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Supporting Information

Crystal and Electronic Structures, Photoluminescent and Photocatalytic Properties of α-$EuZrS_3$

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Table S1. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (U_{eq}[a], Å^2 × 10^3) for α-$EuZrS_3$.

atom	*x*	*y*	*z*	U_{eq}/Å^2
Eu(1)	5668(1)	2500	6787(1)	11(1)
Zr(1)	8274(1)	2500	4426(1)	6(1)
S(1)	4822(2)	2500	8926(1)	7(1)
S(2)	2951(2)	-2500	7173(1)	9(1)
S(3)	3387(1)	2500	4860(1)	9(1)

[a] U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

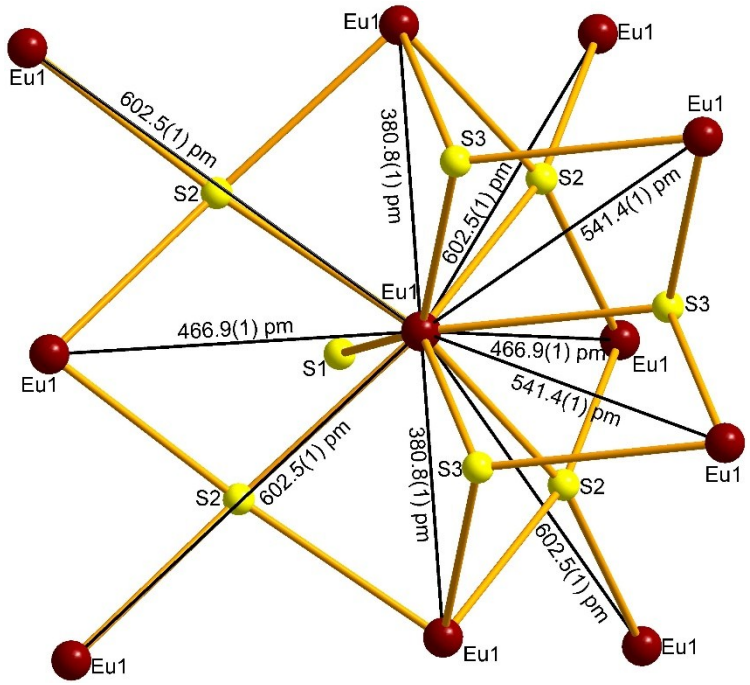

Fig. S1 Neighboring Eu–S and Eu–Eu distances in α-$EuZrS_3$.

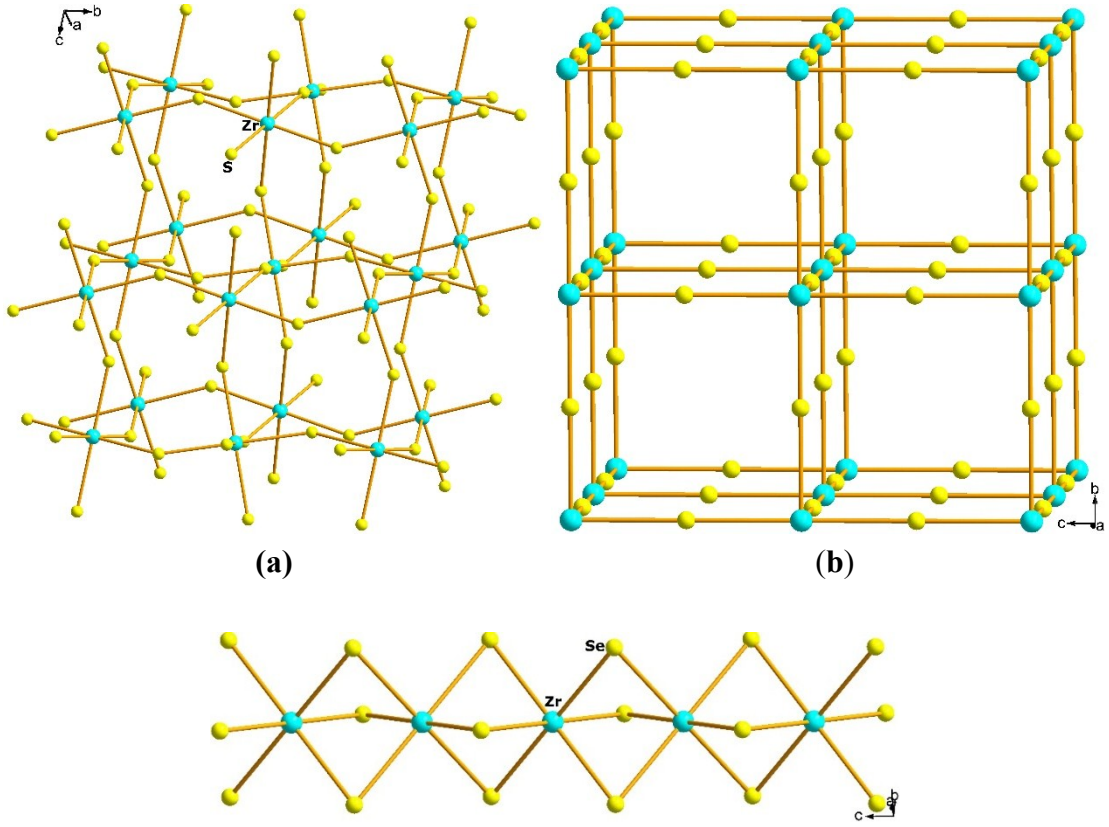

Fig. S2 The structure motifs constructed by Zr–S bonds in β-$EuZrS_3$ (*Pnma*) (**a**) and $BaZrS_3$ (*P*4/*mmm*) (**b**), and Zr–Se bonds in $BaZrSe_3$ ($P6_3/mmc$) (**c**).