Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Photoluminescent Electrospun Submicron Fibers of Hybrid Organosiloxane and Derived Silica

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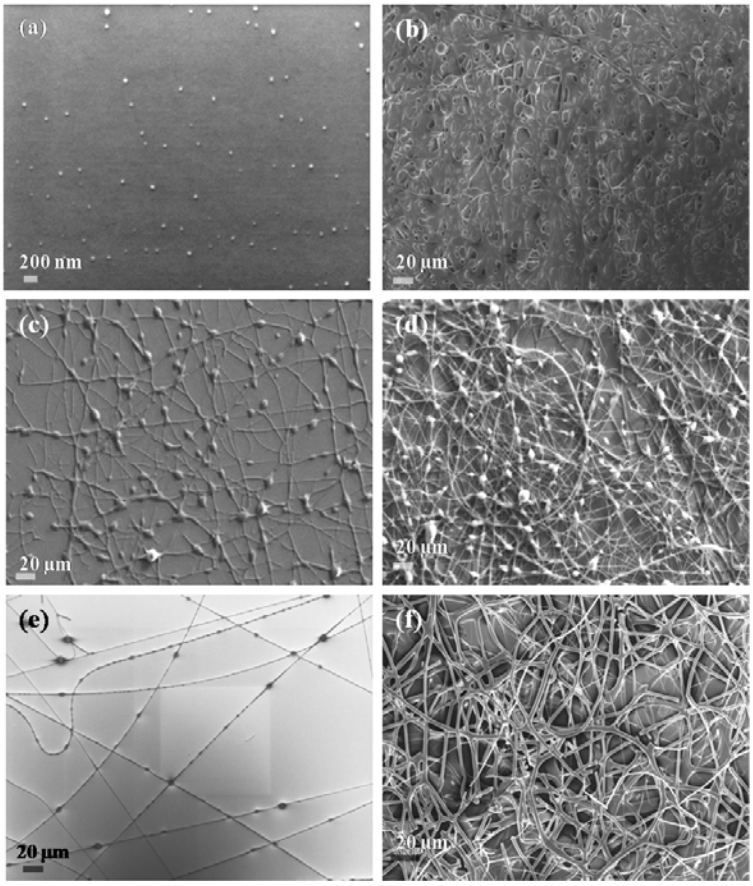


Fig.S1: FESEM micrographs of the products obtained by electrospinning at different volume ratios of the organic/pre-ceramic polymer blend: (a) PMHS, (b) 1:1, (c) 2:1, (d) 3:1, (e) 7:1, (f) 10:1. [Scale bars: (a) 200nm, (b)-(f) 20µm.]

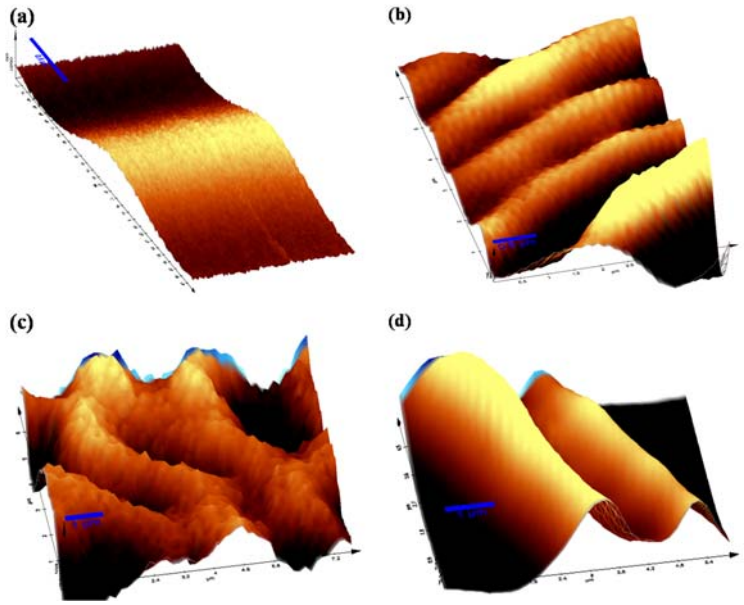


Fig.S2: Confocal micrographs of silica fibers at different calcinations temperatures: (a) 550 ^{o}C, (b) 800 ^{o}C, (c) 1000 ^{o}C and (d) 1400 ^{o}C.

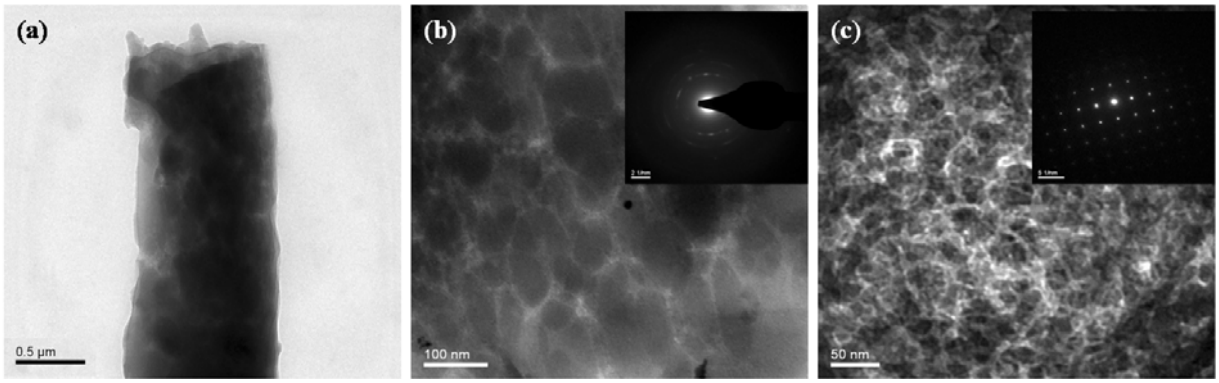
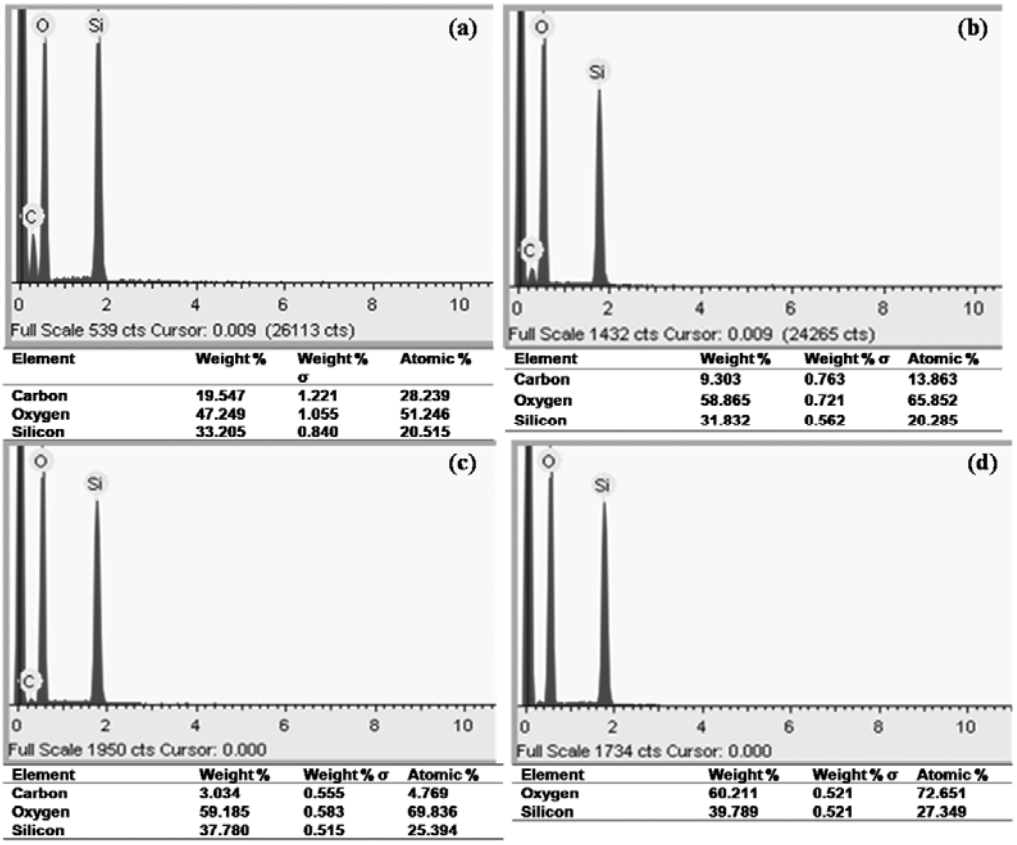


Fig.S3: TEM images ((a)-(c)) and SAED patterns (inset (b) and (c)) of fibers calcined at 800 ^{o}C ((a), (b),) and 1400 ^{o}C ((c)).



Element	Weight %	Weight % σ	Atomic %
Carbon	19.547	1.221	28.239
Oxygen	47.249	1.055	51.246
Silicon	33.205	0.840	20.515

Element	Weight %	Weight % σ	Atomic %
Carbon	9.303	0.763	13.863
Oxygen	58.865	0.721	65.852
Silicon	31.832	0.562	20.285

Element	Weight %	Weight % σ	Atomic %
Carbon	3.034	0.555	4.769
Oxygen	59.185	0.583	69.836
Silicon	37.780	0.515	25.394

Element	Weight %	Weight % σ	Atomic %
Oxygen	60.211	0.521	72.651
Silicon	39.789	0.521	27.349

Fig.S4: EDX Spectrum of silica fibers at different calcinations temperatures: (a) 550 ^{o}C, (b) 800 ^{o}C, (c) 1000 ^{o}C and (d) 1400 ^{o}C.

Table S5: Crystal planes in silica calcined at 1400 ^{o}C.

2θ^{0}	**d-spacing (Å)**	**Crystal plane (hkl)**
22.2	*3.9703*	*(101)*
28.8	*3.09*	*(111)*
31.6	*2.8109*	*(102)*
36.5	*2.4608*	*(200)*

Scherrer formula for calculation of the average crystallite size, incorporating the full width at half-maximum (FWHM) of the major diffraction peak corresponding to the (101) crystal plane

$$\text{Crystallite size (avg.)} = \frac{k\lambda}{B\cos\theta}$$

$$\text{Lattice strain (mean lattice distortion)} = \frac{B}{4\tan\theta}$$

$$B_{size} = B_{obsv} - B_{stnd}$$

$$B_{strain} = (B^2_{obsv} - B^2_{stnd})^{0.5}$$

where, '$B^0(2\theta)$' is the structural broadening, i.e. difference in the integral profile width between a standard and an unknown sample, and 'k', the Scherrer constant, 'θ', the Bragg's diffraction angle and 'λ', the wavelength of X-ray radiation used.

Computation of dislocation density (δ) following Williamson and Smallman's approach:

$$\delta = \frac{1}{D^2}$$

where, 'D' is the average crystallite size

Table S6: Crystallite size, dislocation density and lattice strain as a function of calcination temperature.

Calcination temperature (^{o}C)	Crystallite size, D (nm)	Dislocation density, δ	Lattice strain (%)
800	12.2	0.0070	1.476
1000	15	0.004	1.205
1400	34	0.001	0.527

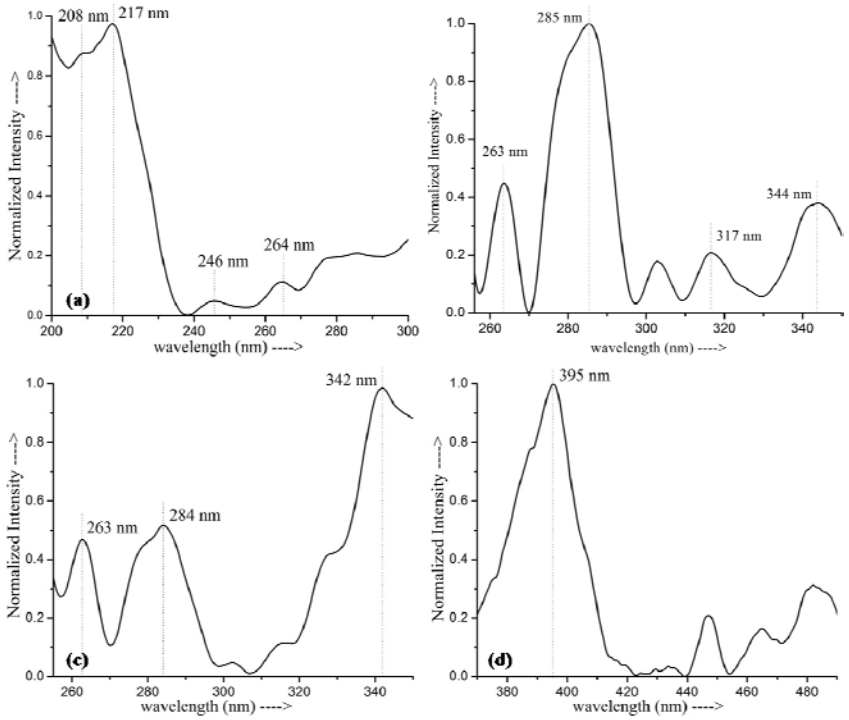


Fig. S7: PLE spectra of silica fibers calined at 550 ^{o}C at $\lambda_{emission}$ (a) 333 nm, (b) 410 nm, (c) 436 nm and (d) 537 nm.

Table S8: Lifetimes and their amplitudes of PMHS/PVP and silica fibers at different calcination temperatures, at λ_{ex} = 267 nm and λ_{em} = 436 nm.

Sample type	A_1	τ_1 (ns)	A_2	τ_2 (ns)
PMHS/PVP	0.869	2.594	0.131	14.310
silica@550 ^oC	0.990	2.092	0.010	13.606
silica@800 ^oC	0.996	1.678	0.004	12.582
silica@1000 ^oC	1.000	1.447	-	-
silica@1400 ^oC	0.999	1.343	0.001	11.216

The decays are fitted with biexponential functions:

$$I(t) = I(0)[A_1\exp(-t/\tau_1) + A_2\exp(-t/\tau_2)]$$

τ_1 and τ_2 are the two lifetimes and A_1 and A_2 are the respective amplitudes, such that $A_1 + A_2 = 1$.

Table S9: Lifetimes and their amplitudes of silica fibers calcined at 550 ^oC at different emission wavelengths at λ_{ex} = 267 nm.

λ_{em} (nm)	A_1	τ_1 (ns)	A_2	τ_2 (ns)
333	1	1.424	-	-
410	0.896	2.059	0.014	13.845
436	0.990	2.092	0.01	13.606
537	1	2.266	-	-

Table S10: Lifetimes and their amplitudes of silica fibers calcined at 550 ^oC at λ_{ex} and λ_{em}.

λ_{em} (nm)	λ_{ex} (nm)	A_1	τ_1 (ns)	A_2	τ_2 (ns)
436	267	0.990	2.092	0.01	13.606
	385	0.999	1.679	0.001	12.316
537	267	1	2.266	-	-
	385	1.000	2.009	-	-
	488	1.000	1.626	-	-

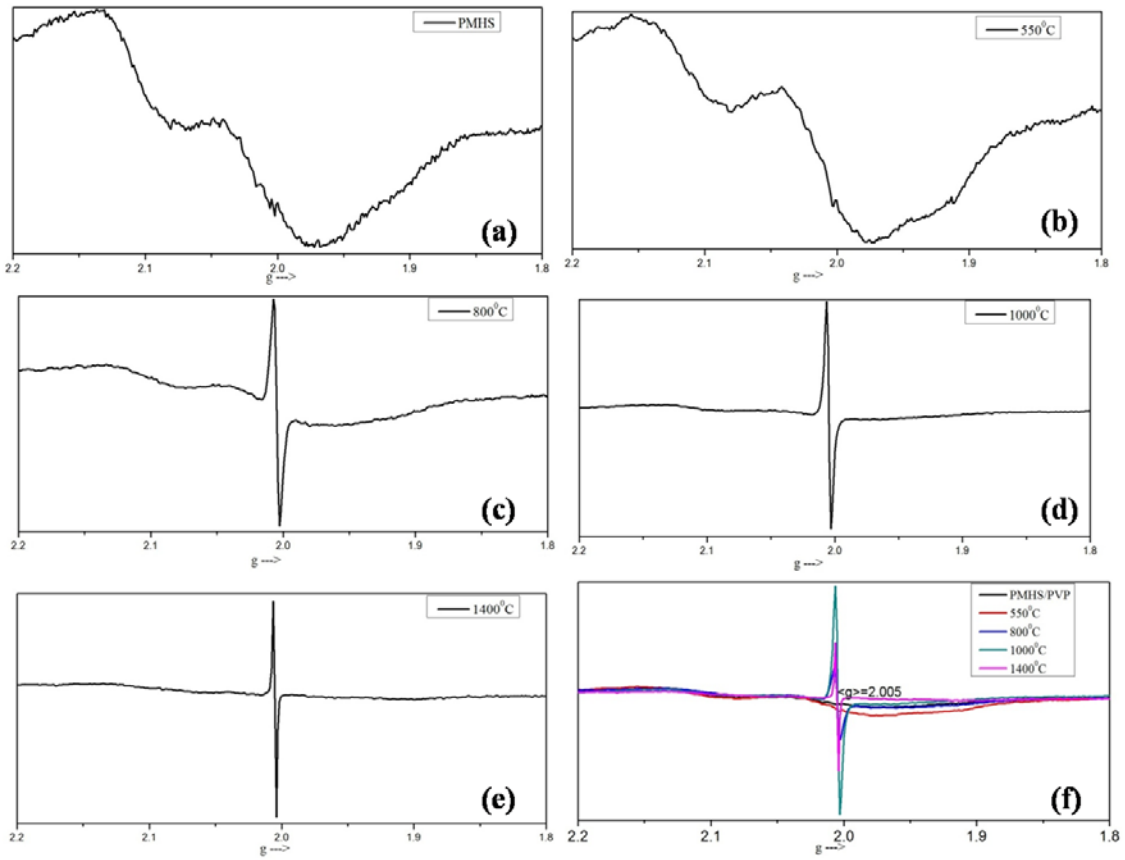


Fig S11: EPR characterization of (a) PMHS/PVP hybrid and silica fibers: (b) 550 ^{o}C, (c) 800 ^{o}C, (d) 1000 ^{o}C, (e) 1400 ^{o}C and (f) (a)-(e) superimposed.