

Electronic Supplementary Information

Quaternary Rare-Earth Selenides with Closed Cavities: Cs[RE₉Mn₄Se₁₈] (RE = Ho–Lu)

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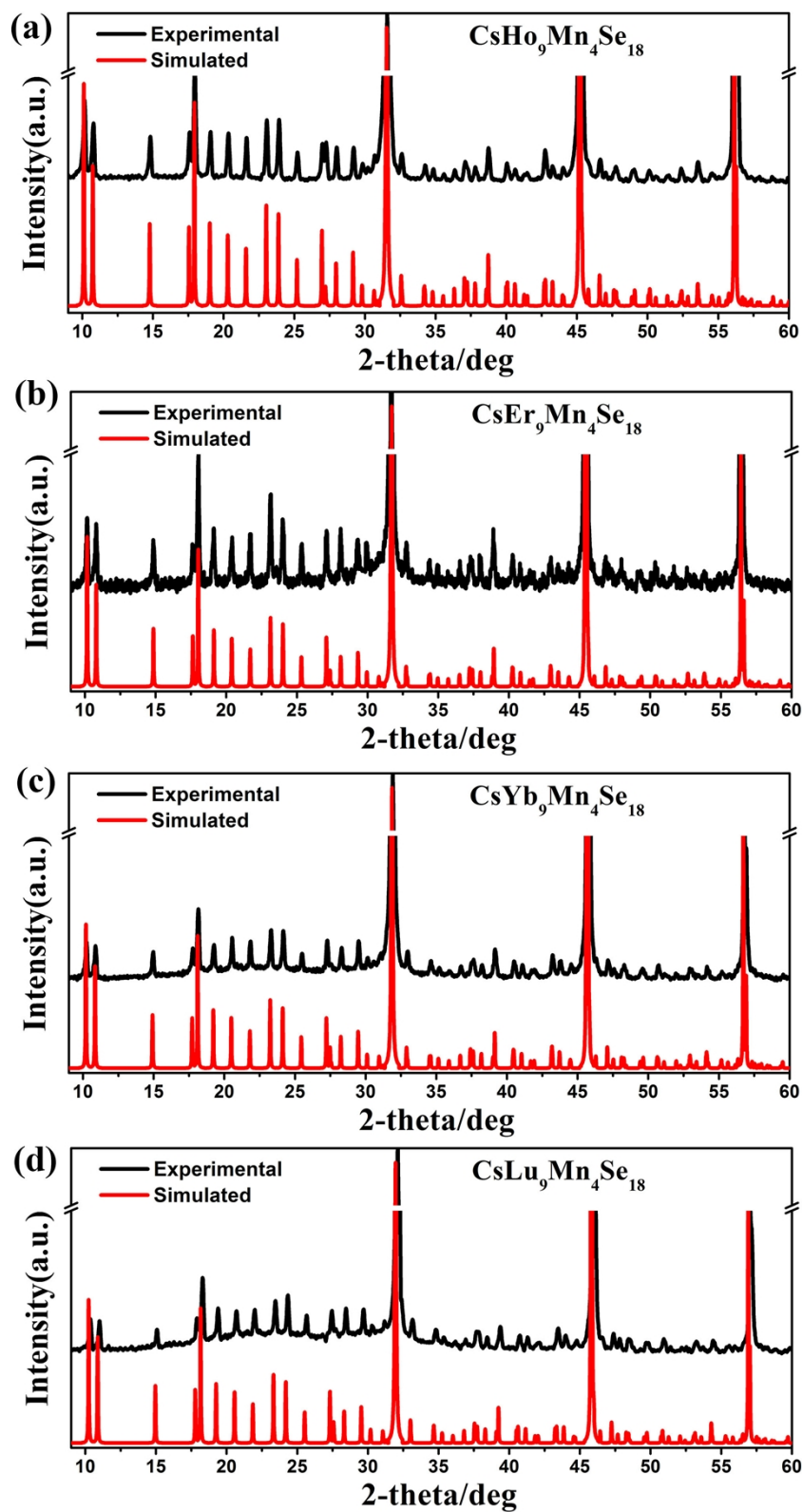


Figure S1. The experimental (black) and simulated (red) powder XRD patterns of $\text{Cs}[\text{RE}_9\text{Mn}_4\text{Se}_{18}]$ (RE = Ho, Er, Yb, Lu).

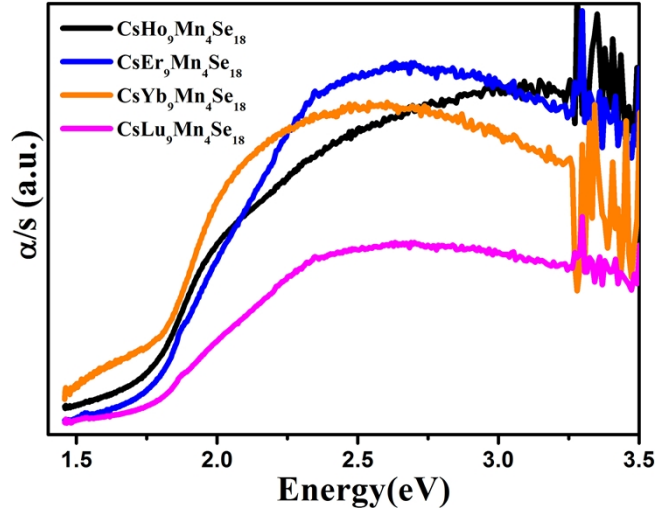


Figure S2. Optical absorption spectrum of Cs[RE₉Mn₄Se₁₈] (RE = Ho, Er, Yb, Lu).

Table S1. The EDX data of Cs[Tm₉Mn₄Se₁₈].

Point-1				Point-2			
Element	Weight%	Atomic%	Formula	Element	Weight%	Atomic%	Formula
MnK	6.60	12.37	3.94	Mn K	6.55	12.29	3.95
Se L	43.20	56.35	17.95	Se L	43.22	56.41	18.14
Cs L	4.05	3.14	1	Cs L	4.01	3.11	1
Tm L	46.15	28.14	8.97	Tm L	46.22	28.20	9.07
Total	100.00			Total	100.00		
Point-3				Point-4			
Element	Weight%	Atomic%	Formula	Element	Weight%	Atomic%	Formula
Mn K	6.54	12.28	3.85	Mn K	6.85	12.82	4.16
Se L	43.10	56.30	17.65	Se L	43.02	56.02	18.19
Cs L	4.11	3.19	1	Cs L	3.98	3.08	1
Tm L	46.25	28.24	8.85	Tm L	46.15	28.09	9.12
Total	100.00			Total	100.00		
Point-5				Average formula: $\text{Cs}_1\text{Mn}_{4.0(1)}\text{Tm}_{9.1(3)}\text{Se}_{18.1(2)}$			
Element	Weight%	Atomic%	Formula				
Mn K	6.68	12.04	4.09				
Se L	43.34	56.53	18.47				
Cs L	3.95	3.13	1				
Tm L	46.03	28.30	9.17				
Total	100.00						

Table S2. Total energy ΔE (in meV/atom) of each Mn-distribution configuration.

Model- ij ($i = a, b, c; j = 1-6$)	ΔE (meV/atom)	
Figure 7a	$a1$	0.00
	$a2$	5.50
	$a3$	20.03
	$a4$	39.35
	$a5$	31.73
	$a6$	43.43
Figure 7b	$b1$	111.18
	$b2$	-18.95
	$b3$	45.47
	$b4$	59.26
	$b5$	-34.77
	$b6$	36.15
Figure 7c	$c1$	-28.40
	$c2$	-33.32
	$c3$	-34.68
	$c4$	-33.19
	$c5$	-34.67
	$c6$	-33.23