Supporting Information for

A carbazole-fluorene molecular hybrid for quantitative detection of TNT with combined fluorescence and quartz crystal microbalance methods

Kalathil K. Kartha,^a Anjamkudy Sandeep,^a Vijayakumar C. Nair,^a Masayuki Takeuchi ^{*b} and Ayyappanpillai Ajayaghosh^{*a}

^aPhotosciences and Photonics Group, Chemical Sciences and Technology Division, National Institute for Interdisciplinary Science and Technology (NIIST), CSIR, Trivandrum 695 019, India

E-mail: ajayaghosh@niist.res.in

^bOrganic Materials Group, Polymer Materials Unit, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, 305-0047, Japan

E-mail: <u>TAKEUCHI.Masayuki@nims.go.jp</u>





Fig. S1 (a) Absorption and (b) emission spectra of CBF in THF (—), water (—) and methylcyclohexane (—) with a conc. of 5×10^{-5} M (l = 1 cm, $\lambda_{ex} = 350$ nm).



Fig. S2 Normalized emission spectra of CBF in (a) solution, (b) corresponding normalised spectra, (c) film state and (d) corresponding normalised spectra, from THF (—), water (—) and MCH (—) with a conc. of 5×10^{-5} M (l = 1 cm, $\lambda_{ex} = 350$ nm). Film prepared from 10 μ L of each solution drop casted on a glass plate and dried under vacuum for 12 h.



Fig. S3 AFM images of (a) CBF nanorods from MCH solution (5 \times 10⁻⁵ M) and (b) CBF nanoparticles from water (1 \times 10⁻⁵ M), respectively.



Fig. S4 Fluorescence changes of CBF nanoparticles upon addition of (a) DNT solution in water and (b) CBF (1 × 10⁻⁶ M) upon addition 10 equiv. DNT solution in THF (l = 1 cm, $\lambda_{ex} = 370$ nm).



Fig. S5 Fluorescence quenching studies of CBF film prepared from (a) water, (b) MCH, and (c) THF upon exposure to TNT vapors ($\lambda_{ex} = 370$ nm).



Fig. S6 (a) Fluorescence quenching studies of CBF film prepared from solution of MCH exposed to DNT vapors (b) A plot of quenching % vs time ($\lambda_{ex} = 370$ nm).

	% Quenching efficiency (QCM freq. shift Hz), approximate weight of adsorbed TNT (ng)		
Time (s)	Nanorods from MCH	Nanoparticles from water	Ill-defined structure from THF
100	36.74 (-2.71), 2.58	34.75 (-2.23), 2.12	6.6 (-1.65), 1.57
200	40.22 (-4.06), 3.86	40.99 (-3.57), 3.39	12.11 (-2.51), 2.39
300	41.94 (-4.74), 4.50	46.20 (-4.55), 4.33	14.10 (-3.01), 2.86
500	45.4 (-5.49), 5.22	63.87 (-6.16), 5.85	23.6 (-3.06), 2.91

 Table S1. A comparison of adsorption and fluorescence quenching by different CBF architectures with time.