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SUPPORTING INFORMATION

Eu^{3+} activated BaF_2 nanostructured thin films: fabrication and a combined experimental and computational study of the energy conversion process

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A scheme of the single zone hot-wall reactor used for this study is reported in Fig. S1.

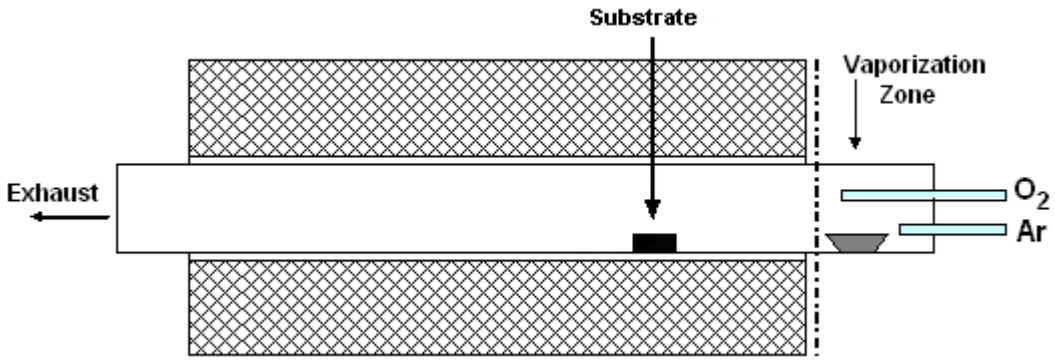
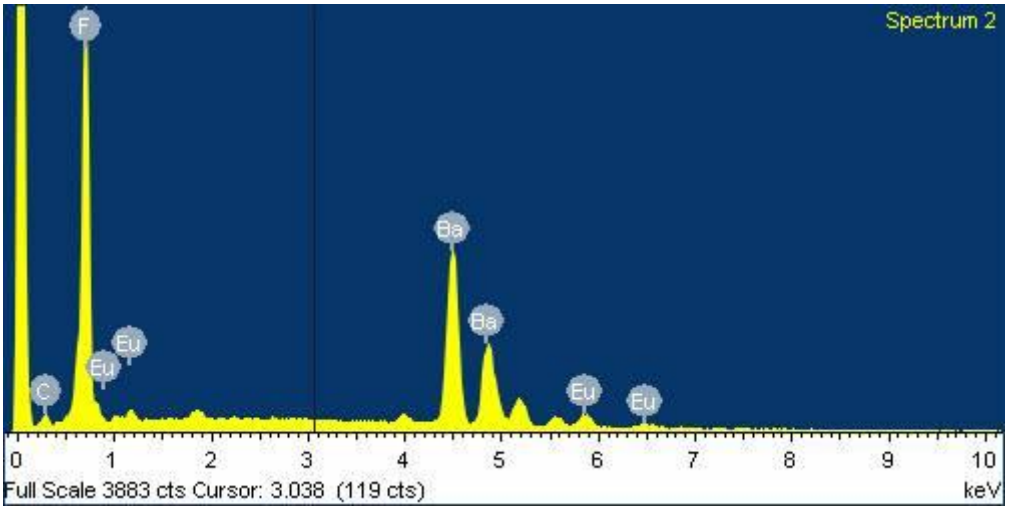


Figure S1. Reactor scheme.

Table S1. Growh rate of BaF_2 films in function of the deposition temperature.

Sample	Deposition Temperature (°C)	Grow Rate (nm/min)
BaF_2 : Eu (1%)	300°C	2.9
	350°C	15.9
	400°C	32.2
	500°C	31.9
	600°C	23.8



BaF2:Eu – EDX Quantitave Data	
	Ba: Eu
Site 1	1 : 0.1
Site 2	1 : 0.1

Figure S2. EDX spectrum (a) and EDX quantitative data (b) of the BaF_2: Eu 10% film deposited on Si (100).

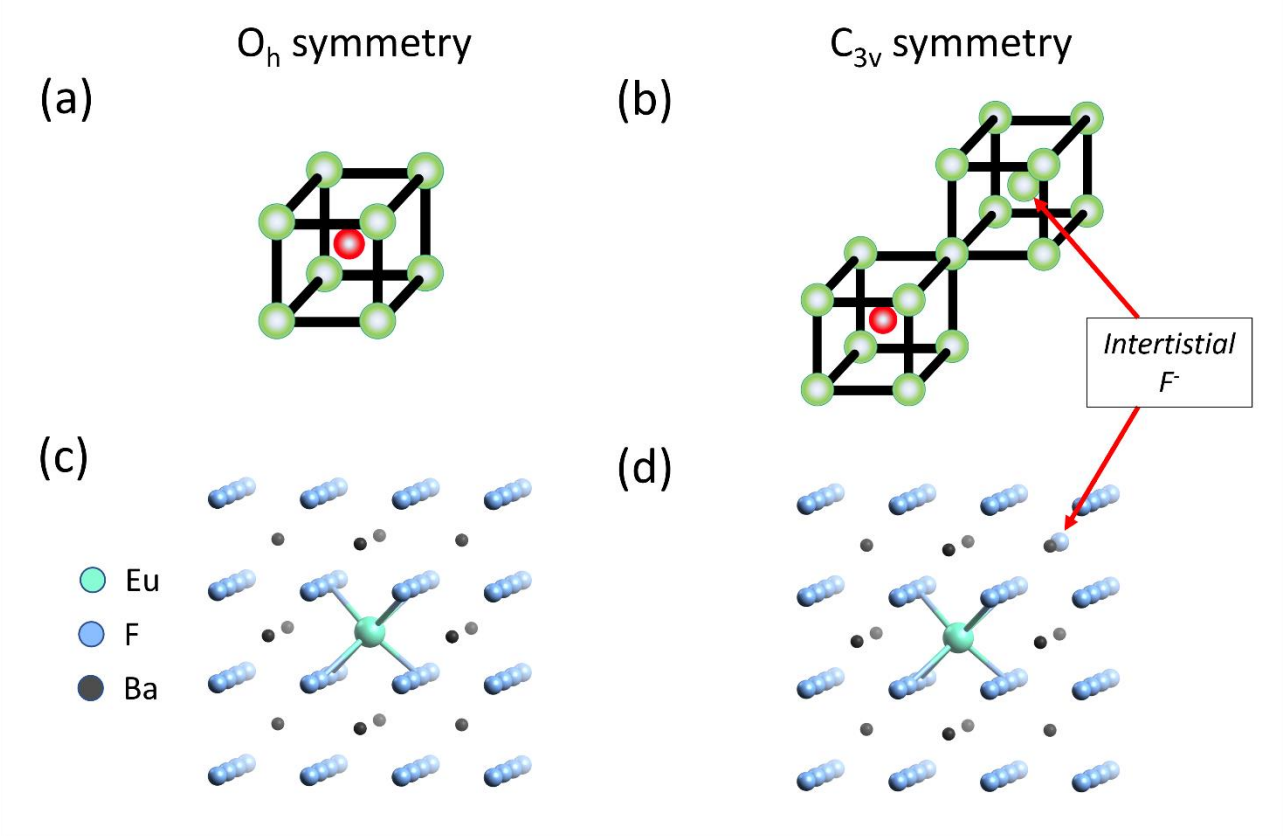


Figure S3: Lattice structure of fluorite-type crystal with a) a metal centre (in red) in O_h symmetry around anions (green); b) a next-nearest neighbour (NNN) anion compensated centre in C_{3v} symmetry. The models for the Eu^{3+} doped BaF_2 crystal structure employed in the *ab initio* simulations for c) O_h and d) C_{3v} symmetry.