

## Electronic Supplementary Information (ESI)

### Dopant site-dependent luminescence from rare-earth doped dibarium octafluorohafnate $\text{Ba}_2\text{HfF}_8$ nanocubes for radiation detection

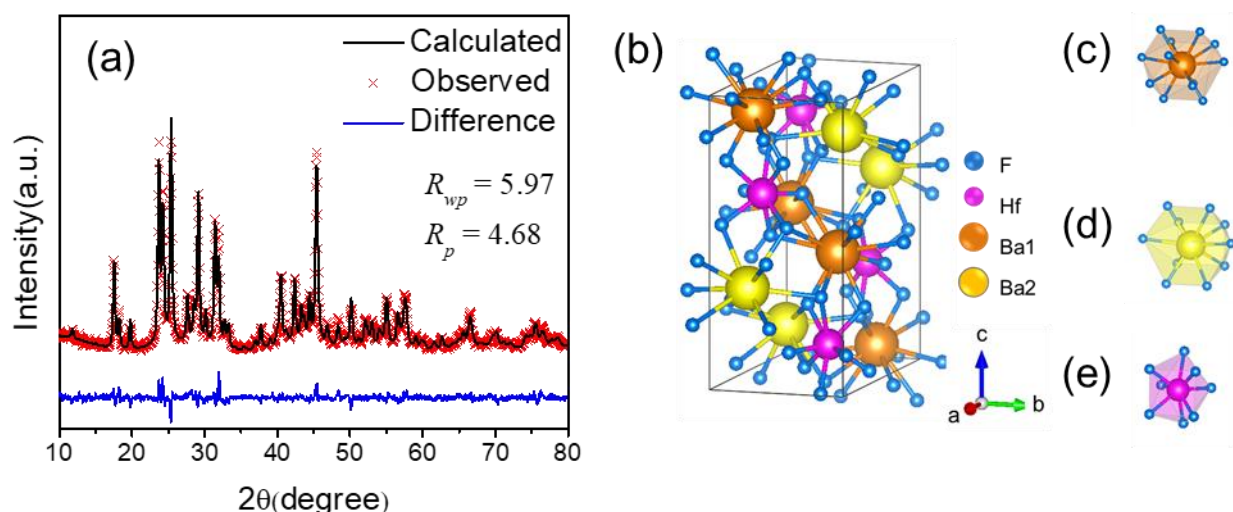
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## Results



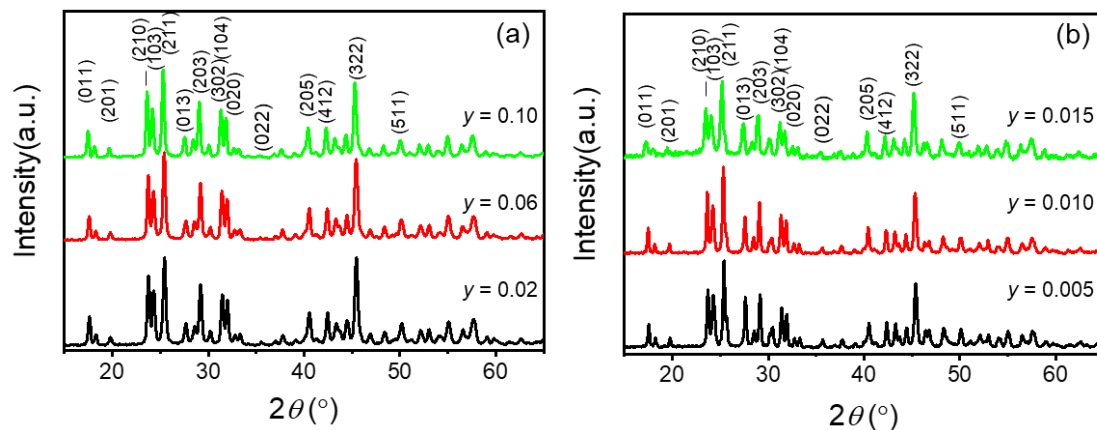
**Fig. S1** (a) XRD Rietveld refinement of  $\text{Ba}_2\text{HfF}_8$ ; (b) crystal structure of  $\text{Ba}_2\text{HfF}_8$ ; (c–e) coordination environment of Ba1, Ba2, and Hf cations, respectively.

**Table S1** Rietveld refined parameters from the XRD patterns of the  $\text{Ba}_2\text{HfF}_8$  [space group  $Pnma$  (62),  $a = 9.798 \text{ \AA}$ ,  $b = 5.636 \text{ \AA}$ ,  $c = 11.920 \text{ \AA}$ ,  $R_{wp} = 5.97\%$ , and  $R_p = 4.68\%$ ].

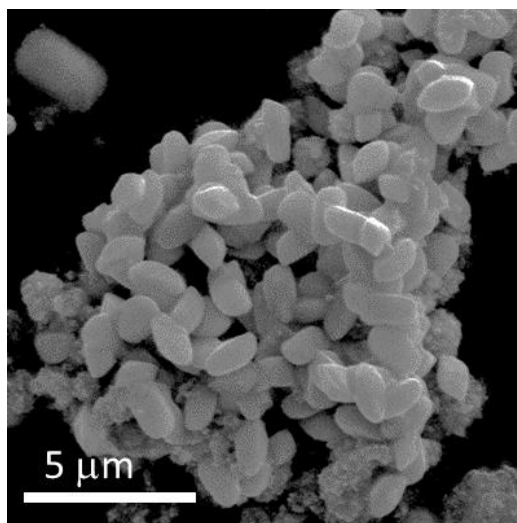
| Atom | Site | x     | y     | z     | Occupancy |
|------|------|-------|-------|-------|-----------|
| Ba1  | 4c   | 0.868 | 0.250 | 0.940 | 1.000     |
| Ba2  | 4c   | 0.438 | 0.250 | 0.155 | 1.000     |
| Hf   | 4c   | 0.246 | 0.250 | 0.858 | 1.000     |
| F    | 8d   | 0.102 | 0.464 | 0.873 | 1.000     |
| F    | 8d   | 0.144 | 0.993 | 0.457 | 1.000     |
| F    | 8d   | 0.346 | 0.462 | 0.739 | 1.000     |
| F    | 4c   | 0.143 | 0.250 | 0.014 | 1.000     |
| F    | 4c   | 0.146 | 0.250 | 0.685 | 1.000     |

**Table S2** Lattice parameters and unit cell volume of  $\text{Ba}_{2-x}\text{HfF}_8\text{:Tb}_x$  ( $x = 0-0.5$ ).

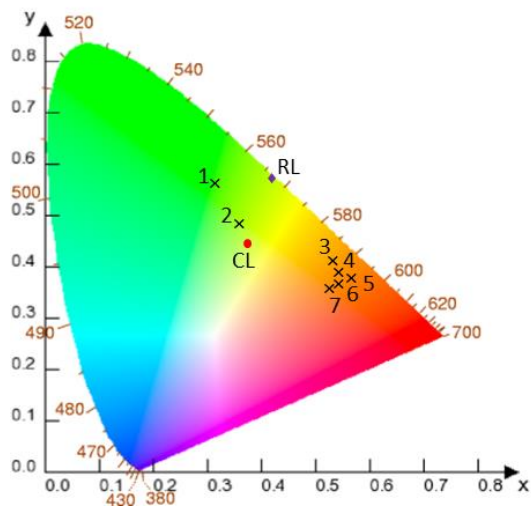
| $x =$ | $a$ (Å) | $b$ (Å) | $c$ (Å) | $V$ (Å <sup>3</sup> ) |
|-------|---------|---------|---------|-----------------------|
| 0     | 9.798   | 5.636   | 11.920  | 658.52                |
| 0.1   | 9.794   | 5.631   | 11.899  | 656.23                |
| 0.3   | 9.759   | 5.616   | 11.883  | 651.36                |
| 0.5   | 9.785   | 5.612   | 11.870  | 650.12                |



**Fig. S2** (a) XRD patterns of  $\text{Ba}_{2-y}\text{HfF}_8\text{:Eu}_y$  samples; (b) XRD patterns of  $\text{Ba}_{1.5-y}\text{HfF}_8\text{:Tb}_{0.5-y}\text{Eu}_y$  samples.



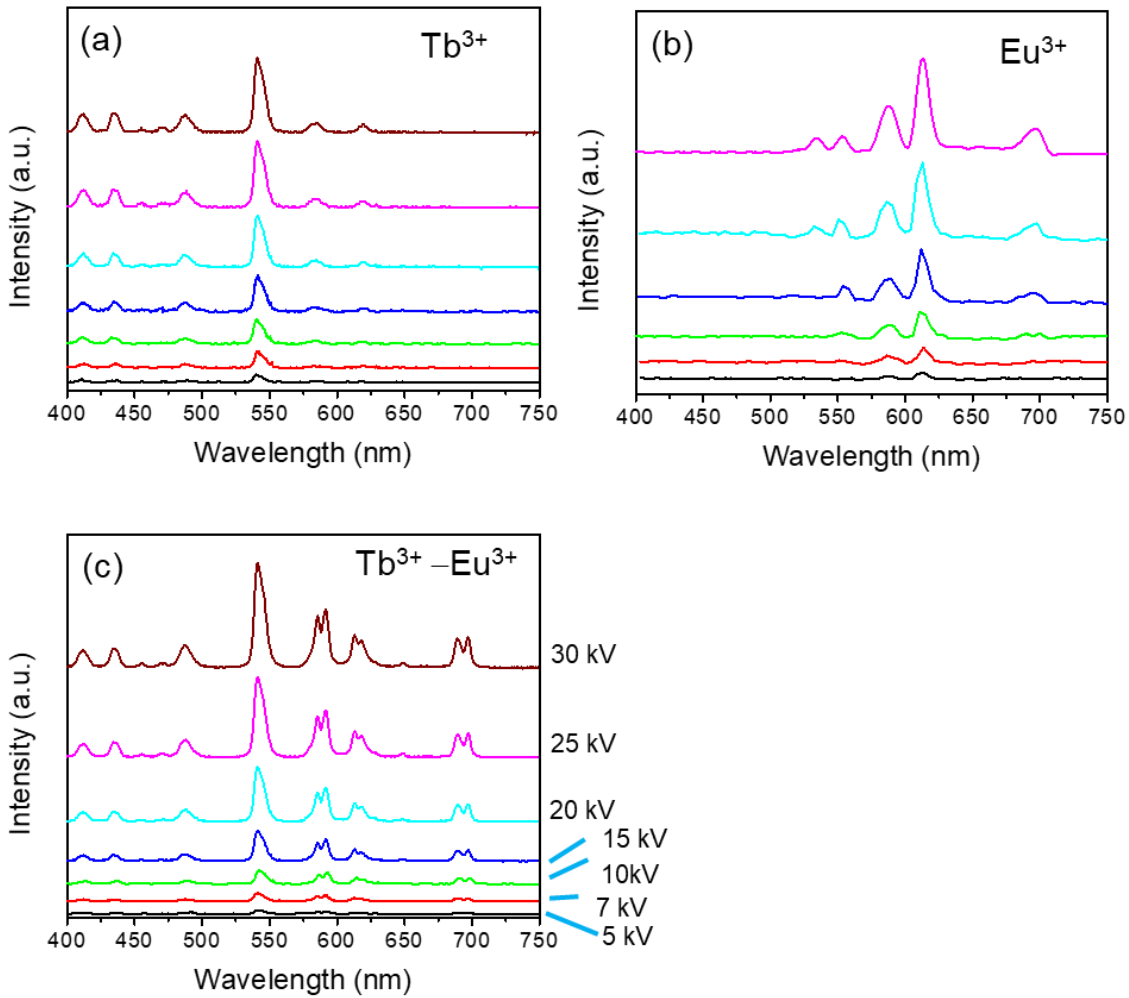
**Fig. S3** SEM image of  $\text{Ba}_{1.485}\text{HfF}_8\text{:Tb}_{0.50}\text{Eu}_{0.015}$  microparticles.



**Fig. S4** PL induced CIE coordinates at various  $\text{Eu}^{3+}$  amount in  $\text{Ba}_{1.5-y}\text{HfF}_8\text{:Tb}_{0.50}\text{Eu}_y$ . For  $y = 0.015$  (sample #6), corresponding CL and RL CIE coordinates are also shown.

**Table S3** CIE Coordinates calculated from the PL spectra of codoped BHF samples.

| No. | Sample composition<br>$\text{Ba}_{1.5-\gamma}\text{HfF}_8:\text{Tb}_{0.5^{3+}}-\text{Eu}_{\gamma^{3+}}$ | CIE (x) | CIE (y) |
|-----|---------------------------------------------------------------------------------------------------------|---------|---------|
| 1   | $\gamma = 0.000$                                                                                        | 0.315   | 0.557   |
| 2   | $\gamma = 0.001$                                                                                        | 0.359   | 0.485   |
| 3   | $\gamma = 0.002$                                                                                        | 0.537   | 0.421   |
| 4   | $\gamma = 0.005$                                                                                        | 0.543   | 0.398   |
| 5   | $\gamma = 0.010$                                                                                        | 0.559   | 0.396   |
| 6   | $\gamma = 0.015$ (PL)                                                                                   | 0.553   | 0.398   |
|     | $\gamma = 0.015$ (CL)                                                                                   | 0.376   | 0.432   |
|     | $\gamma = 0.015$ (RL)                                                                                   | 0.435   | 0.558   |
| 7   | $\gamma = 0.020$                                                                                        | 0.552   | 0.391   |



**Fig. S5** CL spectra of (a)  $\text{Ba}_{1.5}\text{HfF}_8:\text{Tb}_{0.50}$ , (b)  $\text{Ba}_{1.9}\text{HfF}_8:\text{Eu}_{0.1}$ , and (c)  $\text{Ba}_{1.485}\text{HfF}_8:\text{Tb}_{0.50}-\text{Eu}_{0.015}$ . The electron beam voltage, from the bottom plot to the top plot, is 5, 7, 10, 15, 20, 25 and 30 kV, respectively.