Title	Crystal structures, magnetic properties, and DFT calculation of B-site defected 12L-perovskites Ba ₂ La ₂ MW ₂ O ₁₂ (M = Mn, Co, Ni, Zn)
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Supporting Information

Figure S1

Fig. S1 Powder X-ray diffraction profiles for (a) $\text{Ba}_2\text{La}_2\text{MnW}_2\text{O}_{12}$ and (b) $\text{Ba}_2\text{La}_2\text{CoW}_2\text{O}_{12}$. Upper and lower vertical marks mean the Bragg peak positions of main and impurity (BaWO_4) phases, respectively.

Figure S2

Fig. S2 ND profiles calculated for $\text{Ba}_2\text{La}_2\text{NiW}_2\text{O}_{12}$: (a) the comparison between the space group $R-3m$ (a disordered A-site arrangement) and $R-3$ (ordered) and (b) between $R-3$ (disordered) and $R-3$ (ordered). Blue line in each figure means the difference between the profiles.

Figure S3

Fig. S3 Energy dispersions of $\text{Ba}_2\text{La}_2\text{NiW}_2\text{O}_{12}$. The zero energy is placed at the highest occupied state.

Table S1 Structural information for Ba₂La₂MW₂O₁₂ compounds.

M	S.G.	$a / \text{\AA}$	$c / \text{\AA}$	Order/disorder arrangement of Ba and La	XRD/ND	Ref.
Mg	$R\text{-}3m$	5.666	27.44	–	XRD	[17]
	$R\text{-}3m$	5.7276(3)	27.393(2)	order	XRD	[24]
Mn	$R\text{-}3m$	5.7330(4)	27.4134(28)	disorder	ND	[27]
	$R\text{-}3$	5.7235(2)	27.4288(7)	disorder	XRD	This study
	$R\text{-}3m$	5.676	27.40	–	XRD	[17]
Co	$R\text{-}3m$	5.6764(2)	27.3541(11)	disorder	XRD	[27]
	$R\text{-}3$	5.6799(1)	27.3752(4)	order	XRD	This study
	$R\text{-}3m$	5.660	27.35	–	XRD	[17]
Ni	$R\text{-}3m$	5.6647(3)	27.3755(18)	disorder	ND	[27]
	$R\text{-}3$	5.6595(3)	27.3387(13)	order	ND	This study
Cu	Triclinic	^{*1}	^{*1}	–	XRD	[17]
	$R\text{-}3m$	5.676	27.40	disorder	XRD	[17]
	$R\text{-}3m$	5.687	27.395	disorder	XRD	[18]
Zn	$R\text{-}3m$	5.6790(3)	27.3679(20)	disorder	XRD	[25]
	$R\text{-}3$	5.68687(1)	27.39090(4)	order	ND	This study

Note. ^{*1} Monoclinic unit cell with $a = 5.81 \text{ \AA}$, $b = 5.70 \text{ \AA}$, $c = 27.35 \text{ \AA}$, $\alpha \sim 91^\circ$, $\beta \sim 89^\circ$, $\gamma \sim 120.5^\circ$.

Table S2 Structural parameters for Ba₂La₂MW₂O₁₂ (M = Mn, Co, Ni, Zn) determined by the powder X-ray diffraction measurement.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> / Å ²
Ba ₂ La ₂ MnW ₂ O ₁₂					
At room temperature, space group <i>R</i> -3;					
<i>a</i> = 5.7235(2) Å, <i>c</i> = 27.4288(7) Å,					
<i>R</i> _{wp} = 13.13 %, <i>R</i> _p = 8.82 %, <i>R</i> _e = 8.34 %, <i>R</i> _B = 2.44 %, <i>R</i> _F = 1.32 %.					
Ba	6 <i>c</i>	0	0	0.1400(1)	0.58(4)
La	6 <i>c</i>	0	0	0.2923(1)	0.20(4)
Mn	3 <i>a</i>	0	0	0	0.76(9)
W	6 <i>c</i>	0	0	0.4193(1)	0.14(3)
O1	18 <i>f</i>	0.464(4)	0.473(4)	0.1165(3)	0.9(2)
O2	18 <i>f</i>	0.412(2)	0.444(2)	0.2920(4)	0.9
Ba ₂ La ₂ CoW ₂ O ₁₂					
At room temperature, space group <i>R</i> -3;					
<i>a</i> = 5.6799(1) Å, <i>c</i> = 27.3752(4) Å,					
<i>R</i> _{wp} = 9.48 %, <i>R</i> _p = 6.94 %, <i>R</i> _e = 7.14 %, <i>R</i> _B = 2.41 %, <i>R</i> _F = 1.28 %.					
Ba	6 <i>c</i>	0	0	0.1329(1)	0.42(3)
La	6 <i>c</i>	0	0	0.2932(1)	0.25(3)
Co	3 <i>a</i>	0	0	0	0.42(4)
W	6 <i>c</i>	0	0	0.4190(1)	0.12(4)
O1	18 <i>f</i>	0.467(3)	0.470(3)	0.1173(3)	1.0(1)
O2	18 <i>f</i>	0.412(2)	0.449(2)	0.2948(3)	1.0

Table S2 continued

Atom	Site	x	y	z	$B / \text{\AA}^2$
Ba₂La₂NiW₂O₁₂					
At room temperature, space group $R\bar{3}$;					
$a = 5.6604(2) \text{ \AA}$, $c = 27.3522(6) \text{ \AA}$,					
$R_{\text{wp}} = 12.06 \%$, $R_{\text{p}} = 8.71 \%$, $R_{\text{e}} = 8.44 \%$, $R_{\text{B}} = 3.34 \%$, $R_{\text{F}} = 2.45 \%$.					
Ba	$6c$	0	0	0.1324(1)	0.36(4)
La	$6c$	0	0	0.2932(1)	0.39(4)
Ni	$3a$	0	0	0	0.40(6)
W	$6c$	0	0	0.4189(1)	0.25(3)
O1	$18f$	0.471(3)	0.472(3)	0.1174(3)	1.0(2)
O2	$18f$	0.419(2)	0.449(2)	0.2950(4)	1.0
Ba₂La₂ZnW₂O₁₂					
At room temperature, space group $R\bar{3}$;					
$a = 5.6865(2) \text{ \AA}$, $c = 27.3892(7) \text{ \AA}$,					
$R_{\text{wp}} = 15.69 \%$, $R_{\text{p}} = 10.86 \%$, $R_{\text{e}} = 11.54 \%$, $R_{\text{B}} = 3.12 \%$, $R_{\text{F}} = 1.88 \%$.					
Ba	$6c$	0	0	0.1331(1)	0.47(5)
La	$6c$	0	0	0.2929(1)	0.22(6)
Zn	$3a$	0	0	0	0.48(9)
W	$6c$	0	0	0.4190(1)	0.18(9)
O1	$18f$	0.485(5)	0.487(5)	0.1186(4)	1.2(2)
O2	$18f$	0.419(3)	0.453(3)	0.2943(4)	1.2