Supplementary Information

Sub-nano MgF_2 embedded in carbon nanofiber and electrospun MgF_2 nanofiber by one-step electrospinning as highly efficient catalysts for 1,1,1-trifluoroethane dehydrofluorination

Wenfeng Han*, Chunpeng Zhang, Haili Wang, Shenglan Zhou, Haodong Tang*, Luteng Yang, Zhikun Wang

Institute of Industrial Catalysis, Zhejiang University of Technology, Hangzhou 310032, Zhejiang, PR China

*Corresponding Author. Email: hanwf@zjut.edu.cn (W.H)

tanghd@zjut.edu.cn (H.D. Tang)

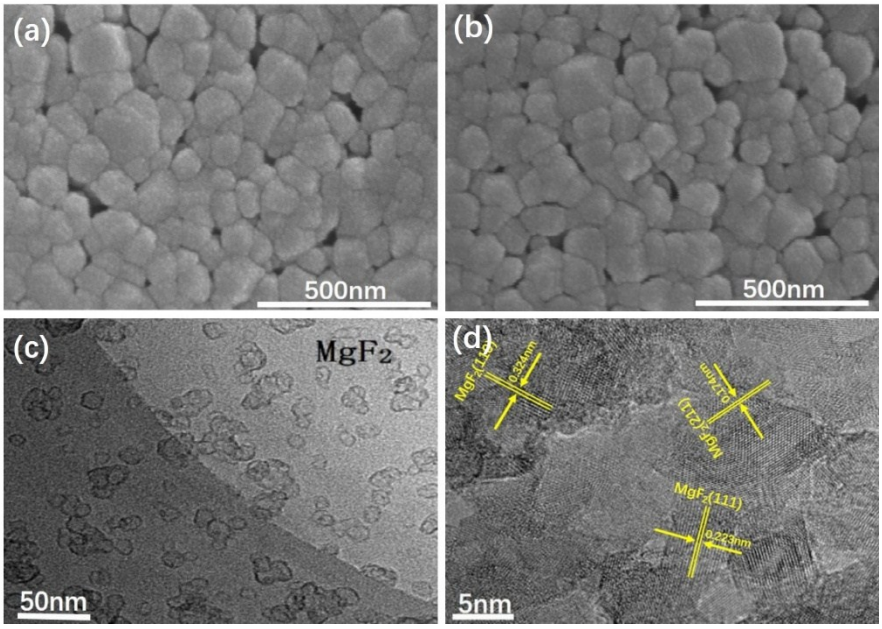

Figure S1 SEM images (a and b) and TEM images (c and d) of precipitated MgF_2.

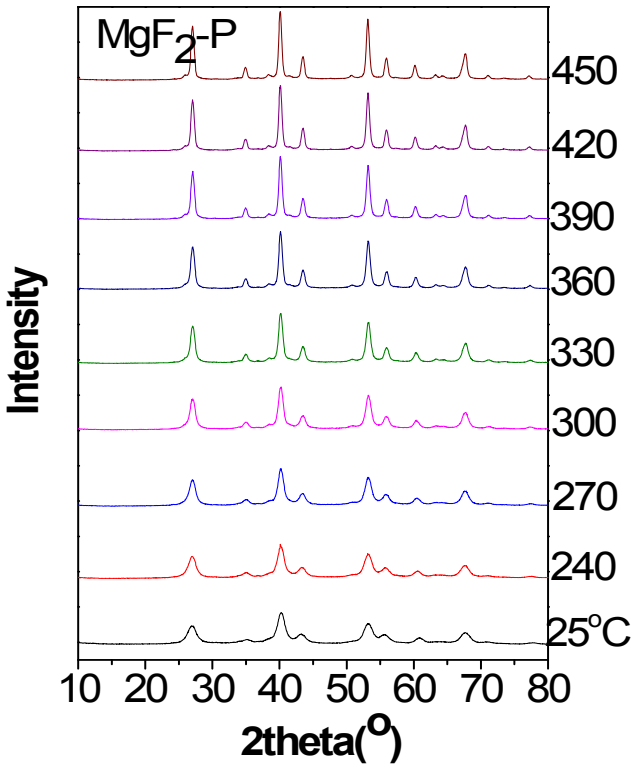

Figure S2 In situ XRD spectra of precipitated MgF_2 at temperatures between 25 °C and 450 °C.

Table S1 Increase of crystalline size of precipitated MgF_2 with temperature

T, °C	Crystalline size (nm)		
	(110)	(111)	(211)
25	5.3	6.6	5.7
240	6.1	7.7	6.9
270	6.1	7.7	5.2
300	8.9	10.7	10.0
330	10.9	12.7	12.5
360	13.1	14.5	14.5
450	16.4	17.5	19.3

Table S2 Crystalline size of precipitated MgF_2 after calcination at 650 °C for 5 h.

Catalyst	Crystalline size(nm)		
	110	111	211
Precipitated MgF_2 (Fresh)	85	94.9	80.3
Spent (Reaction at 450℃)	>100	>100	>100
Spent (Reaction at 500℃)	>100	>100	>100

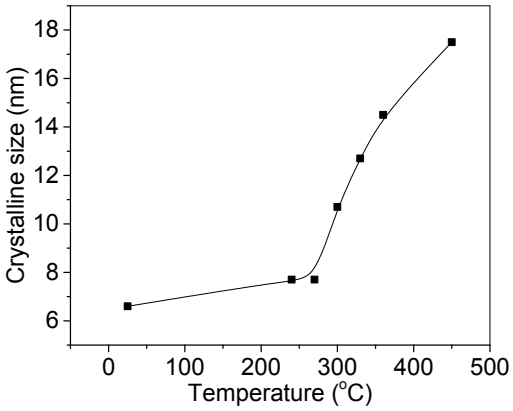

Figure S3 Crystalline size of plane (111) at temperatures between 25 °C and 500 °C for precipitated MgF_2.

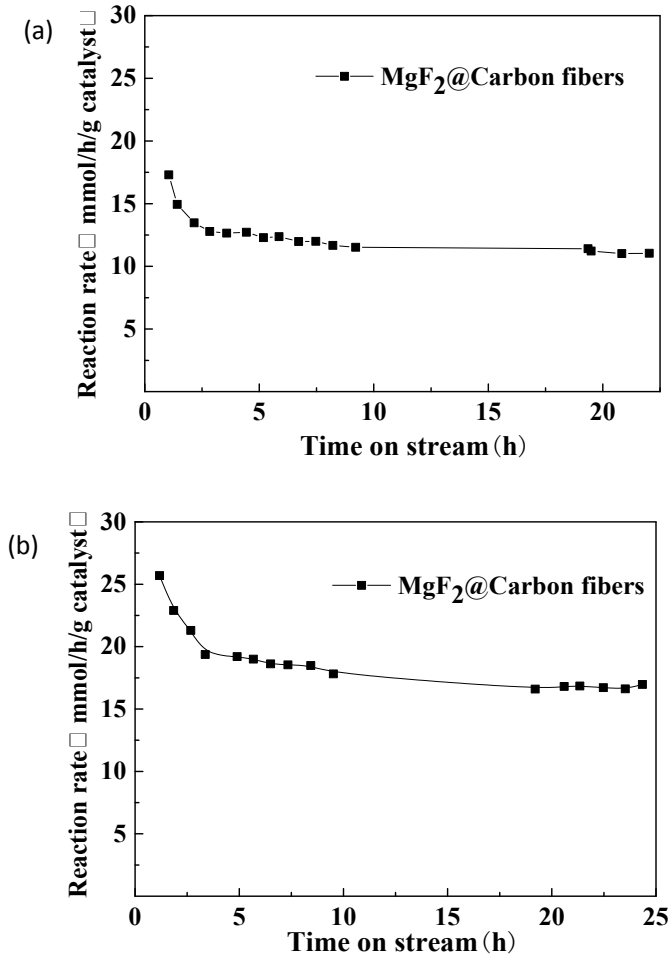

Figure S4 Dehydrofluorination of 1,1,1-trifluoroethane over nano MgF_2 embedded in nanofiber at (a) 450 °C and (b) 500 °C. GHSV for 1,1,1-trifluoroethane of 1200h^{-1} and diluted by equimolar N_2.

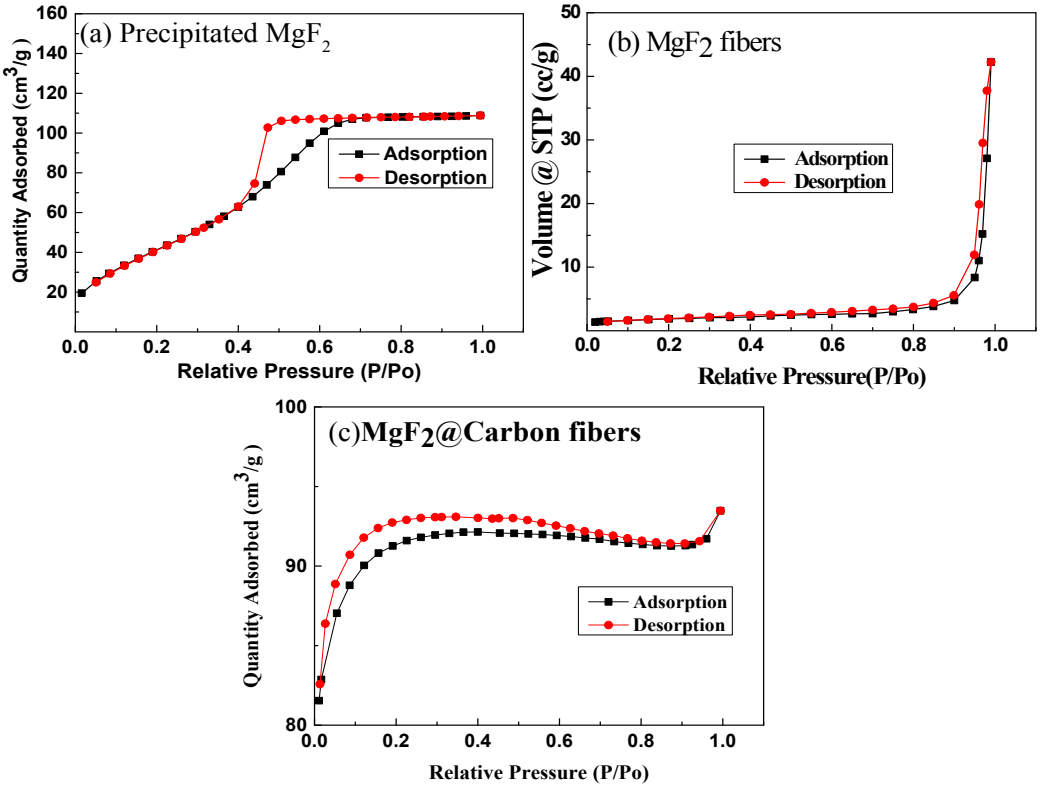

Figure S5 N_2 adsorption–desorption isotherms of (a) precipitated MgF_2, (b)electrospun MgF_2 fibers and (c) nano MgF_2 embedded in carbon nanofiber.

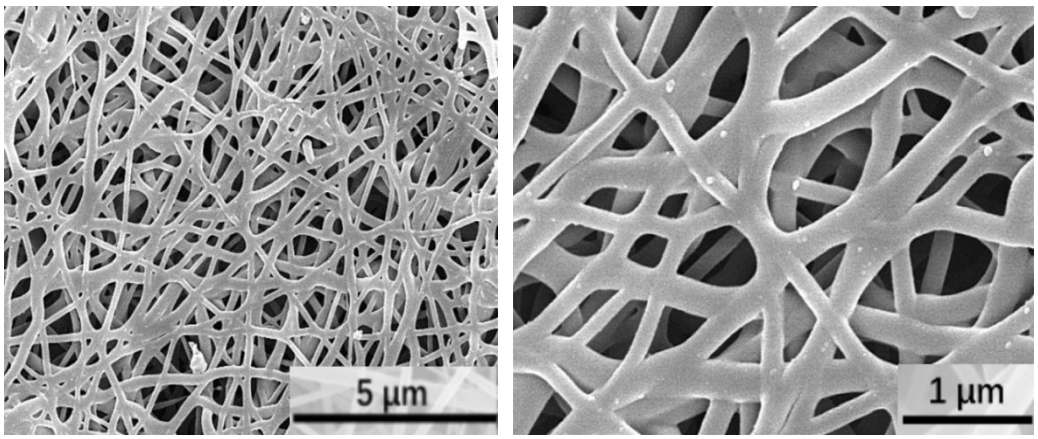

Figure S6 SEM images nano MgF_2 embedded in nanofiber after reaction at 450 °C.

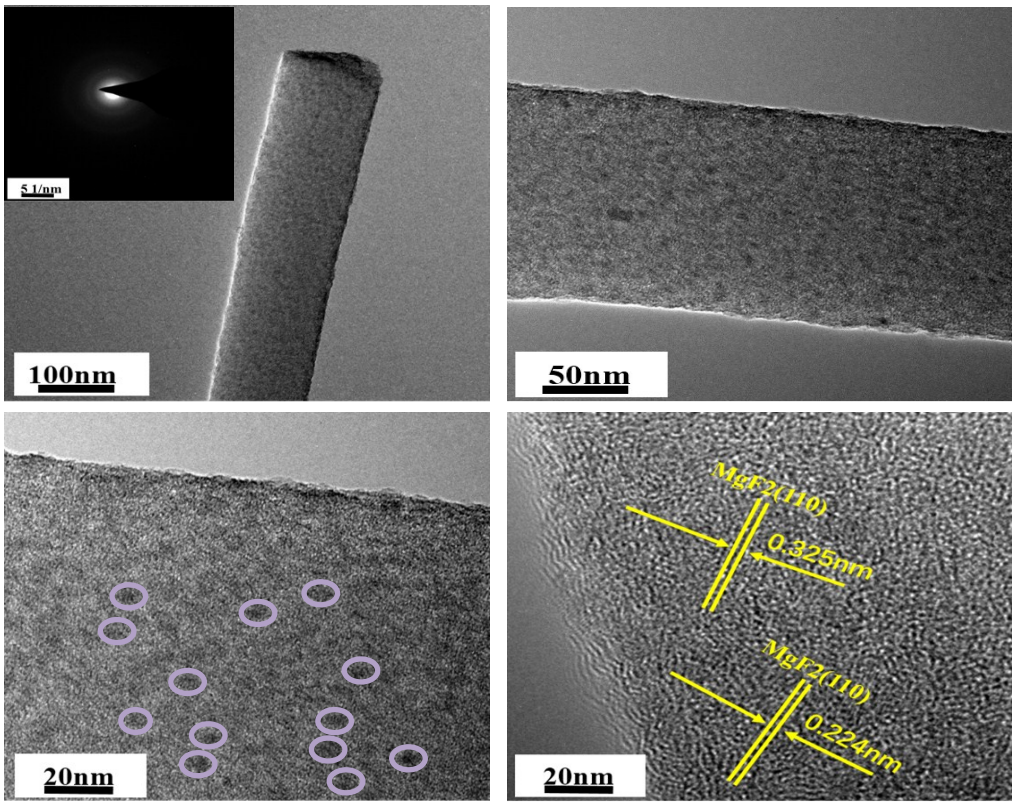

Figure S7 TEM images nano MgF_2 embedded in nanofiber after reaction at 450 ^oC.

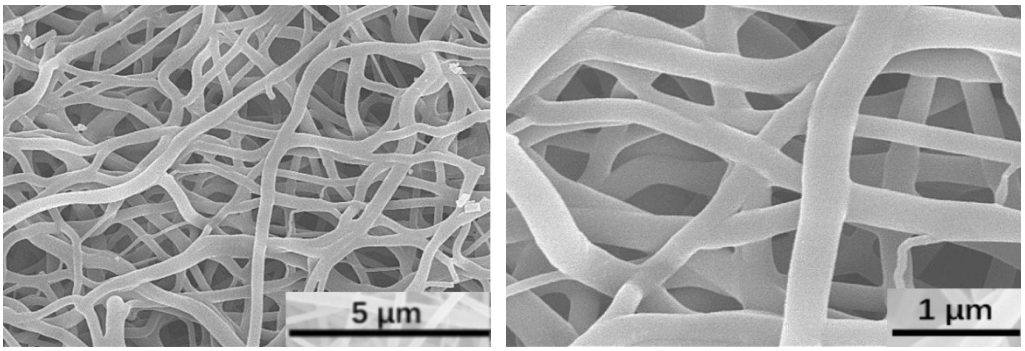

Figure S8 SEM images nano MgF_2 embedded in nanofiber after reaction at 500 ^oC.

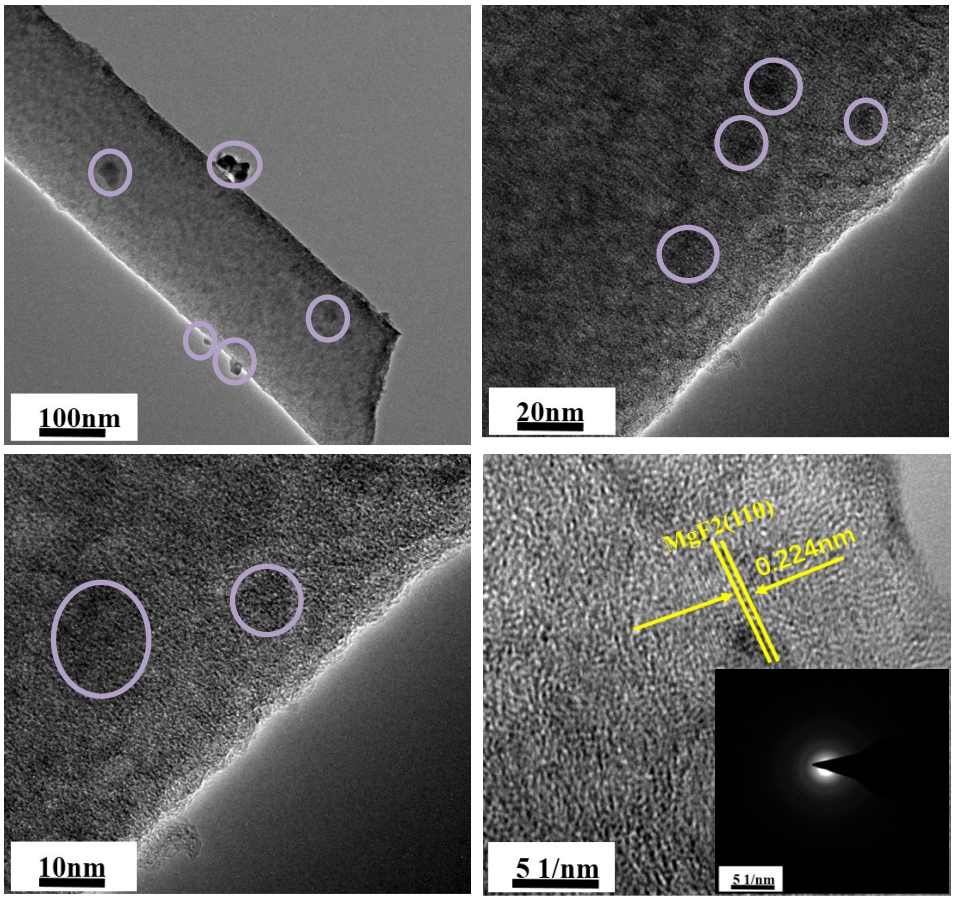

Figure S9 TEM images nano MgF_2 embedded in nanofiber after reaction at 500 ^oC.

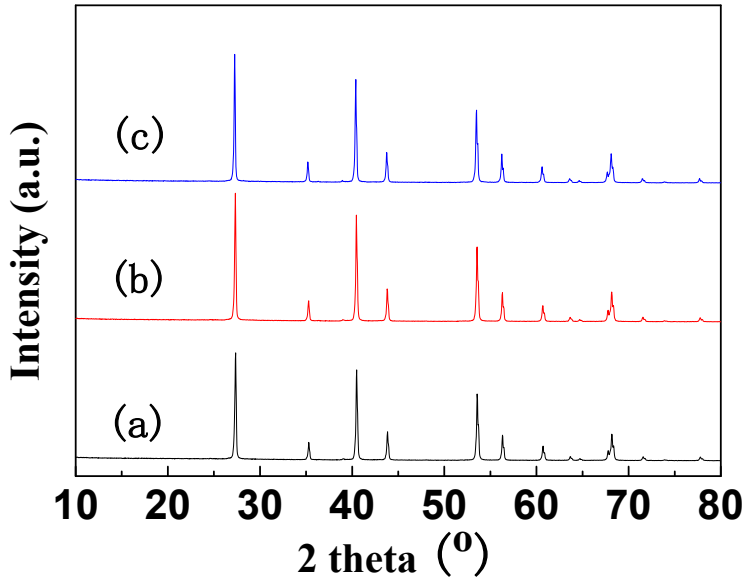

Figure S10 X-ray diffraction (XRD) patterns of precipitated MgF_2 following calcination at 650 ^oC for 5 h. (a) before reaction, (b) spent MgF_2 after reaction at 450 ^oC and (c) spent MgF_2 after reaction at 500 ^oC.

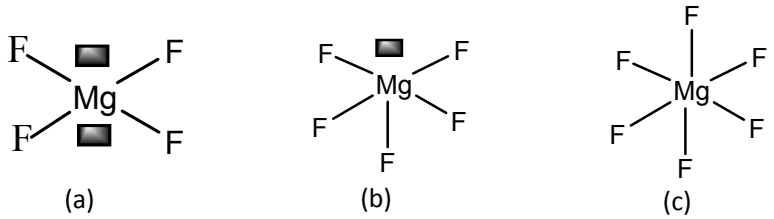

Figure S11 (a) 4-fold coordinated, (b) 5-fold coordinated and (c) 6-fold coordinated MgF_2.

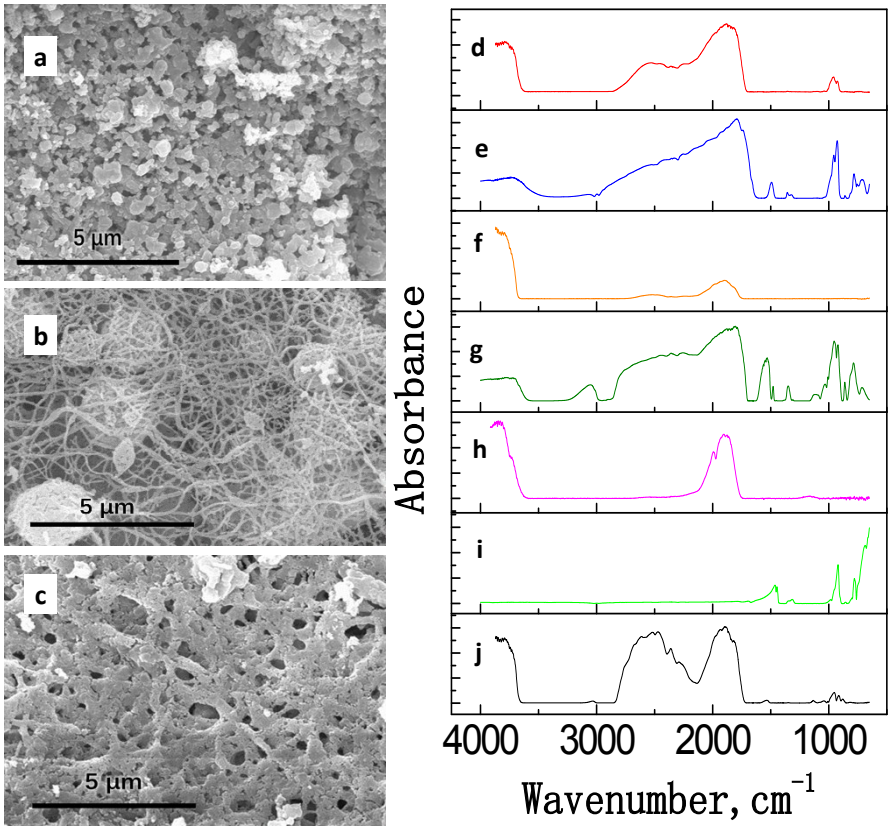

Figure S12 SEM images of MgF_2 with (a) absence of PVP in electrospinning solution; (b) 0.05 g/mL PVP in electrospinning solution; (c) 0.1 g/mL in electrospinning solution and FT-IR spectra of fibers derived from the electrospinning solution (d) PVDF + PVP + $Mg(CH_3COO)_2{\cdot}4H_2O$ + DMF; (e) PVDF + $Mg(CH_3COO)_2{\cdot}4H_2O$ + DMF; (f) PVP + $Mg(CH_3COO)_2{\cdot}4H_2O$ + DMF; (g) PVP + PVDF + DMF; (h) $Mg(CH_3COO)_2{\cdot}4H_2O$; (i) PVDF+DMF; (j) PVP+DMF

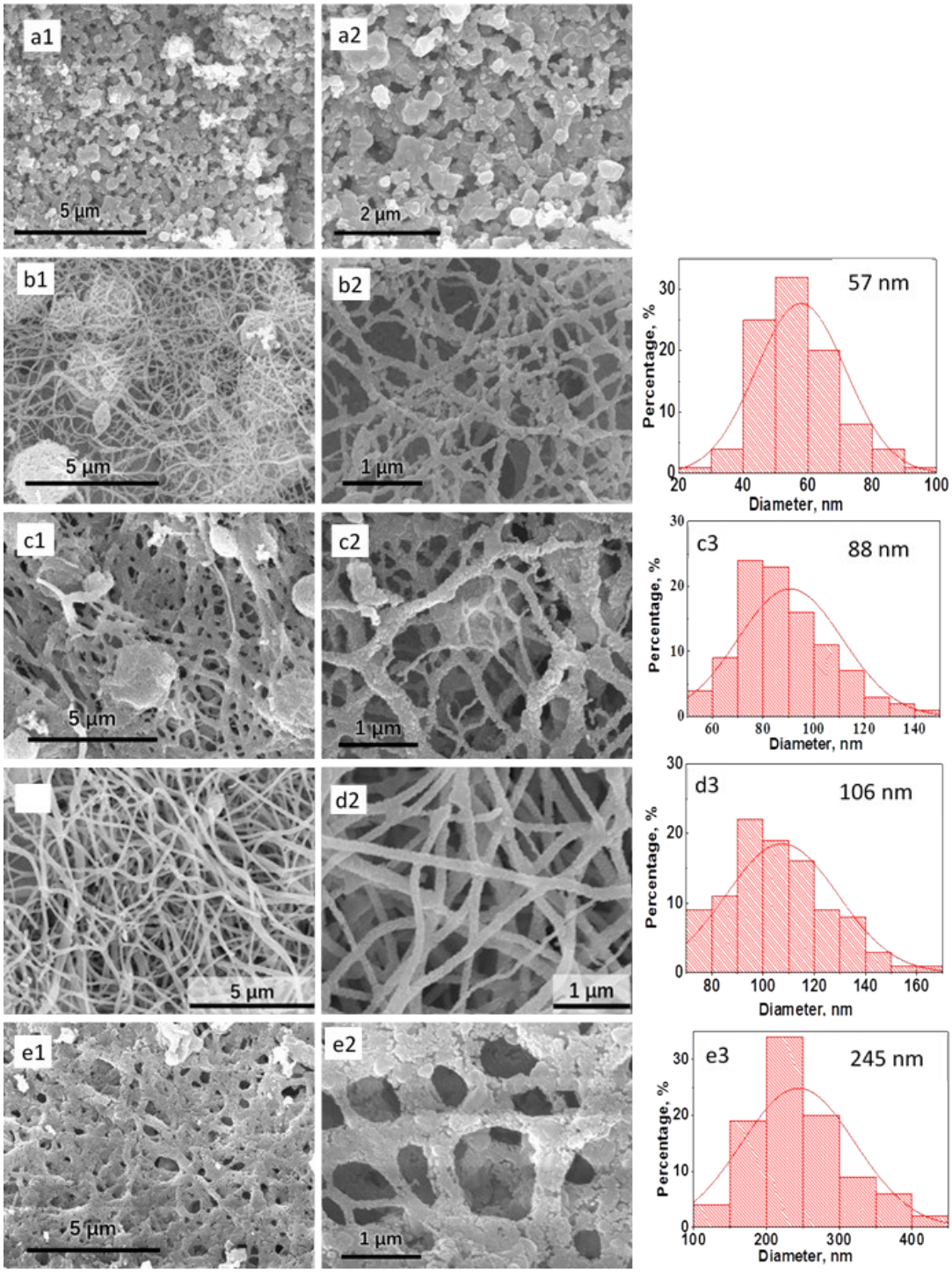

Fig. S13 Effect of PVP concentration on the Electrospun MgF_2 nanofibers. SEM images and fiber diameter distribution of MgF_2 with PVP concentration (a) 0 g/mL; (b) 0.05 g/mL (c) 0.07 g/mL; (d) 0.08 g/mL and (d) 0.10 g/mL in the electrospinning solution.

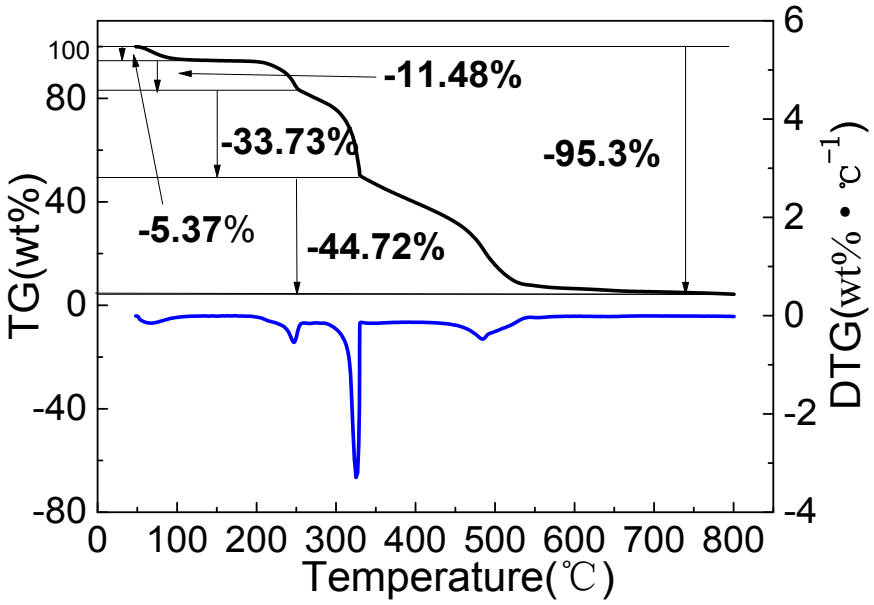

Figure S14 TG-DTG of PVP/PVDF/$Mg(CH_3COO)_2{\cdot}4H_2O$ nanofibers with ramp rate of 10 ^oC/min in air atmosphere.