Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Correlation of oxygen vacancy and upconversion of Er^{3+} incorporated $BaTiO_3$

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Instrumental information

The diffraction patterns of Er^{3+} incorporated $BaTiO_3$ (E-BT) were acquired by using an X-ray diffractometer (SmartLab multi-purpose X-ray diffractometer, Rigaku) with Cu Kα radiation. X-ray photoelectron spectra were measured by using X-ray photoelectron spectroscopy (NEXSA, Thermo Fisher Scientific). The photographs of E-BT under 980 nm excitation were taken by Nikon D5500. The upconversion emission spectra were obtained by using a focused 980 nm laser (1999 CHP, 3SP technologies) and detectors (HR2000+, Ocean insight).

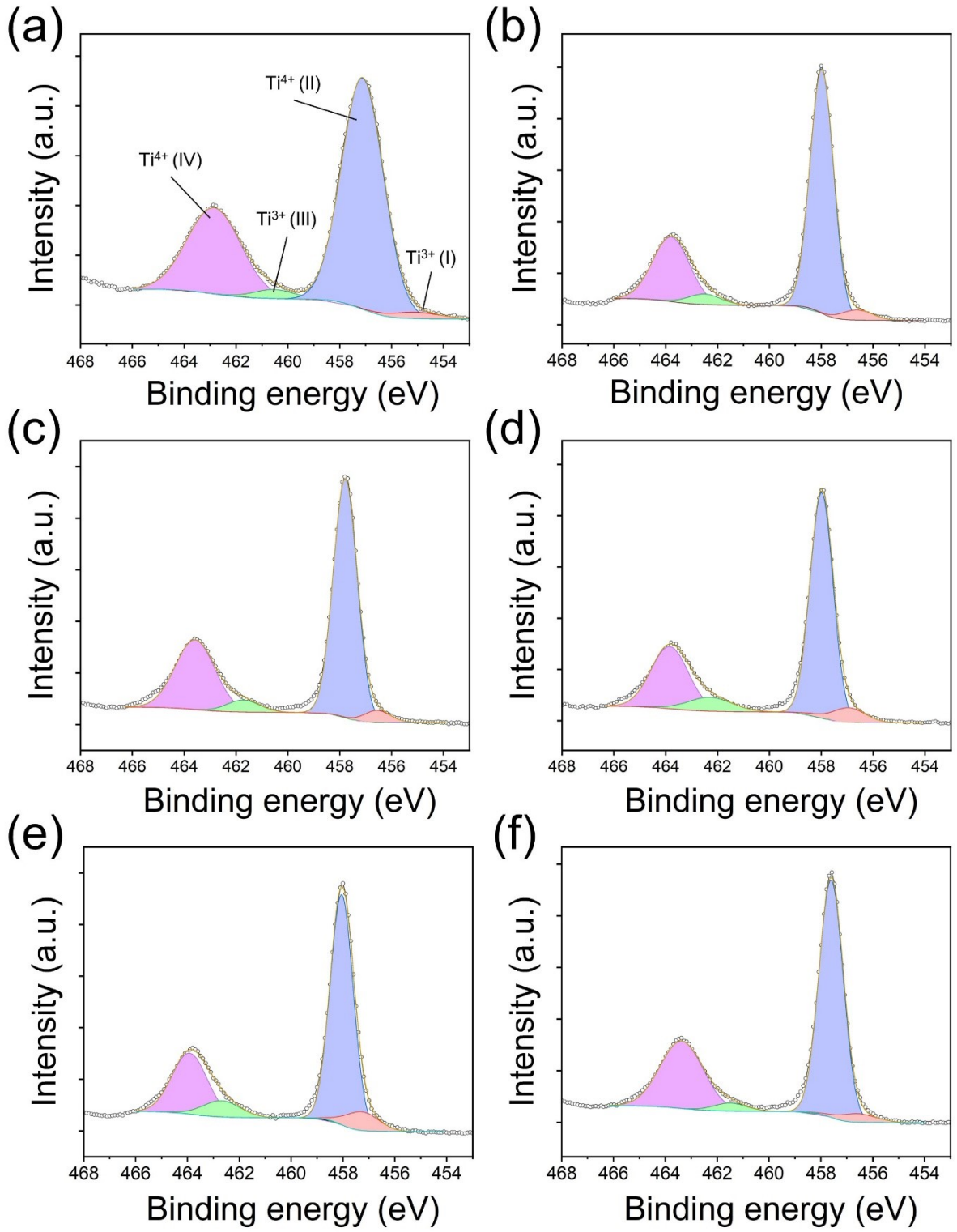

Figure S1. Ti 2p XPS spectra of E-BT annealed at 600 °C for different times. (a) - (f): E-BT was annealed for 0, 2, 4, 6, 8, and 12 h, respectively.

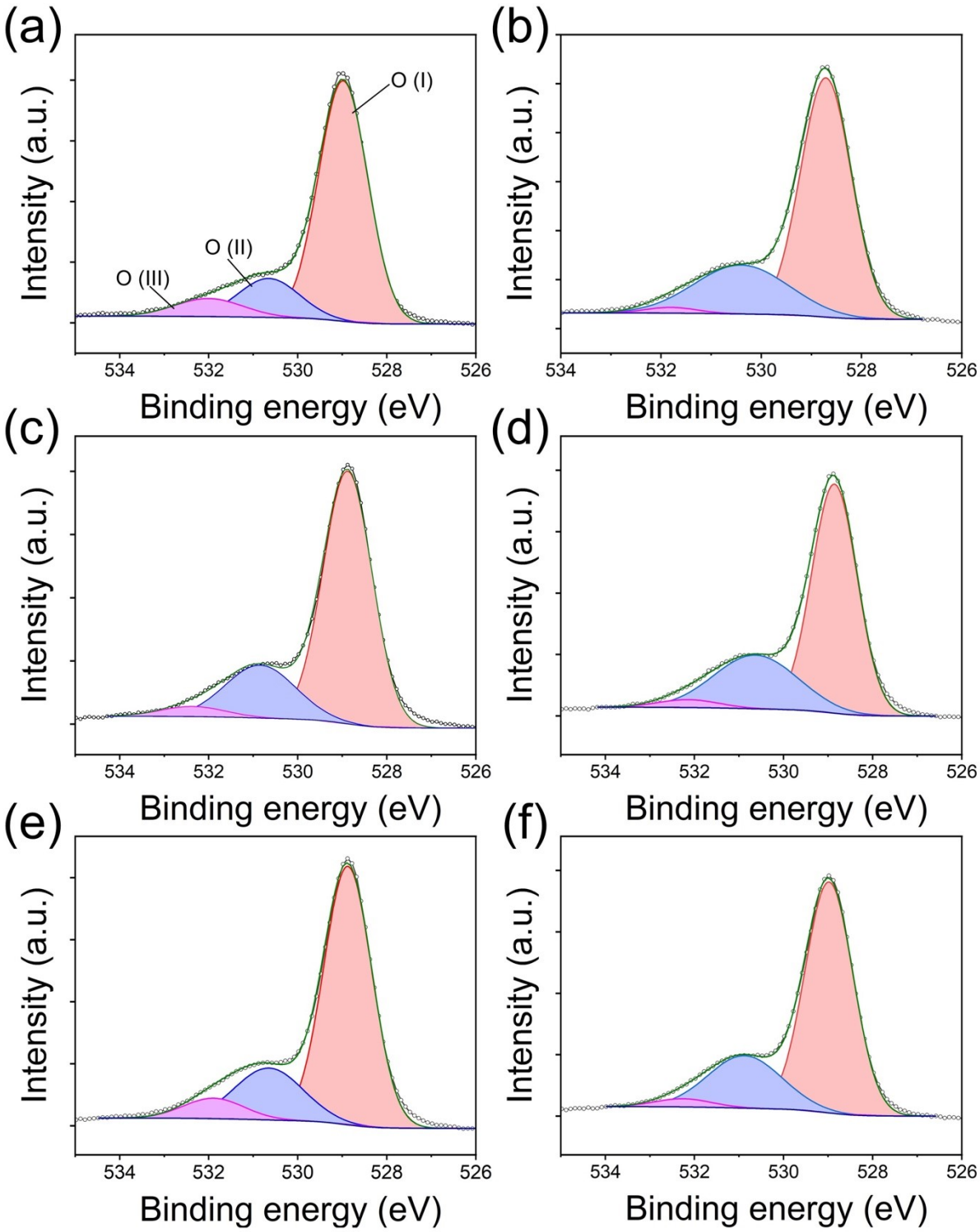

Figure S2. O 1s XPS spectra of E-BT annealed at different temperatures and times. (a) and (b): annealed at 600 °C for 6 and 12 h. (c) and (d): annealed at 800 °C for 6 and 12 h. (e) and (f): annealed at 1000 °C for 6 and 12 h. The integrated area value (A) of O (III) represents the amount of oxygen vacancy. Overall, the value of O (III) for 6 h annealing is larger the one for 12 h annealing.

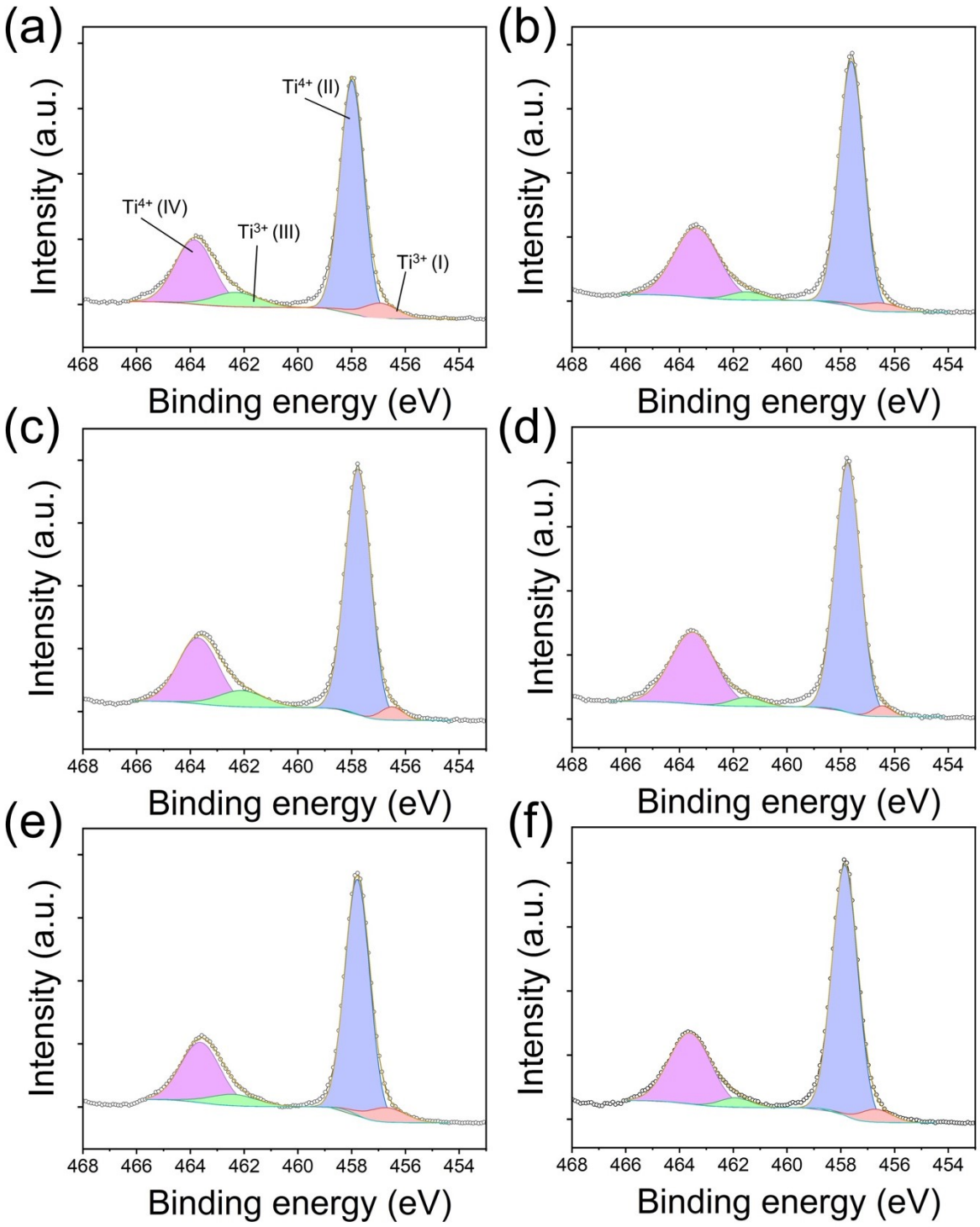

Figure S3. Ti 2p XPS spectra of E-BT annealed at different temperatures and times. (a) and (b): annealed at 600 °C for 6 and 12 h. (c) and (d): annealed at 800 °C for 6 and 12 h. (e) and (f): annealed at 1000 °C for 6 and 12 h. The integrated area value (A) of Ti^{3+} (I and III) represents the amount of oxygen vacancy. As same as O 1s XPS, the values of Ti (I) and (III) for 6 h annealing are larger the one for 12 h annealing.

Annealing time (h)	$A_{O\text{-}I}$	$A_{O\text{-}II}$	$A_{O\text{-}III}$	$A_{Ti\text{-}I}$	$A_{Ti\text{-}II}$	$A_{Ti\text{-}III}$	$A_{Ti\text{-}IV}$
0	120472.01	66658.13		2678.69	84918.51	3251.87	40308.47
2	141464.37	45399.56	3336.55	4666.42	85454.22	5126.36	35332.19
4	184296.47	41446.08	11980.62	5806.40	107066.54	7375.59	49152.87
6	102727.72	23887.01	13707.80	5945.46	63694.18	7492.02	28443.69
8	82389.78	21068.54	4904.96	4956.52	50491.74	6720.02	18775.32
12	123959.83	46740.71	2997.57	4320.94	80767.31	3676.83	40537.94

Table S1. Integrated area values (*A*) of O 1s and Ti 2p XPS spectra of E-BT annealed at 600 ^{o}C for 0, 2, 4, 6, 8, and 12 hours. Since the amount of O_V in 0 h annealed E-BT, the XPS peak was not confirmed.

Annealing Temperature (^{O}C)	Annealing time (h)	$A_{O\text{-}I}$	$A_{O\text{-}II}$	$A_{O\text{-}III}$	$A_{Ti\text{-}I}$	$A_{Ti\text{-}II}$	$A_{Ti\text{-}III}$	$A_{Ti\text{-}IV}$
600	6	102727.72	23887.01	13707.80	5945.46	63694.18	7492.02	28443.69
	12	123959.83	46740.71	2997.57	4320.94	80767.31	3676.83	40537.94
800	6	148802.03	44453.54	7768.10	4504.39	93524.96	8269.58	40361.76
	12	128565.12	55218.66	5871.76	2719.34	83491.71	3752.69	42038.73
1000	6	168947.61	48007.70	16781.38	8886.79	104971.79	8839.21	42190.57
	12	137395.43	47812.55	5703.26	5410.98	84273.80	3906.13	38796.27

Table S2. Integrated area values (*A*) of O 1s and Ti 2p XPS spectra of E-BT. E-BT annealed at 600, 800, and 1000 ^{o}C for 6 and 12 hours.

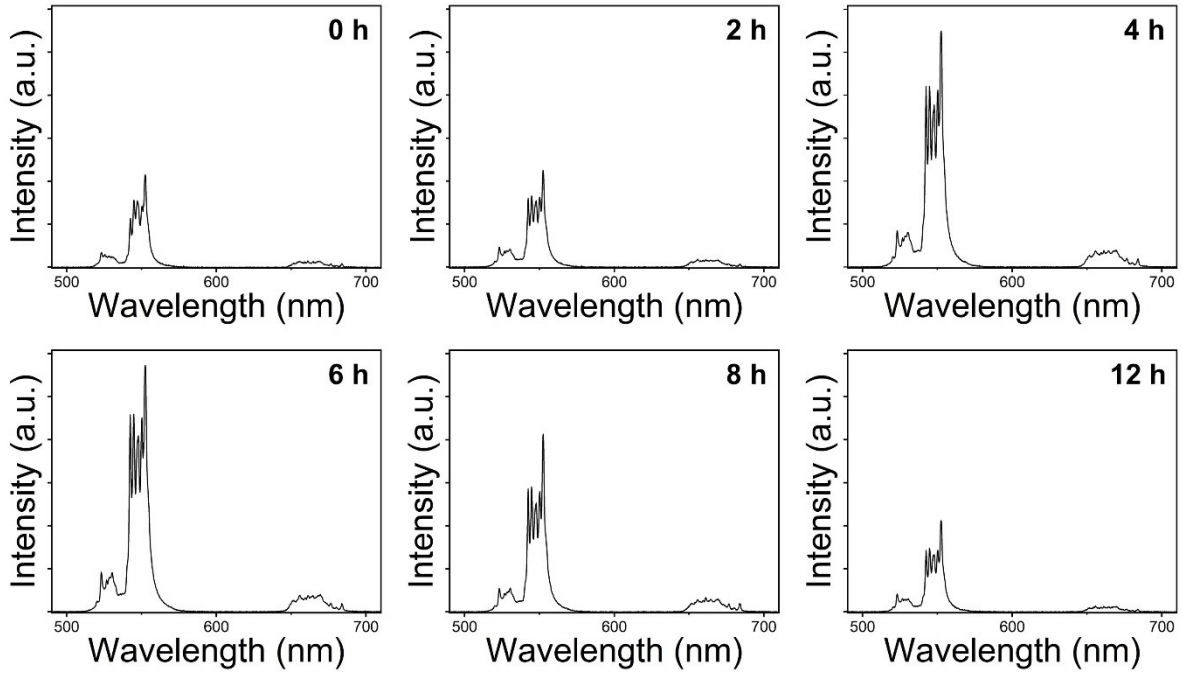

Figure S4. UC spectrea of annealed E-BT, from 0 to 12 h (Under 980 nm excitation).

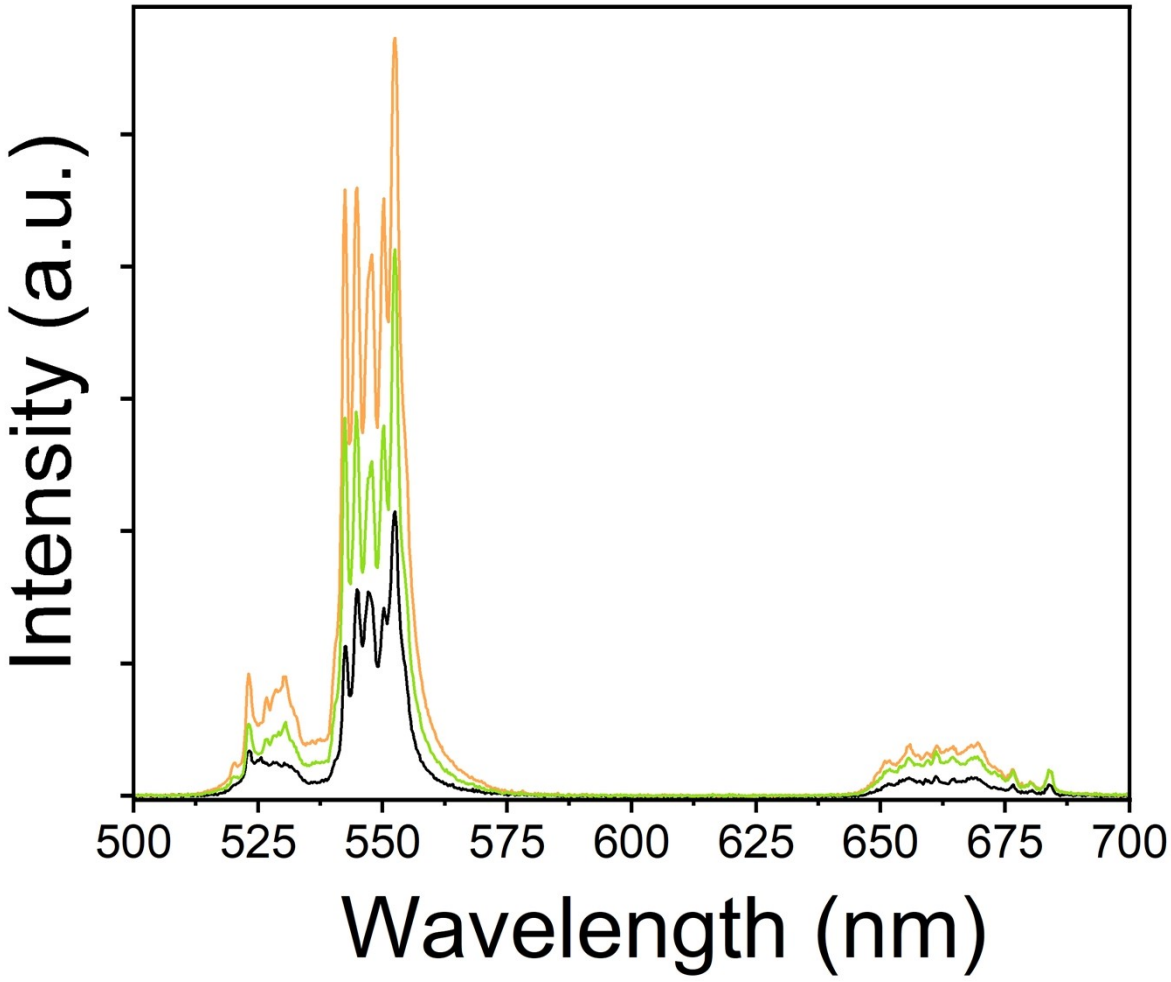

Figure S5. Comparison for UC spectra of E-BT annealed at 600 °C. Black is 0 h, orange is 6 h, and green is 8 h annealed E-BT (Under 980 nm excitation).

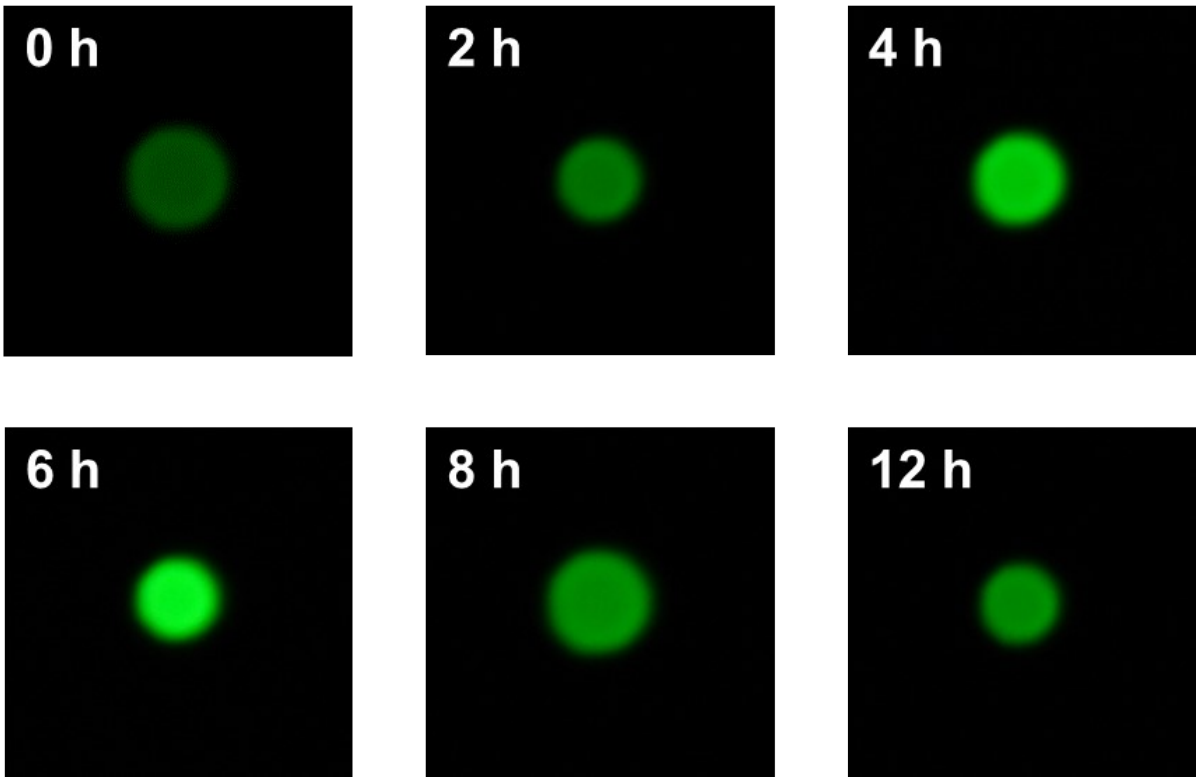

Figure S6. Photographs of post-annealed E-BT (Under 980 nm excitation).

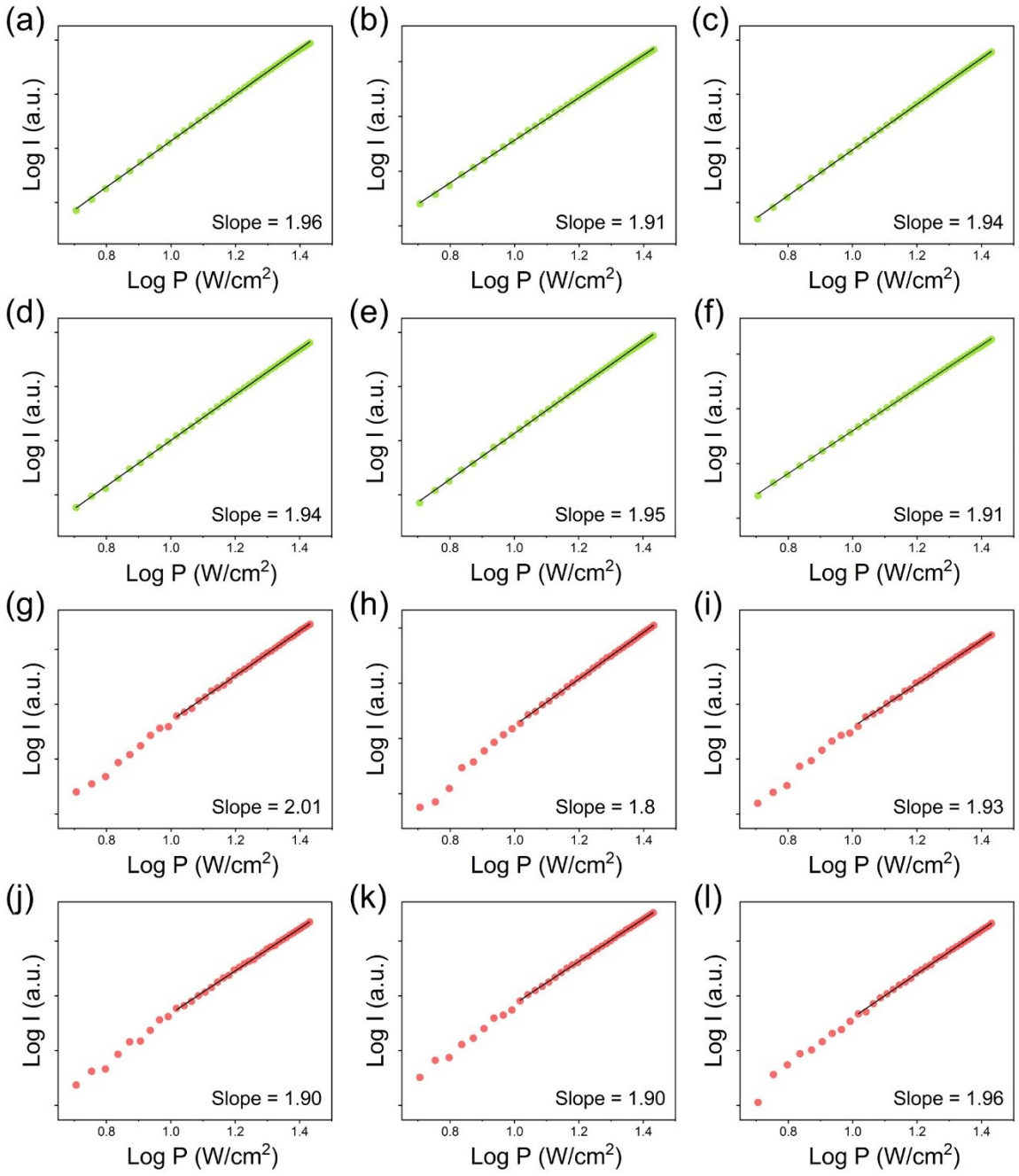

Figure S7. (a-f) Pump-power dependence of $^2H_{11/2}$, $^4S_{3/2} \rightarrow {}^4I_{15/2}$ (green) emission of annealed E-BT for 0, 2, 4, 6, 8, and 12 h, respectively, and (g-i) $^4F_{9/2} \rightarrow {}^4I_{15/2}$ (red) emission of annealed E-BT for 0, 2, 4, 6, 8, and 12 h, respectively.