Electronic Supplementary Information

Hydrothermal Synthesis of defect induced pristine α-$NaCe(WO_4)_2$: a novel material for solid state lightening and gas sensing

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Table S1: Coordination environment of triclinic NCWO structure.

Coordinates atoms	x	y	Z	Occupancy	Site occupancy	symmetry
Na1	0.2815	0.7733	0.1567	1.0	1a	1
Na2	0.7184	0.2266	0.8432	1.0	1a	1
Ce1	0.1740	0.2878	0.4547	1.0	1a	1
Ce2	0.2860	0.7121	0.5452	1.0	1a	1
O1	0.1823	0.3500	0.7987	1.0	1a	1
O2	0.8176	0.6500	0.2012	1.0	1a	1
O3	0.4619	0.6413	0.2627	1.0	1a	1
O4	0.5380	0.4586	0.7372	1.0	1a	1
O5	0.8659	0.0119	0.1955	1.0	1a	1
O6	0.1340	0.9880	0.8044	1.0	1a	1
O7	0.7074	0.0107	0.4898	1.0	1a	1
O8	0.2925	0.9893	0.5101	1.0	1a	1
O9	0.1740	0.6339	0.5530	1.0	1a	1
O10	0.8259	0.3660	0.4469	1.0	1a	1
O11	0.4847	0.8316	0.0074	1.0	1a	1
O12	0.5152	0.1683	0.9925	1.0	1a	1
O13	0.0578	0.3132	0.1062	1.0	1a	1

O14	0.9421	0.6868	0.8937	1.0	1a	1
O15	0.3906	0.1712	0.2675	1.0	1a	1
O16	0.6093	0.8287	0.7324	1.0	1a	1
W1	0.2753	0.2990	0.0396	1.0	1a	1
W2	0.7246	0.7009	0.9603	1.0	1a	1
W3	0.6569	0.1086	0.2887	1.0	1a	1
W4	0.3430	0.8913	0.7112	1.0	1a	1

Table S2: The details of the deconvolution of the FTIR bands

Samples	Peak position (cm^{-1})		Area (cm^2)	FWHM	χ^2
$NCWO_{120^0C}$	660-717	668.644	0.446	5.089	3.24
		679.572	0.112	7.247	
		698.572	0.172	13.993	
		707.462	0.065	8.798	
	718-777	742.568	0.477	15.444	3.30
		762.311	0.614	14.002	
	778-910	811.177	3.500	29.541	2.1
		852.943	5.599	38.620	
		879.857	3.377	28.367	
$NCWO_{140^0C}$	660-717	669.343	0.181	5.242	2.24
		680.665	0.047	5.993	
		700.475	0.118	13.643	
		704.758	0.042	15.349	
	718-777	738.186	0.342	12.033	3.81
		751.922	0.700	21.808	

	778-910	814.374	4.428	36.893	2.43
		852.670	5.636	40.724	
		881.042	3.264	26.692	

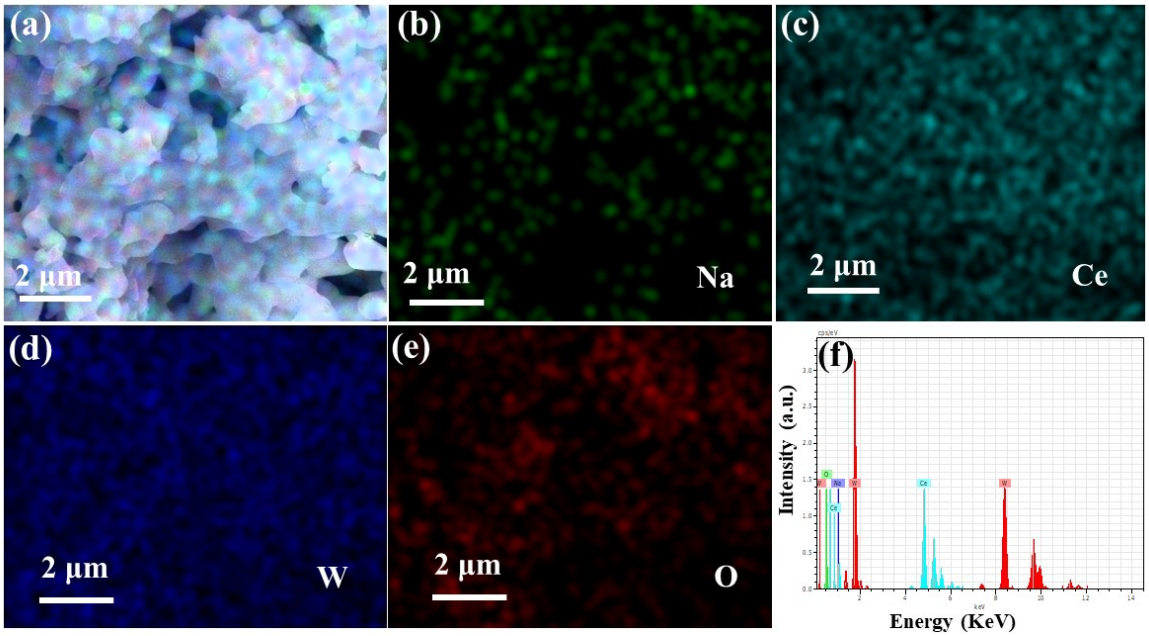

Figure S1: The elemental mapping of $NCWO_{120}{}^{0}{}_{C}$

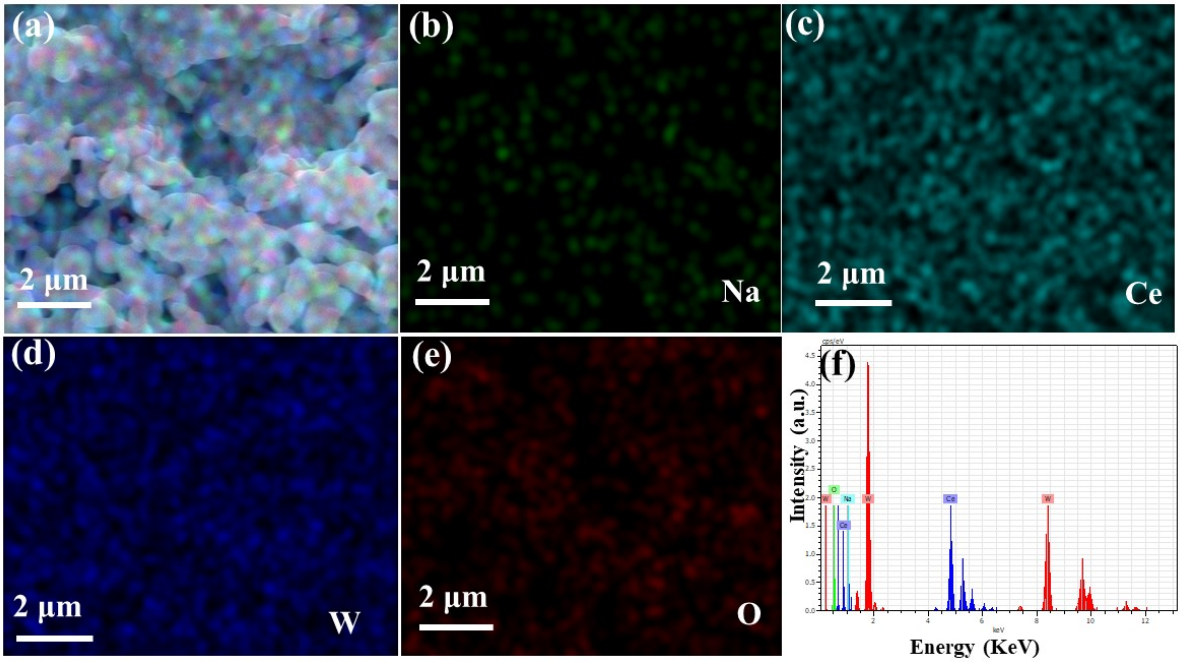

Figure S2: The elemental mapping of $NCWO_{140^0C}$

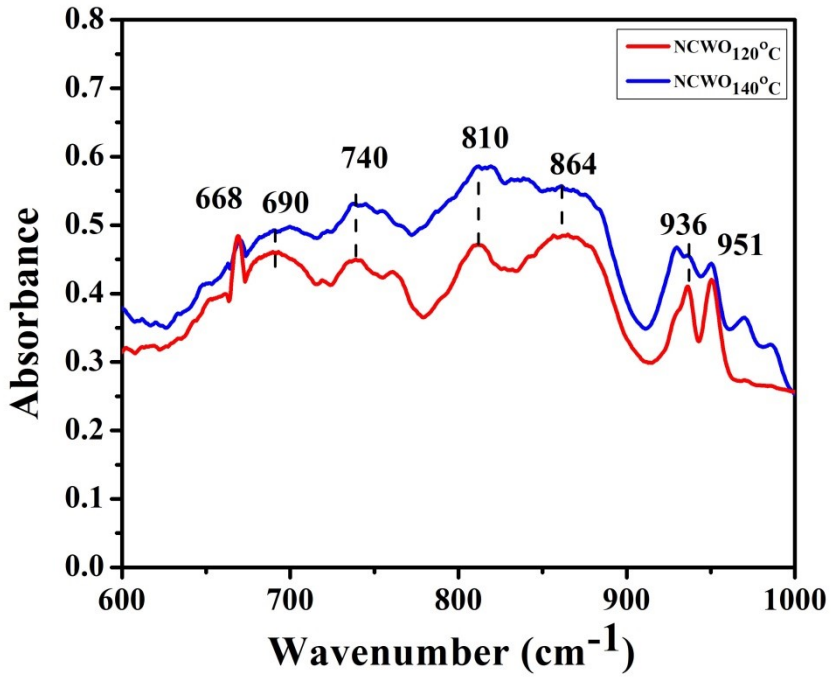

Figure S3: FTIR spectra of $NCWO_{120^0C}$ and $NCWO_{140^0C}$.

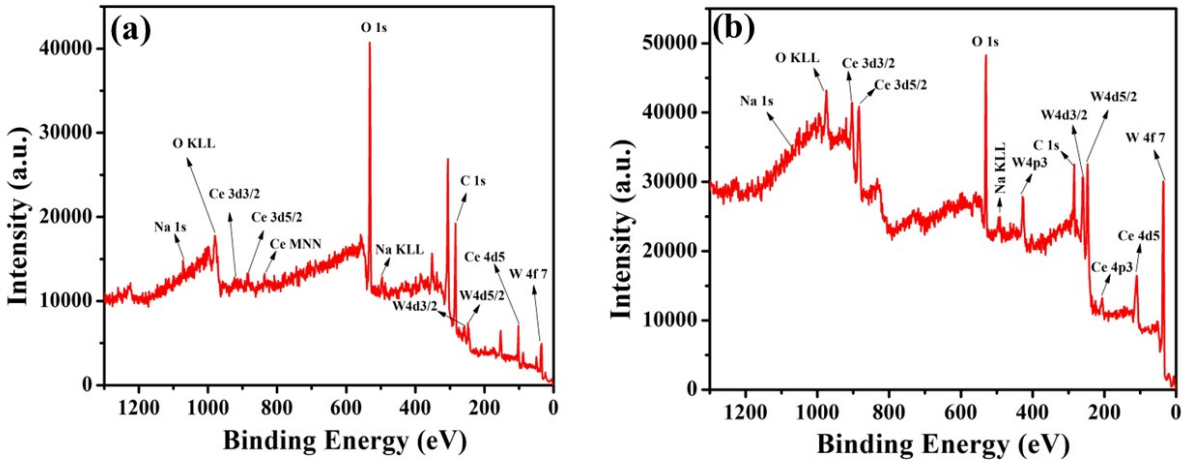

Figure S4: XPS wide spectrum of Ce-3d, W-4f, O-1s, Na-1s of (a) $NCWO_{120}{}^{0}C$ and (b) $NCWO_{140}{}^{0}C$ respectively.

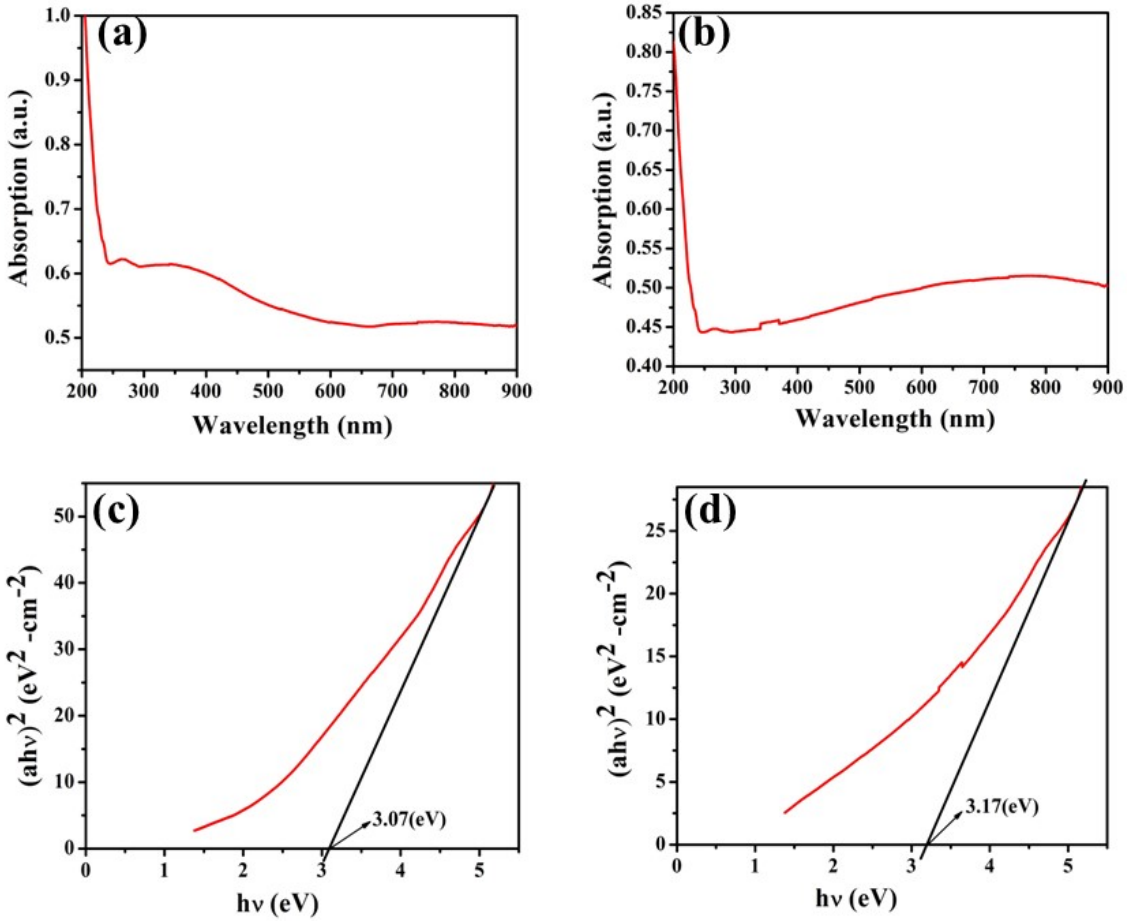

Figure S5: UV spectra (a, b) and corresponding band gap calculation (c, d) of $NCWO_{120}{}^{0}{}_{C}$ and $NCWO_{140}{}^{0}{}_{C}$ respectively.