Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information for

Dimensionality Reduction upon Calcium Incorporation in $Cs_{0.3}(Ca_{0.3}Ln_{0.7})PS_4$ and $Cs_{0.5}(Ca_{0.5}Ln_{0.5})PS_4$

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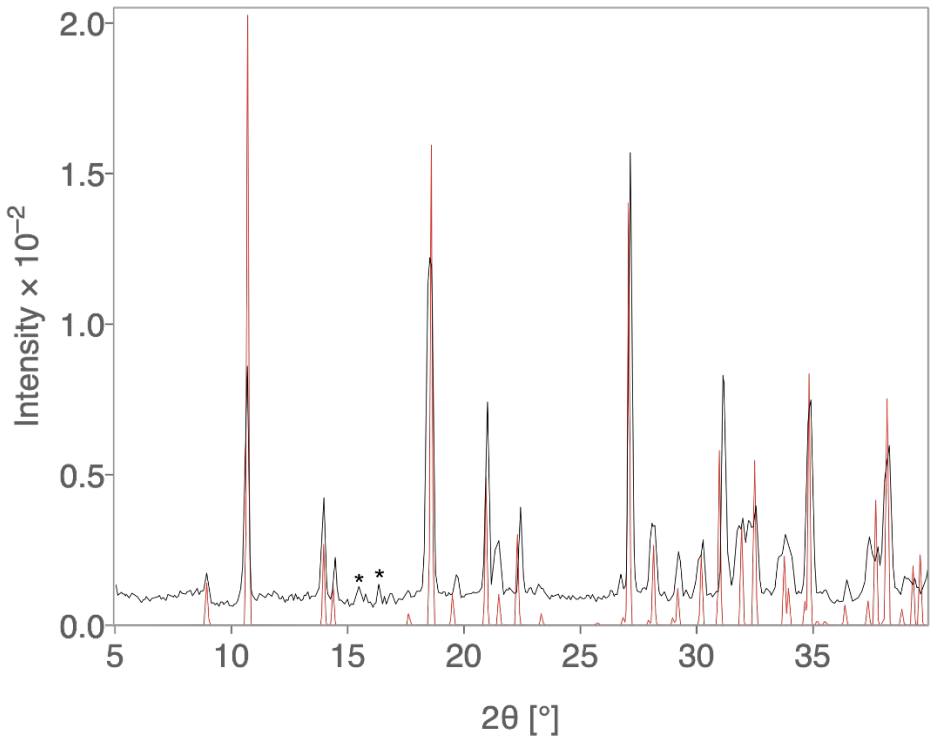

Figure S1. Experimental (black) and calculated (red) PXRD patterns of $Cs_{0.3}(Ca_{0.3}Pr_{0.7})PS_4$. Stars (*) denote the peaks that correspond to $Ca_2P_2S_6$ impurity.

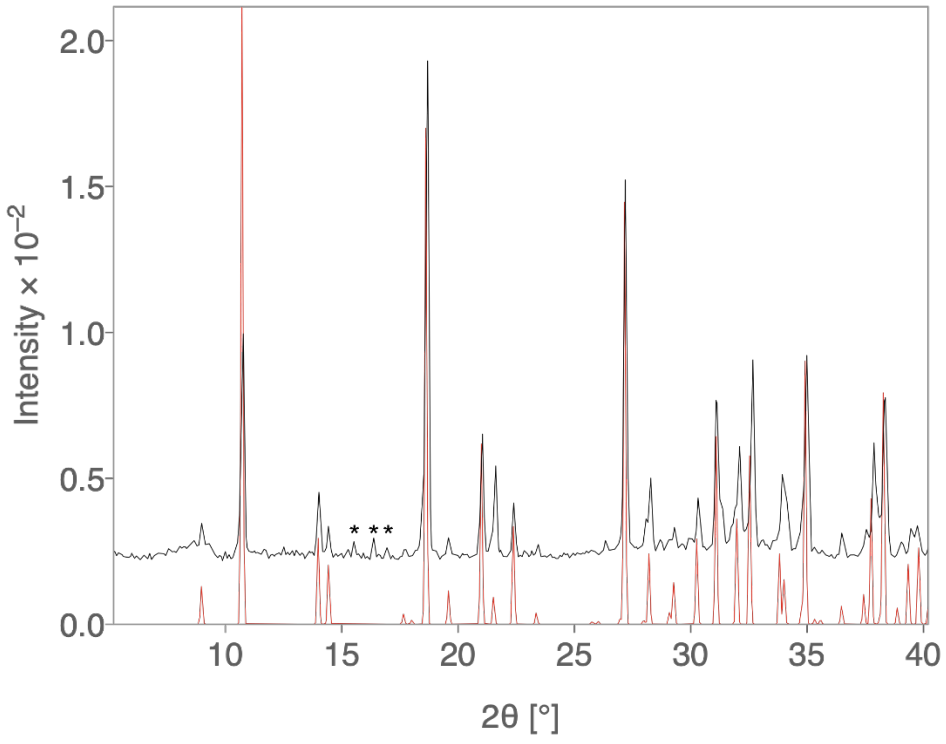

Figure S2. Experimental (black) and calculated (red) PXRD patterns of $Cs_{0.3}(Ca_{0.3}Pr_{0.7})PS_4$. Stars (*) denote the peaks that correspond to $Ca_2P_2S_6$ impurity.

Table S1. Elemental compositions of the thiophosphates determined by EDS.

$Cs_{0.3}(Ca_{0.3}Ce_{0.7})PS_4$		$Cs_{0.3}(Ca_{0.3}Pr_{0.7})PS_4$		$Cs_{0.3}(Ca_{0.3}Nd_{0.7})PS_4$	
Element	Atom %	Element	Atom %	Element	Atom %
Ce	11.29	Pr	9.91	Nd	11.63
Cs	6.40	Cs	5.38	Cs	6.41
Ca	6.08	Ca	5.41	Ca	6.03
P	16.45	P	23.45	P	15.56
S	59.77	S	55.85	S	60.37
$Cs_{0.3}(Ca_{0.3}Sm_{0.7})PS_4$		$Cs_{0.3}(Ca_{0.3}Tb_{0.7})PS_4$		$Cs_{0.3}(Ca_{0.3}Dy_{0.7})PS_4$	
Sm	10.67	Tb	13.33	Dy	12.22
Cs	6.17	Cs	9.38	Cs	7.57
Ca	6.09	Ca	6.56	Ca	7.56
P	14.99	P	23.12	P	22.16
S	62.09	S	47.61	S	50.49
$Cs_{0.5}(Ca_{0.5}Pr_{0.5})PS_4$		$Cs_{0.5}(Ca_{0.5}Nd_{0.5})PS_4$		$Cs_{0.5}(Ca_{0.5}Tb_{0.5})PS_4$	
Pr	9.75	Nd	8.42	Tb	8.94
Cs	9.57	Cs	7.53	Cs	9.27
Ca	9.86	Ca	7.61	Ca	9.52
P	17.52	P	14.21	P	17.65
S	53.31	S	62.23	S	54.62
$Cs_{0.5}(Ca_{0.5}Dy_{0.5})PS_4$					
Dy	10.01				
Cs	10.40				
Ca	10.04				
P	21.20				
S	46.36				

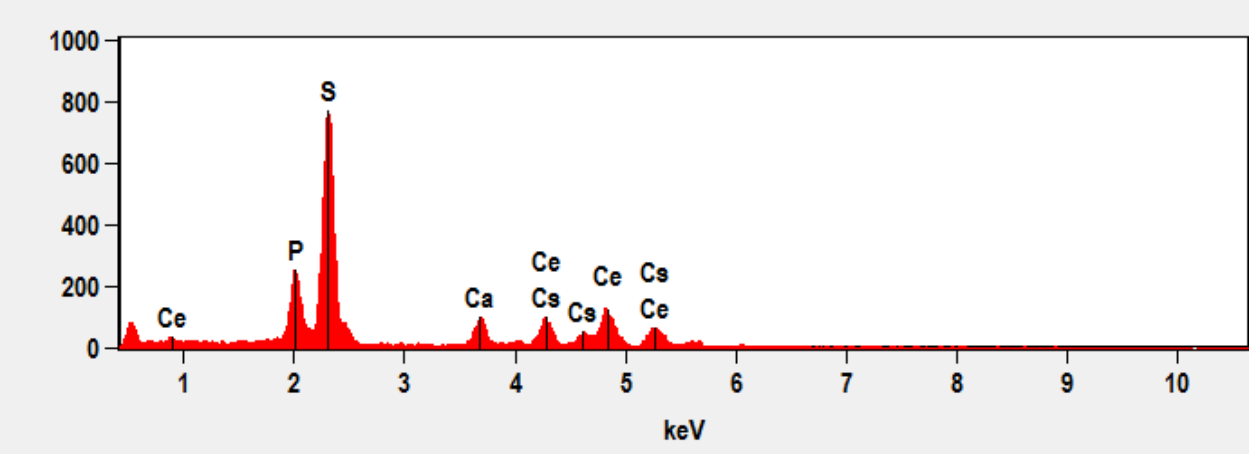

Figure S3. EDS spectrum of $Cs_{0.3}(Ca_{0.3}Ce_{0.7})PS_4$.

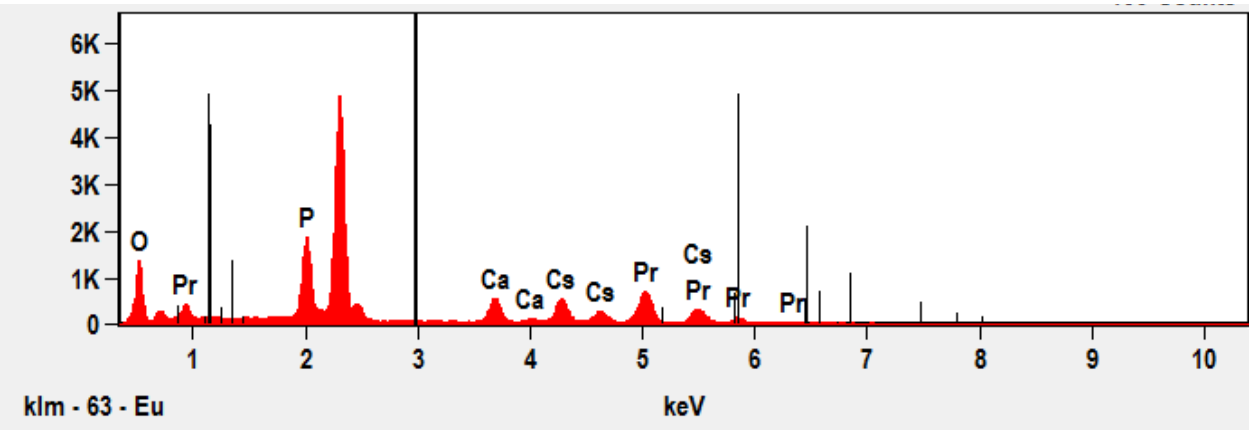

Figure S4. EDS spectrum of $Cs_{0.3}(Ca_{0.3}Pr_{0.7})PS_4$.

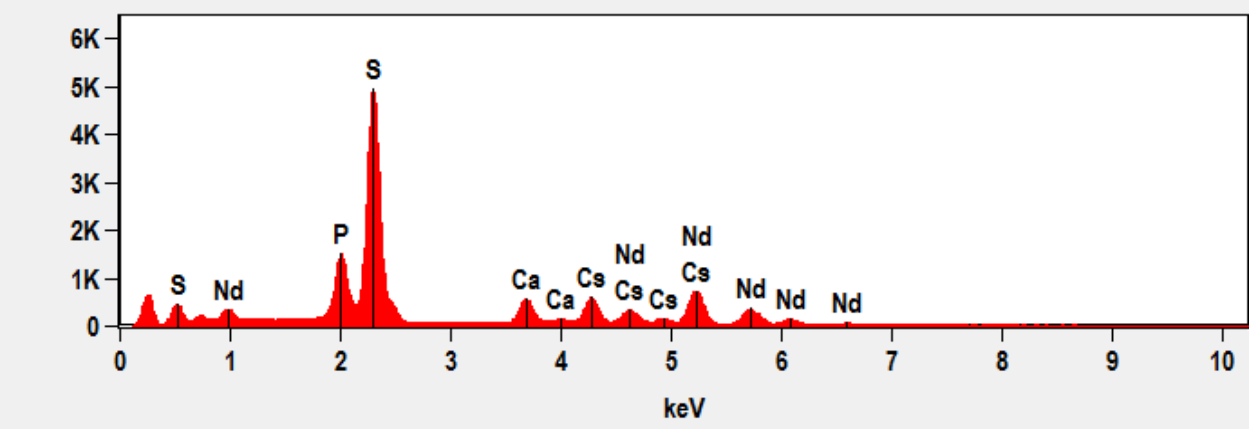

Figure S5. EDS spectrum of $Cs_{0.3}(Ca_{0.3}Nd_{0.7})PS_4$.

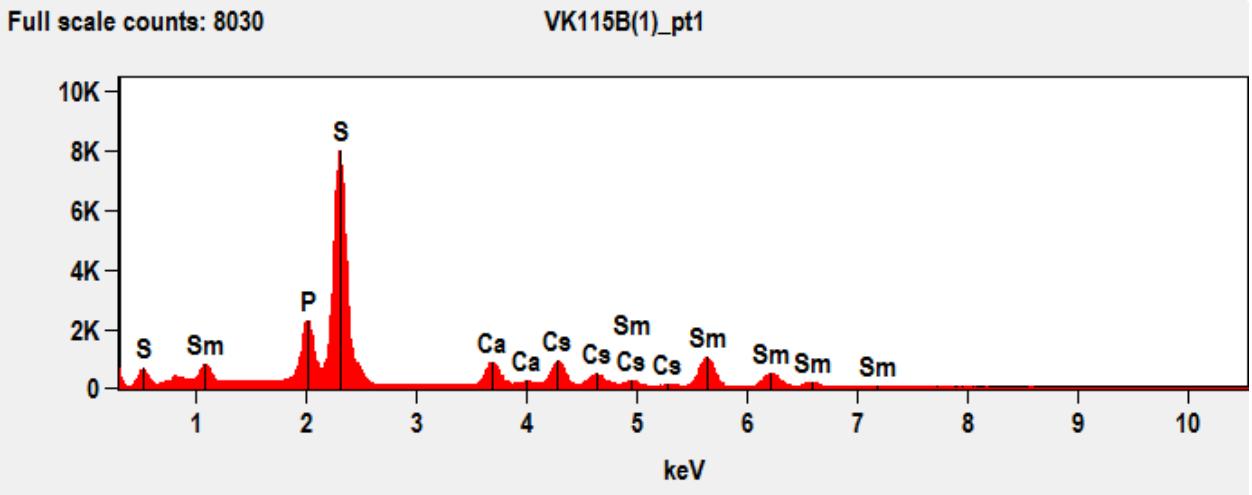

Figure S6. EDS spectrum of $Cs_{0.3}(Ca_{0.3}Sm_{0.7})PS_4$.

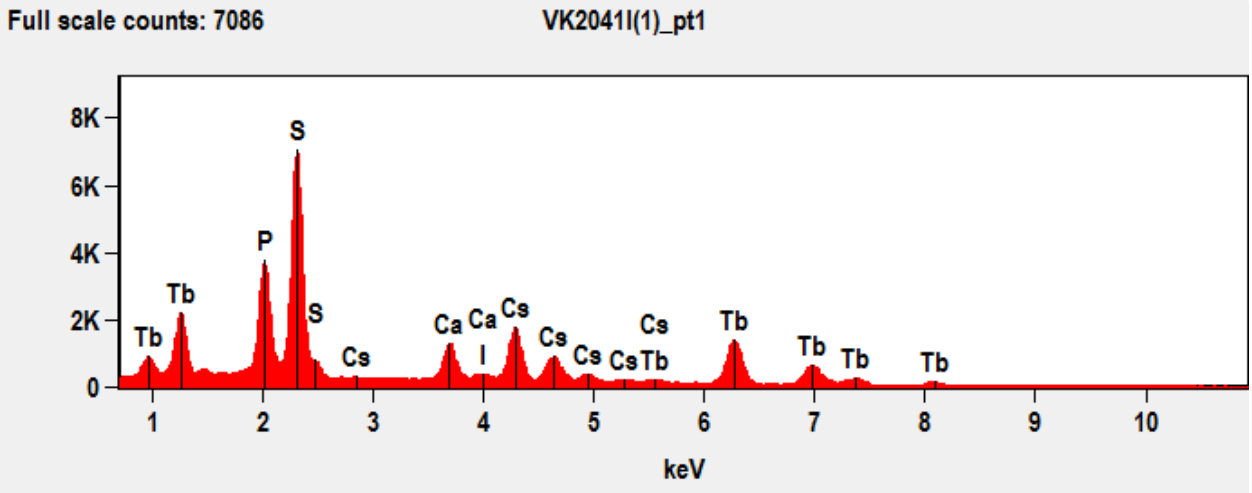

Figure S7. EDS spectrum of $Cs_{0.3}(Ca_{0.3}Tb_{0.7})PS_4$.

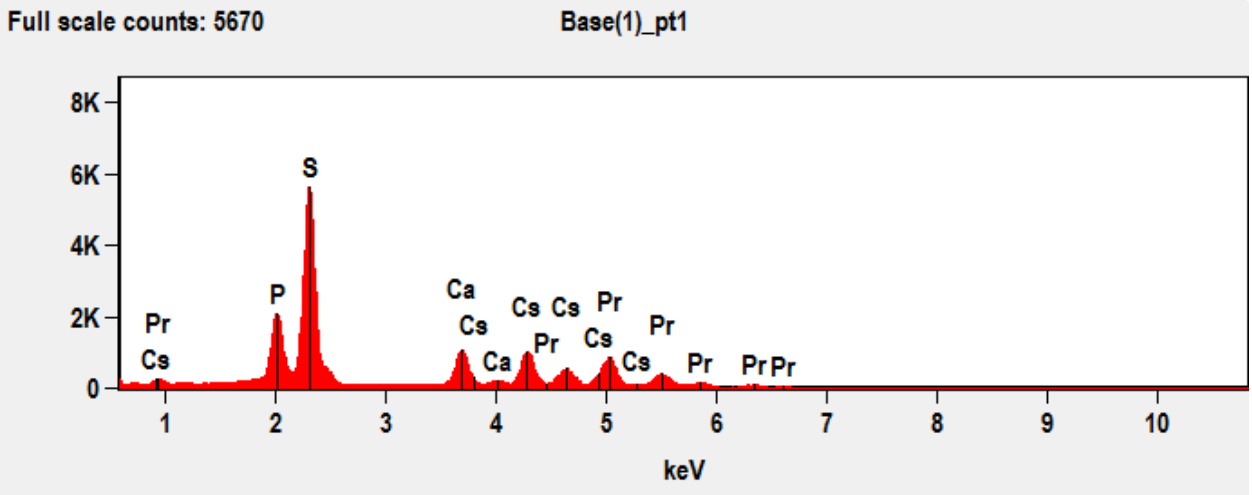

Figure S8. EDS spectrum of $Cs_{0.5}(Ca_{0.5}Ce_{0.5})PS_4$.

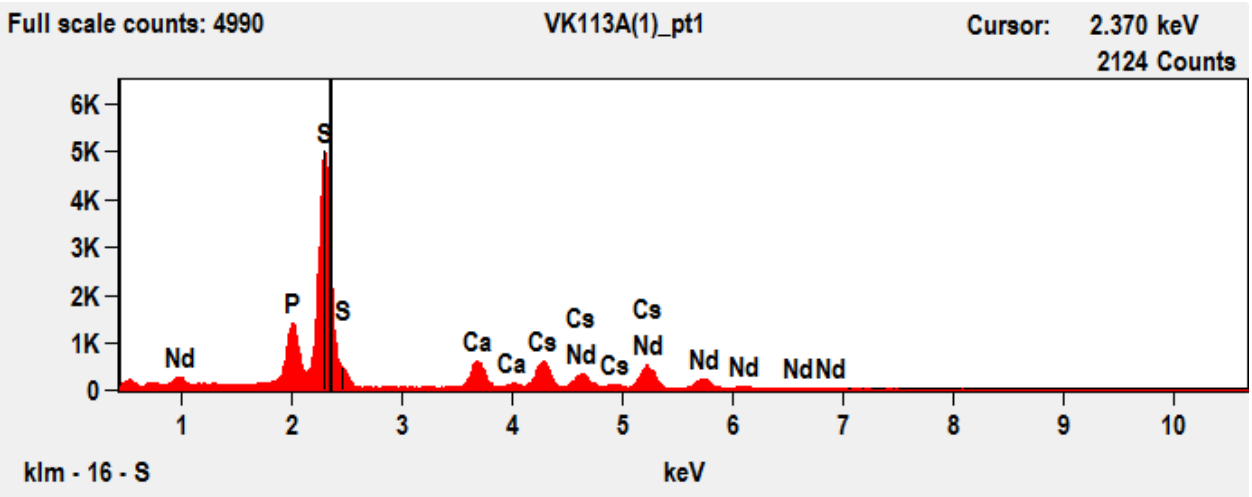

Figure S9. EDS spectrum of $Cs_{0.5}(Ca_{0.5}Nd_{0.5})PS_4$.

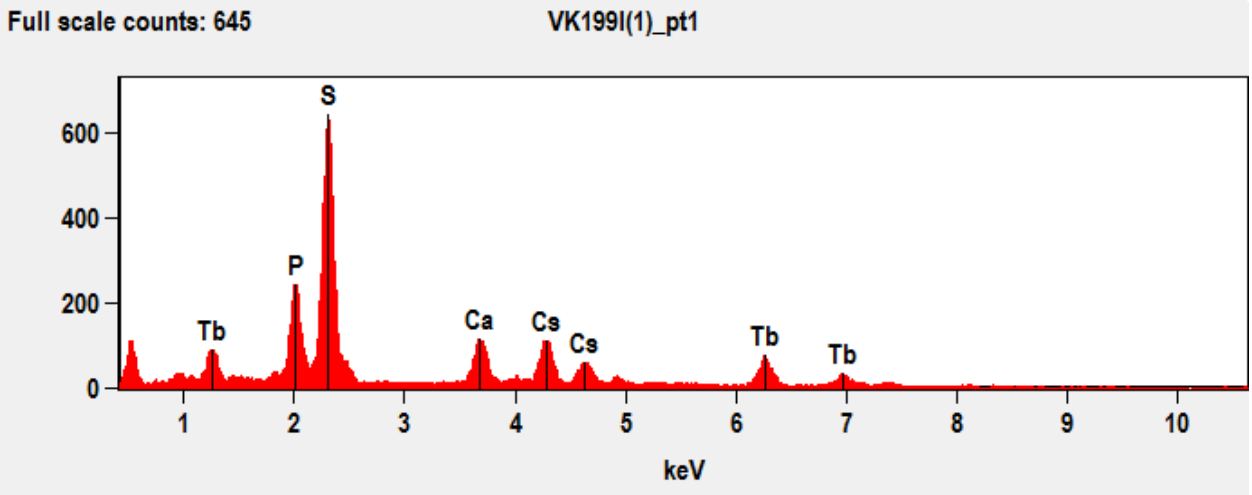

Figure S10. EDS spectrum of $Cs_{0.5}(Ca_{0.5}Tb_{0.5})PS_4$.

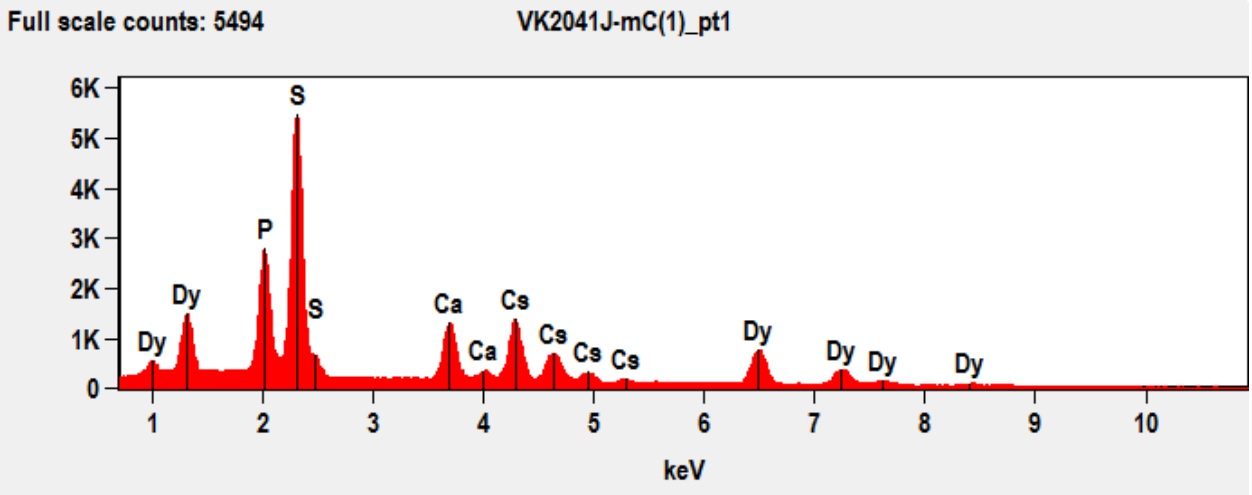

Figure S11. EDS spectrum of $Cs_{0.5}(Ca_{0.5}Dy_{0.5})PS_4$.

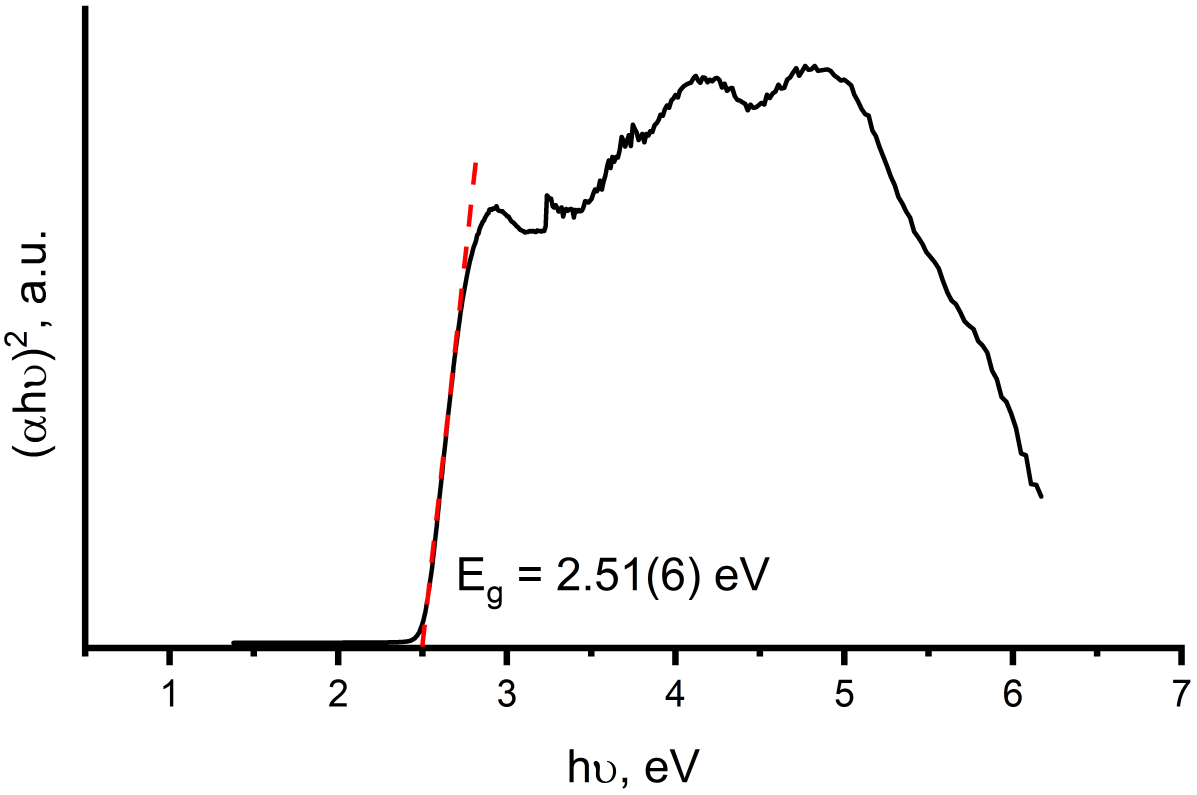

Figure S12. Tauc plot and band gap for $Cs_{0.3}(Ca_{0.3}Ce_{0.7})PS_4$.

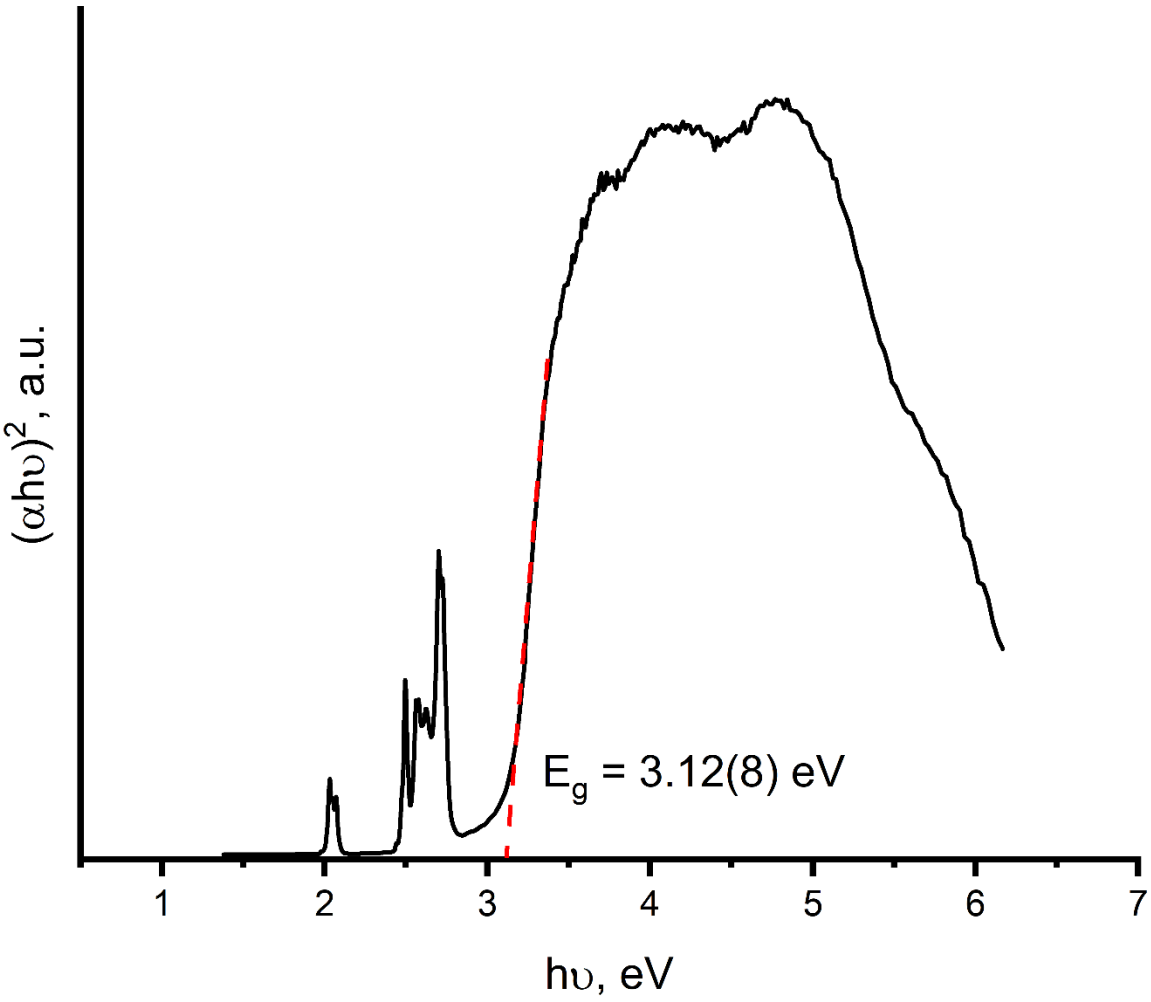

Figure S13. Tauc plot and band gap for $Cs_{0.3}(Ca_{0.3}Pr_{0.7})PS_4$.

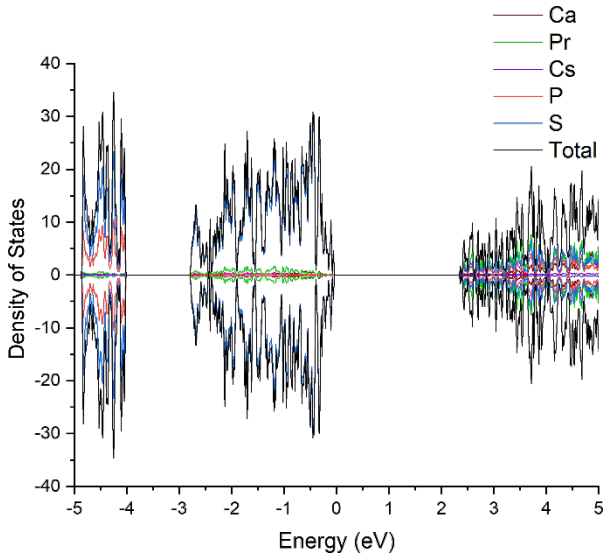

Figure S14. Calculated density of states of $Cs_{0.5}(Ca_{0.5}Pr_{0.5})PS_4$.

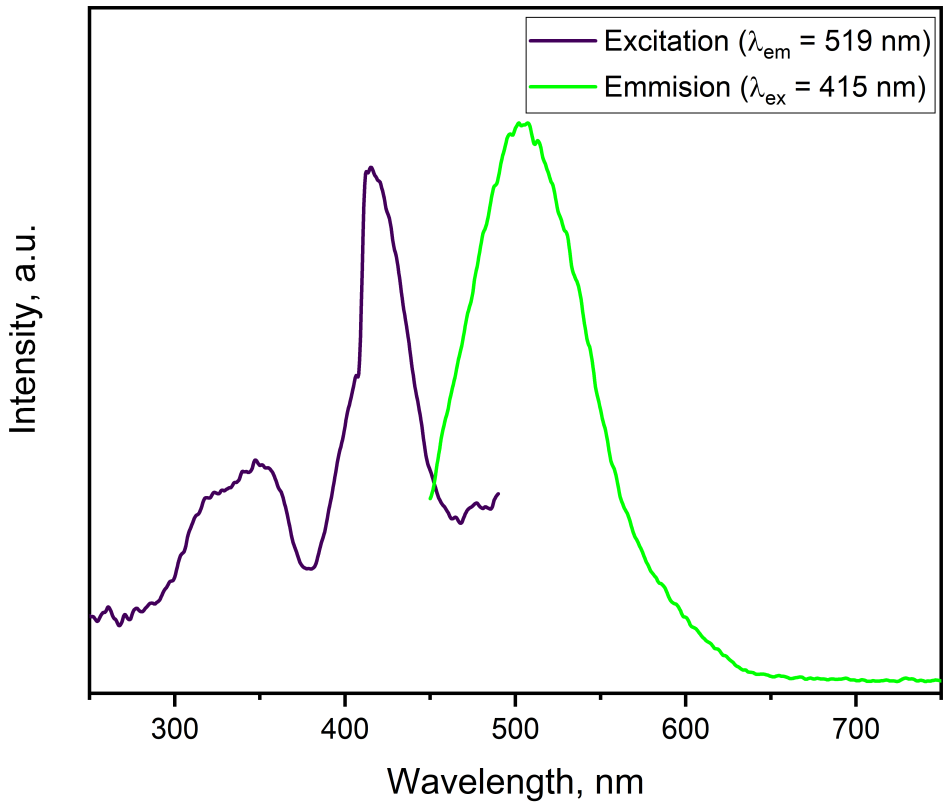

Figure S15. Fluorescence excitation and emission spectra of $Cs_{0.3}(Ca_{0.3}Ce_{0.7})PS_4$.