Supplementary Material (ESI) for Chemical Communications
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Visible-Light Harvesting Periodic Mesoporous Organosilica

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Supporting Information

Experimental details

Regents. All regents and solvents were of the highest commercial quality and used without further purification.

2,7-bis(triethoxysilyl)acridone (BTEAD). To a mixture of $[Rh(CH_3CN)_2(cod)]BF_4$ (131 mg, 0.345 mmol) and 2,7-dibromo-9(10*H*)-acridone[1] (2.03 g, 5.75 mmol) was added distilled DMF (80 mL) and triethylamine (4.81 mL, 34.5 mmol). The mixture was stirred at room temperature for 30 min, after which triethoxysilane (4.25 mL, 23.0 mmol) was added dropwise at 0 °C, and stirring was continued at 80 °C for 2 h. The reaction mixture was then concentrated under vacuum to remove DMF. The resulting mixture was treated with Et_2O to give a solution of BTEAD in Et_2O, which was filtered through a Celite plug, and the filter cake was rinsed with Et_2O. The combined filtrates were concentrated under vacuum to yield BTEAD. It was passed through charcoal to give highly purified BTEAD (1.60 g, 54%). ^{1}H NMR ($CDCl_3$) δ 11.92 (s, 1H) , 8.49 (s, 2H) , 7.85(d, J = 8.10 Hz, 2H) , 7.63 (d, J = 8.10 Hz, 2H), 3.84(q, J = 7.02 Hz, 12H) , 1.19 (t, J = 7.02 Hz, 18H), ^{13}C NMR ($CDCl_3$) δ 142.2, 138.5, 133.6, 122.7, 120.4, 117.3, 58.5, 18.4. HRMS (ES$^+$) $[M+Na]^+$ calcd for $C_{25}H_{37}O_7NNaSi_2$ 542.2001, found 542.1995.

1) (a) Kajigarshi, S.; Kakinami, T.; Moriwaki, M.; Tanaka, T.; Fujisaki, S.; Okamoto, T. *Bull. Chem. Soc. Jpn.* **1989**, 62, 439. (b) Mircea, V.; Ioan, A. S.; Radu, C.; Monica, C. *Synthetic. Commun.* **1995**, 25, 3493.

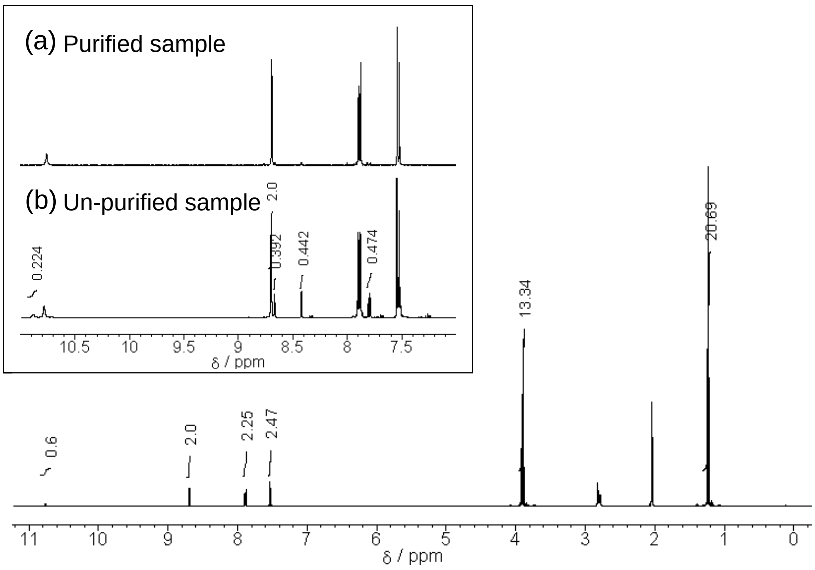

Fig. S1 ^{1}H NMR spectrum of the highly purified BTEAD in acetone-d_6. The spectrum of the unpurified sample in the range of the aromatic protons was also shown in inset. The contaminant was 2-bromo-7-(triethoxysilyl)acridone which was determined by combined analysis with ESI-MS. The purity of the unpurified sample was 60.8 mol% while the purified one was > 98 mol% in purity.

DCM doped Acd-PMO. Acd-PMO powder (20 mg) was suspended in 20 ml of an aqueous solution of 50 mM C_{18}TMACl surfactant and mixed with DCM dye at appropriate concentrations (0.02 – 0.2 mM). The suspensions were stirred at rt for 12 h and filtered, and the recovered powders were dried in vacuo. The concentration of adsorbed DCM was determined from the DCM concentrations in the filtrate by UV-vis absorption spectroscopy. The value of 297.37 g/mol was used as the molecular weight of acridone groups in the Acd-PMO powder based on the chemical unit ($SiO_{1.5}$-$C_{13}H_7O$-$SiO_{1.5}$).

General measurements. Powder X-ray diffraction (XRD) patterns were obtained with a Rigaku RINT-TTR diffractometer using Cu-Kα radiation (50 kV, 300 mA). The adsorption/desorption isotherms of nitrogen at the temperature of liquid nitrogen (77 K) were measured using a Quantachrome NOVA 3000e system. The samples were out-gassed for 4 h at 60°C before the measurements. The Brunauer-Emmett-Teller (BET) surface areas were calculated from the data at relative pressures of 0.05 – 0.2, and the pore-size distributions were calculated using the Barrett-Joyner-Halenda (BJH) model from the adsorption branch isotherms. ^{1}H- and ^{13}C-NMR spectra of the BTEAD solution were recorded on a JEOL ECX-400 spectrometer at 395.88 MHz for ^{1}H and 99.55 MHz for ^{13}C. The solid-state ^{29}Si and ^{13}C magic angle spinning nuclear magnetic resonance (MAS NMR) spectra were recorded on a Bruker AVANCE 400 spectrometer at 70.49 MHz for ^{29}Si and 100.61 MHz for ^{13}C. Chemical shift in both the ^{29}Si and ^{13}C NMR was shown relative to the peak of trimethylsilane (TMS) at 0 ppm. UV-Vis spectra were recorded on a Jasco V-670 spectrometer. An integrating sphere unit was equipped for the UV-Vis diffuse reflectance (DR) spectra of powder samples. PMO powder samples (1 mg) were diluted by mixing with KBr (500 mg) in a mortar before the measurements. FT-IR spectra of PMO powder samples were recorded on a Nicolet AVATAR-360 spectrometer with an ATR (Attenuated Total Reflection) unit. ESI (electrospray ionization)-MS spectra were recorded on a Micromass Q-TOF mass-spectrometer using CH_3CN as eluent. SEM and FE-SEM images were obtained using a HITACHI S-5500 electron microscope with acceleration voltages of 2.0 kV and 10 kV, respectively. The powder sample was supported on a collodion. TEM images were obtained on a Kodak SO-163 film using a JEOL JEM-2000EX electron microscope with acceleration voltage of 200 kV. The powder sample was dispersed in ethanol after the pulverization in mortar.

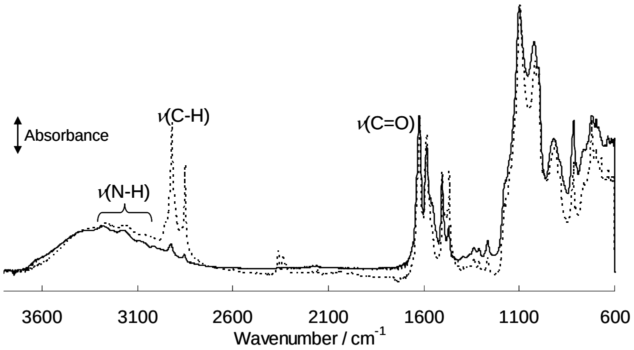

Fig. S2 FT-IR (ATR) spectra of the Acd-PMO powders before (dotted line) and after (solid line) the surfactant extraction. The diminishing of the ν(C-H) peaks shows almost complete removing of the surfactant by the extraction process.

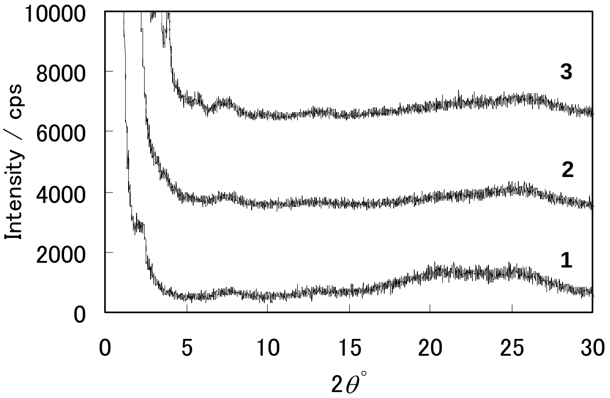

Fig. S3 XRD patterns of the Acd-PMO powders (entry 1, 2, and 3) at the wider angle.

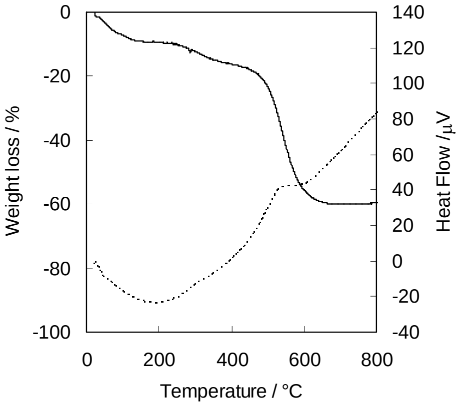

Fig. S4 Thermogravimetry of the Acd-PMO powder (entry 3) in air; TGA-curve (solid line) and DTA-curve (dotted line).

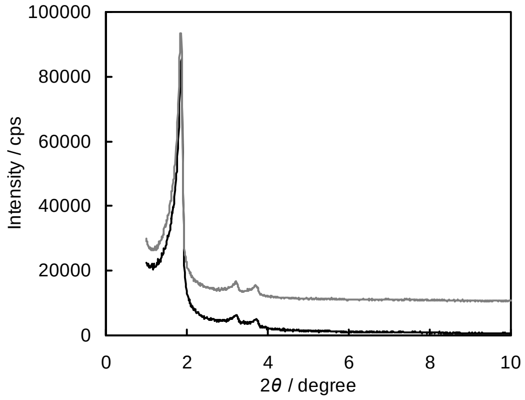

Fig. S5 XRD patterns of the Acd-PMO samples (entry 3) before (solid line) and after (gray line) boiling in water for 8h.

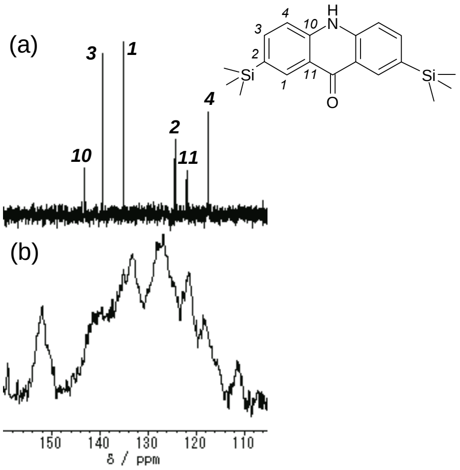

Fig. S6 (a) ^{13}C NMR spectrum of the BTEAD precursor in d_6-acetone and the assignment (b) ^{13}C CP-MAS NMR spectrum of the Acd-PMO powder synthesized without the post-synthesis HCl treatment under a strong basic condition: BTEAD: C_{18}TMACl: NaOH: H_2O = 1.00: 1.05: 6.42: 670 [mol].

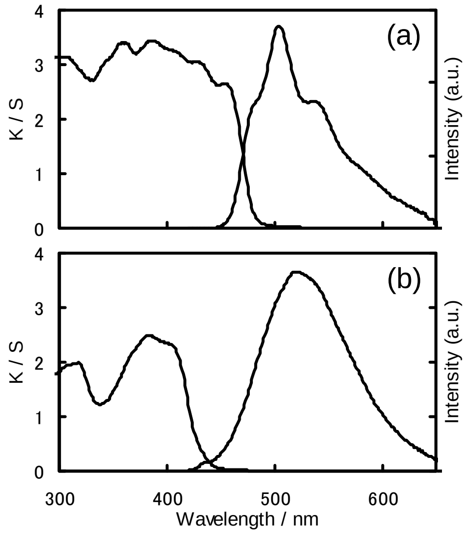

Fig. S7 UV-Vis (DR) and fluorescence emission spectra of the Acd-PMO powders prepared without (a) or with (b) the post-synthesis HCl treatment.

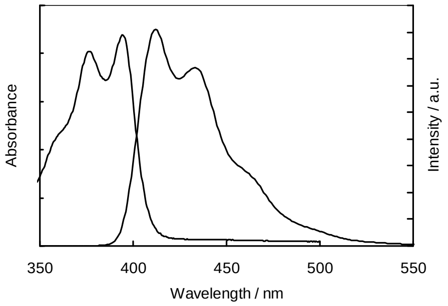

Fig. S8 UV-Vis and fluorescence emission spectra of BTEAD in 2-propanol.