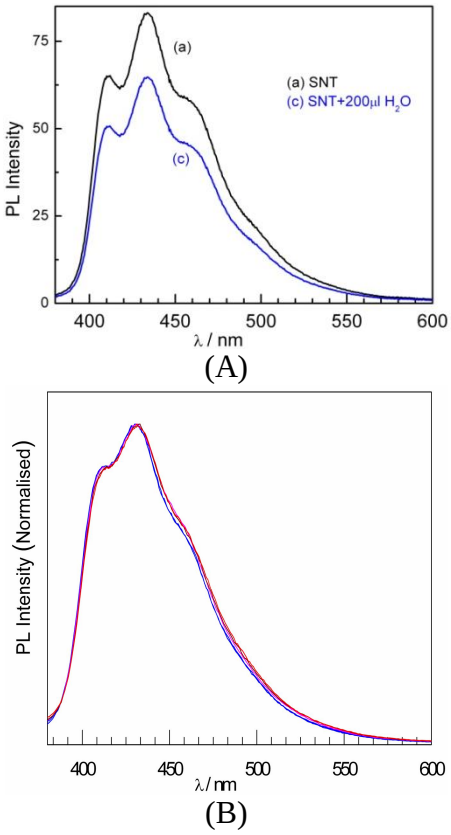

Figure S6. (A) No effect of addition of water on the blue PL of SNT dispersed in ethanol, λ_{ex}= 360 nm. Black line corresponds to the PL peak without $NaClO_4$ and the blue line corresponds to the PL spectra after the addition of 200µl water. **(B)** No effect of addition of $NaClO_4$ on the blue PL of SNT dispersed in ethanol, λ_{ex}= 360 nm. Blue line corresponds to the PL peak without $NaClO_4$ and the red line corresponds to the PL spectra after the addition of 0.43 M $NaClO_4$.

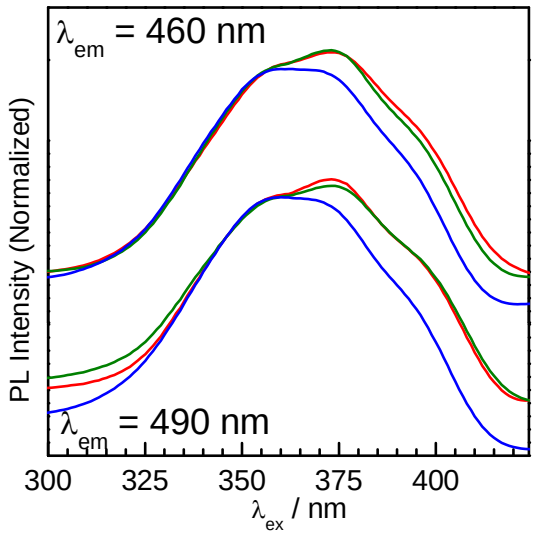

Figure S7. Excitation spectra before (blue) and after the addition of HCl (red) and HClO4 (green) to the ethanolic dispersion of SNT. λem = 460 nm (top panel) and 490 nm (bottom panel).

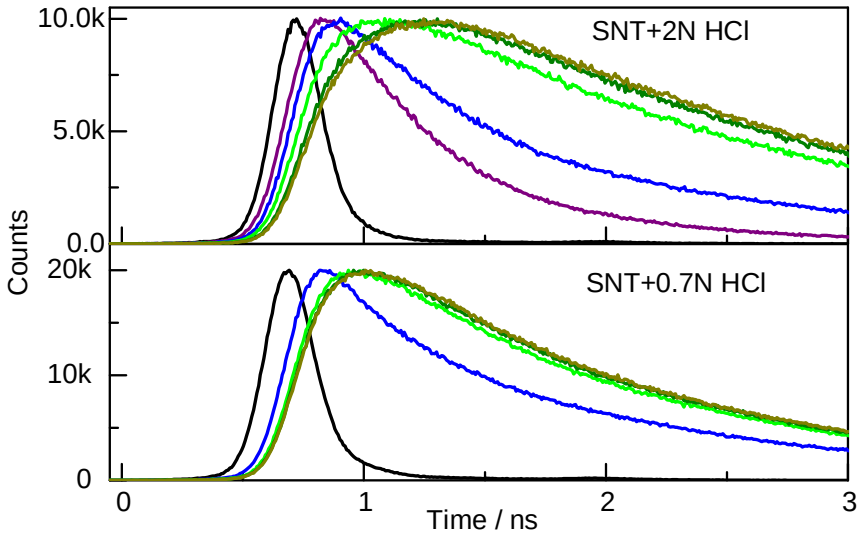

Figure S8. PL decays of silica nanotubes treated with HCl. The concentrations of the acid are mentioned in the Figure. λ_{ex} = 375 nm. The decays have been recorded at 430 nm (purple), 460 nm (blue), 500 nm (green), 530 nm (olive) and 560 nm (dark yellow). The instrument response function is shown in black. The counts are shown in a linear scale and the decays are truncated at 3 ns, in order to highlight the differences at shorter times.

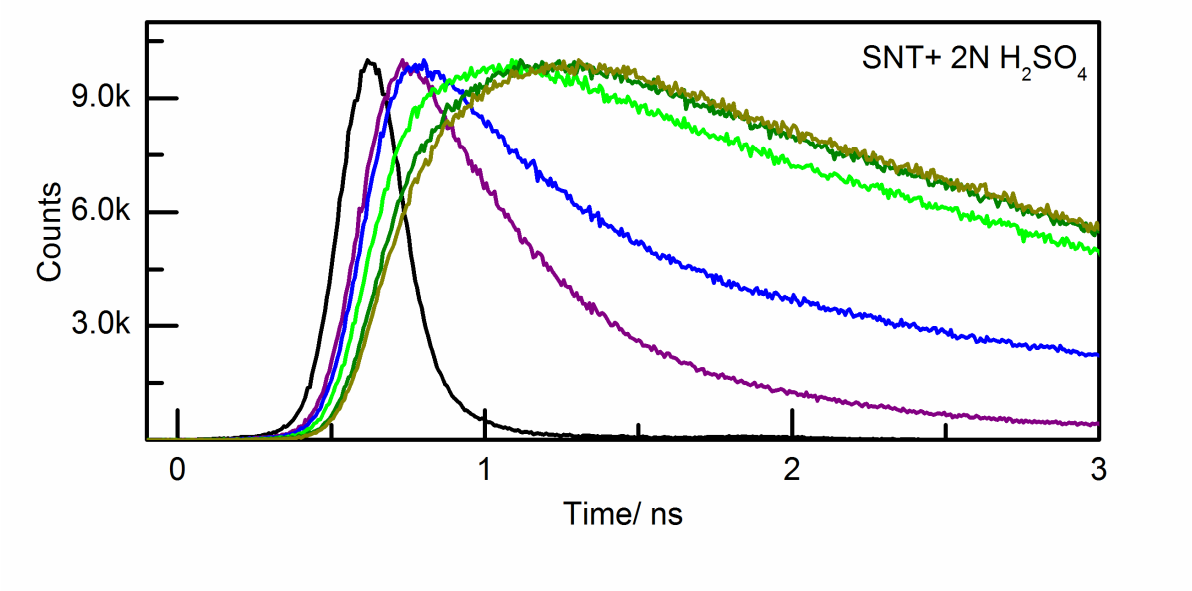

Figure S9. PL decays of silica nanotubes treated with 2N H_2SO_4. λ_{ex} = 375 nm. The decays have been recorded at 430 nm (purple), 460 nm (blue), 500 nm (green), 530 nm (olive) and 560 nm (dark yellow). The instrument response function is shown in black. The counts are shown in a linear scale and the decays are truncated at 3 ns, in order to highlight the differences at shorter times.

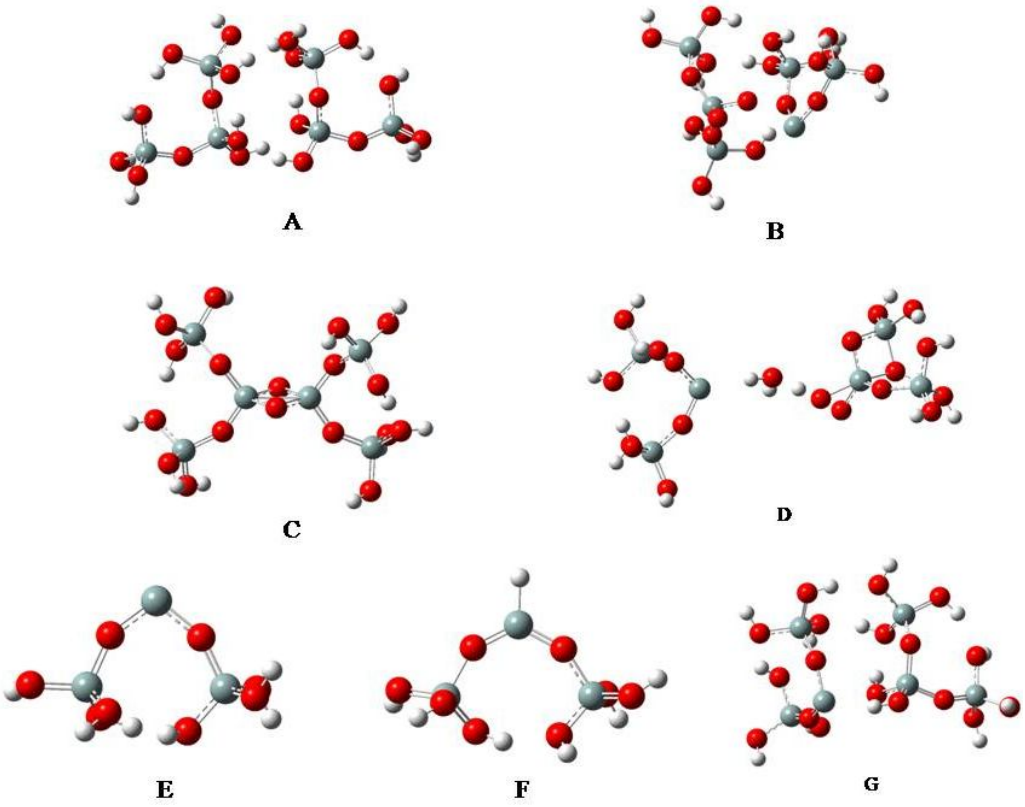

Figure S10. Optimized structures of different schemes, the calculations are done at B3LYP/6-31G(D) level of theory.

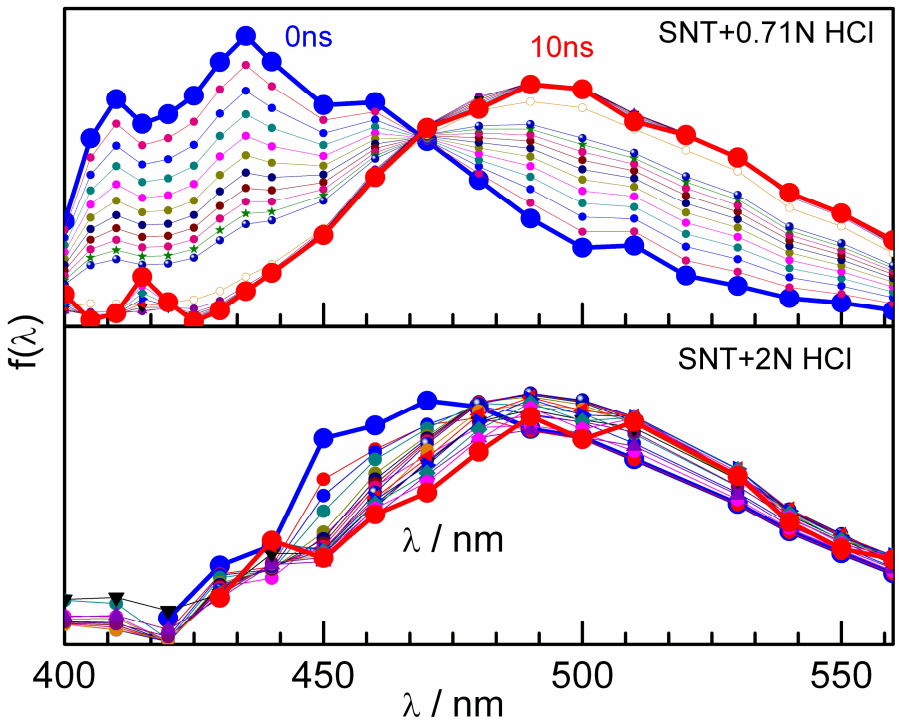

Figure S11. Time-resolved area-normalized emission spectra (TRANES) of SNT in ethanol treated with HCl between time 0 and 10 ns, The spectra between 0 and 1 ns are at intervals of 100 ps. Those between 1 and 10 ns are at intervals of 1 ns. The arrows denote the direction of increase in time.

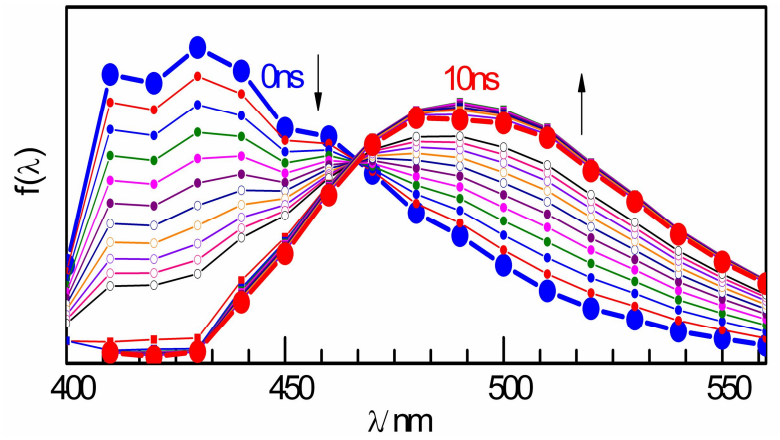

Figure S12. Time-resolved area-normalized emission spectra (TRANES) of SNT in ethanol treated with 2 N H_2SO_4 between time 0 and 10 ns, The spectra between 0 and 1 ns are at intervals of 100 ps. Those between 1 and 10 ns are at intervals of 1 ns. The arrows denote the direction of increase in time.

Table S1. Photoluminescence lifetimes and their amplitudes of SNT after and before the addition of acid.

Sample	[Acid]/ N	λ_{em}	A_1	τ_1 (ns)	A_2	τ_2 (ns)	A_3	τ_3(ns)	χ^2
SNT	No acid	400	0.98	1.33	0.02	3.40			1.10
		410	0.98	1.32	0.02	3.04			1.07
		420	0.95	1.28	0.05	2.38			1.03
		430	0.96	1.32	0.04	2.70			1.00
		440	0.99	1.33	0.01	4.06			1.02
		450	0.99	1.34	0.01	4.08			1.06
		460	0.99	1.37	0.01	4.23			1.10
		470	0.99	1.36	0.01	4.83			1.00
		480	0.99	1.38	0.01	5.87			1.12
		490	0.99	1.37	0.01	5.26			1.18
		500	0.99	1.38	0.01	5.73			1.06
		510	0.99	1.36	0.01	5.72			1.11
		520	0.99	1.35	0.01	6.10			1.07
		530	0.98	1.36	0.02	6.32			1.07
		540	0.98	1.37	0.02	6.88			1.07
		550	0.99	1.42	0.01	6.66			1.01
		560	0.97	1.39	0.03	6.31			1.19
SNT+$HClO_4$	0.4	400	0.96	0.54	0.04	2.56			1.14
		410	0.98	0.52	0.02	2.53			1.18
		420	0.98	0.52	0.02	2.20			1.14
		430	0.97	0.51	0.03	1.99			1.15
		440	0.96	0.49	0.04	1.88			1.20
		450	0.97	0.51	0.03	2.06			1.15
		460	0.95	0.50	0.05	1.98			1.18
		470	0.48	0.51	0.52	2.23			1.15
		480	0.23	0.55	0.77	2.26			1.08
		490	-0.01	1.23	1.01	2.26			1.07
		500	-0.19	0.55	1.19	2.24			1.10
		510	-0.42	0.44	1.42	2.22			1.05
		520	-0.61	0.51	1.61	2.25			1.07
		530	-0.47	0.59	1.47	2.26			1.08
		540	-0.81	0.51	1.81	2.26			1.11
		550	-0.83	0.54	1.83	2.26			1.04
		570	-0.88	0.54	1.88	2.26			1.09
		580	-0.97	0.53	1.97	2.26			1.06
		590	-0.93	0.53	1.89	2.27	0.04	6.47	1.06
		600	-0.99	0.50	1.94	2.28	0.05	7.30	1.01
		610	-1.16	0.49	2.11	2.31	0.05	7.66	1.00

Sample	[Acid]/ N	λ_{em}	A_1	τ_1 (ns)	A_2	τ_2 (ns)	A_3	τ_3(ns)	χ^2
SNT+$HClO_4$	2.0	460	0.50	0.22	0.50	2.25			1.16
		470	0.32	0.36	0.68	2.27			1.05
		480	0.26	0.38	0.74	2.25			1.07
		490	0.20	0.43	0.80	2.26			1.15
		500	0.18	0.45	0.82	2.26			1.08
		510	0.16	0.52	0.84	2.26			1.11
		520	0.12	0.55	0.88	2.24			1.15
		530	0.16	0.54	0.84	2.28			1.20
		540	0.19	0.81	0.81	2.35			1.10
		550	0.21	0.79	0.79	2.37			1.20
		560	0.14	0.86	0.86	2.26			1.17
		570	0.17	0.83	0.83	2.27			1.13
		580	0.17	0.82	0.82	2.23	0.01	5.86	1.11
		590	0.21	0.75	0.75	2.25	0.03	7.37	1.08
		600	0.23	0.71	0.71	2.26	0.06	6.82	1.07
		610	0.23	0.70	0.70	2.25	0.08	6.66	1.10
SNT+HCl	0.7	400	0.95	0.47	0.05	1.77			1.20
		410	0.97	0.42	0.03	1.47			1.04
		420	0.96	0.41	0.04	1.56			1.04
		430	0.94	0.42	0.06	1.34			1.15
		440	0.87	0.42	0.12	1.44			1.02
		450	0.74	0.43	0.26	1.43			1.20
		460	0.58	0.43	0.42	1.43			1.09
		470	0.36	0.49	0.64	1.44			1.10
		480	0.07	0.84	0.93	1.43			1.07
		490	-0.34	0.26	1.34	1.44			1.04
		500	-0.35	0.38	1.35	1.43			1.11
		510	-0.57	0.43	1.57	1.40			1.06
		520	-0.72	0.42	1.72	1.41			1.02
		530	-0.49	0.50	1.49	1.43			1.05
		540	-0.70	0.42	1.70	1.44			1.04
		550	-1.67	0.43	2.67	1.43			1.08
		570	-1.09	0.38	2.09	1.44			1.17
		580	-1.09	0.41	2.09	1.46			1.10
		590	-0.89	0.38	1.89	1.49			1.03
		600	-0.88	0.30	1.88	1.51			1.06
		610	-0.74	0.28	1.66	1.68	0.08	3.76	1.00

Sample	[Acid]/ N	λ_{em}	A_1	τ_1 (ns)	A_2	τ_2 (ns)	A_3	τ_3(ns)	χ^2
SNT+HCl	2.0	460	0.49	0.30	0.51	1.26			1.09
		470	0.35	0.24	0.65	1.23			1.10
		480	0.21	0.31	0.79	1.24			1.07
		490	0.20	0.71	0.80	1.28			1.04
		500	0.15	0.71	0.85	1.26			1.03
		510	0.15	0.72	0.85	1.26			1.13
		520	0.12	0.55	0.88	2.24			1.11
		530	0.20	0.81	0.80	1.30			1.10
		540	0.13	0.71	0.87	1.27			1.11
		550	0.10	0.73	0.90	1.26			1.12
		560	0.20	0.81	0.80	1.30			1.08
		570	0.08	0.77	0.92	1.26			1.10
		580			0.97	1.22	0.03	2.59	1.42
		590			0.99	1.18	0.01	2.27	1.20
		600			0.84	1.18	0.16	2.42	1.12
		610			0.76	1.15	0.24	2.32	1.08
$SNT+H_2SO_4$	2.0	400	0.94	0.44	0.06	1.96			1.19
		410	0.98	0.41	0.02	2.21			1.24
		420	0.97	0.41	0.03	1.86			1.07
		430	0.94	0.42	0.05	2.18			1.19
		440	0.87	0.40	0.14	2.11			1.11
		450	0.73	0.40	0.27	2.17			1.09
		460	0.59	0.38	0.40	2.20			1.14
		470	0.40	0.38	0.60	2.22			1.12
		480	0.15	0.34	0.85	2.22			1.13
		490	-0.02	0.29	1.02	2.21			1.09
		500	-0.25	0.66	1.25	2.10			1.07
		510	-0.34	0.50	1.34	2.20			1.07
		520	-0.96	0.40	1.96	2.18			1.04
		530	-0.94	0.39	1.94	2.19			1.11
		540	-1.39	0.42	2.39	2.17			1.05
		550	-0.55	0.47	1.55	2.21			1.16
		560	-2.09	0.36	3.08	2.21			1.13
		570	-1.41	0.38	2.41	2.18			1.11
		580	-0.53	0.41	1.51	2.18	0.03	7.21	1.06
		590	-1.01	0.31	1.93	2.32	0.07	7.62	1.03
		600	-0.46	0.38	1.33	2.21	0.14	6.38	1.19
		610	-0.89	0.28	1.75	2.38	0.14	7.14	1.09

[a]The decays are fitted with a multiexponential function: $I(t) = I(0)\sum A_i\, e^{-t/\tau_i}$, where the lifetimes are denoted as τ_i and amplitudes are denoted as A_i. $\sum A_i = 1$. λ_{ex} = 375 nm.

Table S2. The wavelengths (nm) corresponding to the singlet-to-singlet transitions of the model clusters obtained by the time-dependent DFT method

Transition No.	**A**	**B**	**C**	**D**	**E**	**F**	**G**
1	178.29	244.80	183.86	316.97	238.63	233.35	244.80
2	178.13	235.88	183.10	272.03	212.33	218.60	235.88
3	174.05	223.17	179.47	257.69	203.31	210.08	223.17
4	173.91	216.65	175.75	235.97	201.38	209.00	216.65
5	171.99	211.25	174.14	235.76	192.33	199.08	211.25
6	171.56	204.35	173.04	229.58	188.49	194.30	204.35
7	169.70	199.46	171.95	227.40	183.34	190.81	199.46
8	169.34	198.47	171.06	220.31	180.74	187.88	198.47
9	166.51	197.58	170.07	218.00	179.38	185.42	197.58
10	166.21	185.53	168.79	216.64	175.29	183.20	185.53