

Supporting Information for

Investigation of crystal structure and electrochemical performance of Gd doped $\text{LaNb}_{0.9}\text{Mo}_{0.1}\text{O}_{4.05}$

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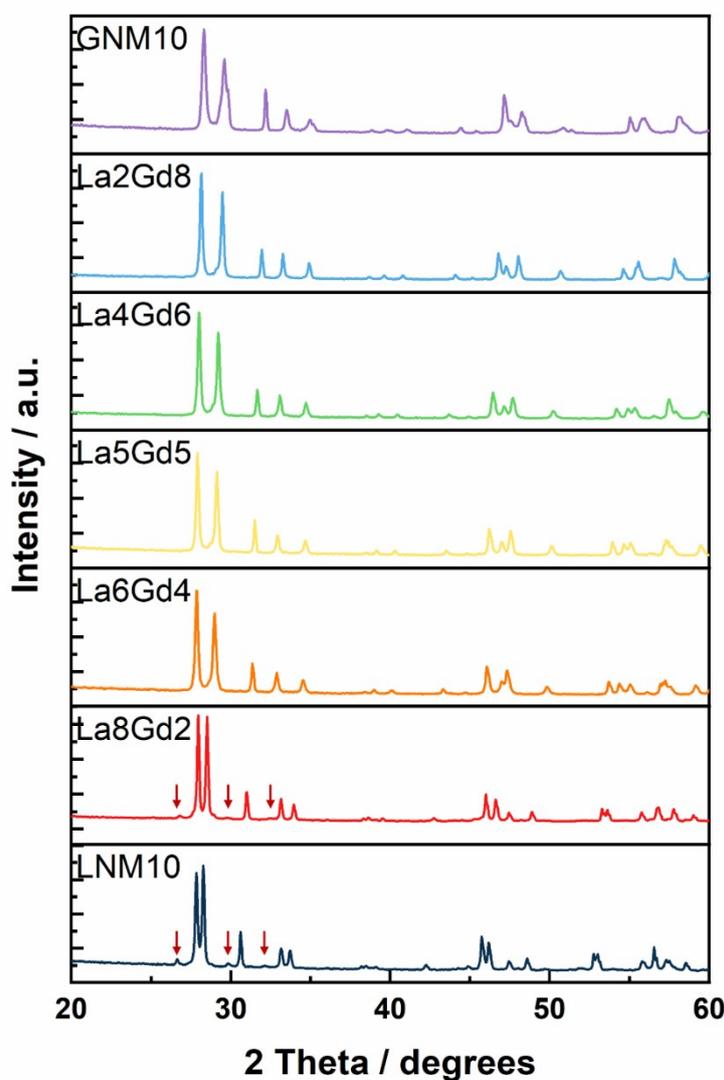


Figure S1. Room temperature XRD patterns of $\text{La}_{1-x}\text{Gd}_x\text{Nb}_{0.9}\text{Mo}_{0.1}\text{O}_{4.05}$ series. The satellite reflections of modulated structure are marked by the arrows.

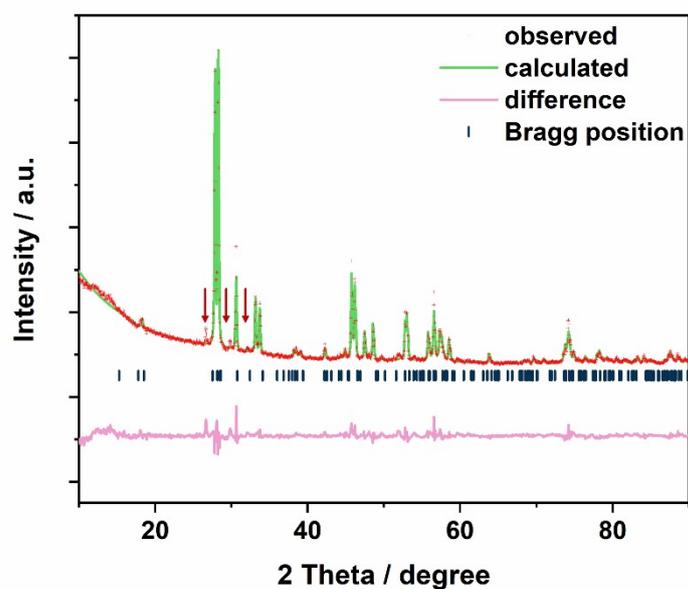


Figure S2. Rietveld refinement results for XRD data of LNM10 at 25 °C with $R_{wp} = 3.89\%$, $\chi^2 = 1.83$. The satellite reflections of modulated structure are marked by the arrows.

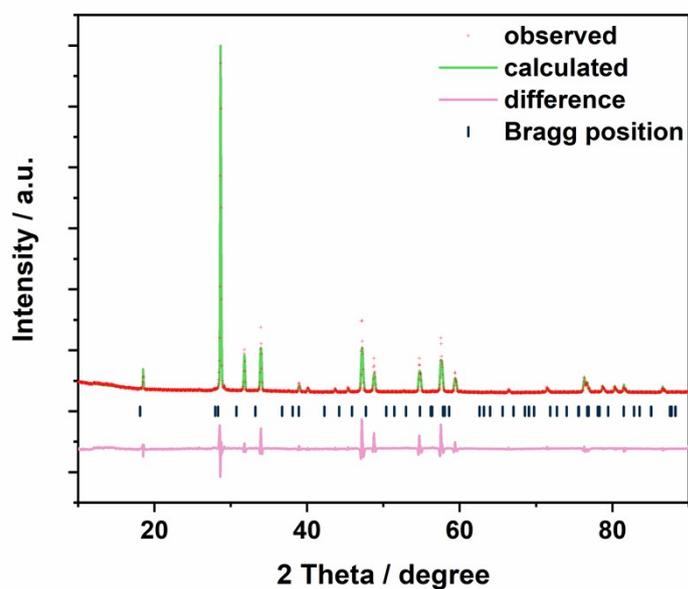


Figure S3. Rietveld refinement results for XRD data of GNM10 at 900 °C with $R_{wp} = 5.59\%$, $\chi^2 = 7.56$.

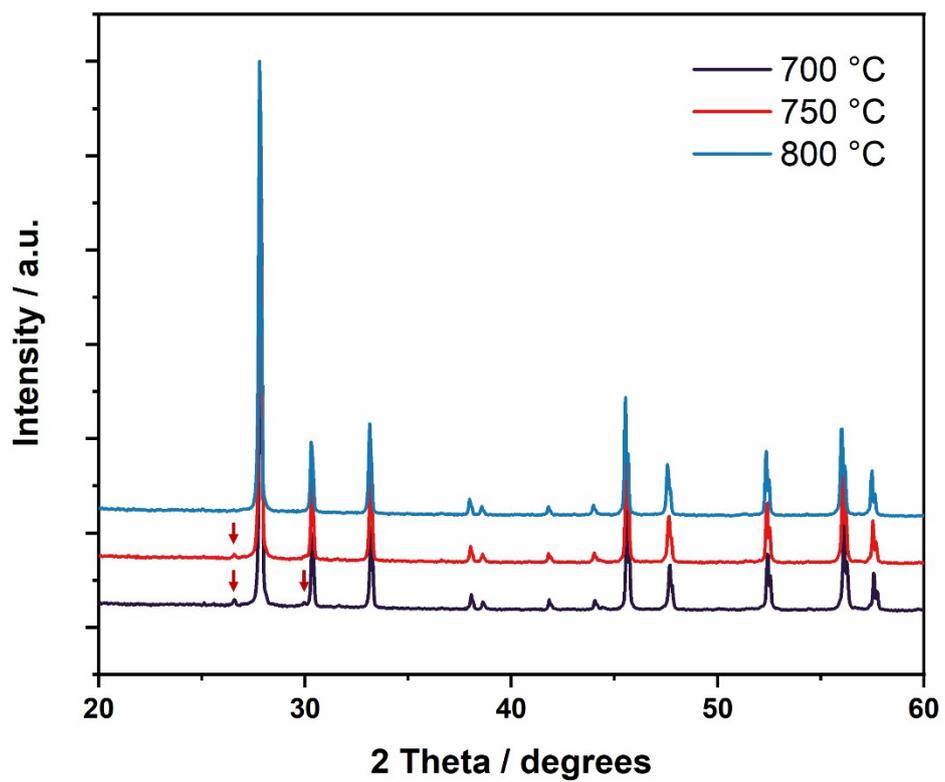


Figure S4. XRD patterns of LNM10 recorded at 700 °C, 750 °C and 800 °C, respectively. The satellite reflections of the modulated structure are marked by the arrows.

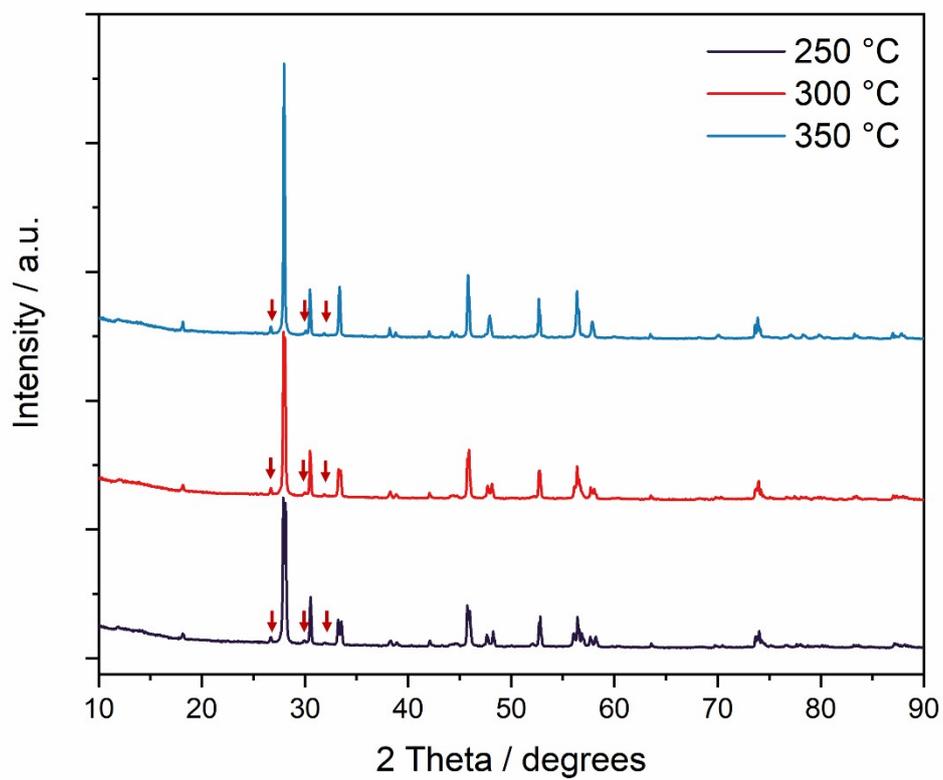


Figure S5. XRD patterns of LNM10 recorded at 250 °C, 300 °C and 350 °C, respectively. The satellite reflections of the modulated structure are marked by the arrows.

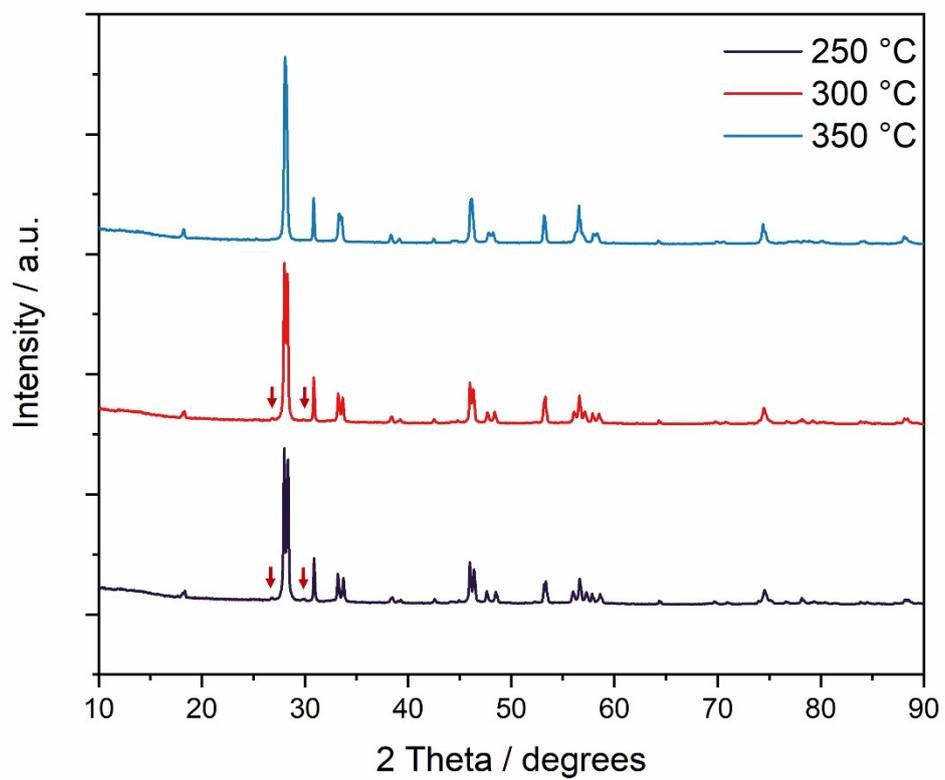


Figure S6. XRD patterns of La₈Gd₂ recorded at 250 °C, 300 °C and 350 °C, respectively. The satellite reflections of the modulated structure are marked by the arrows.

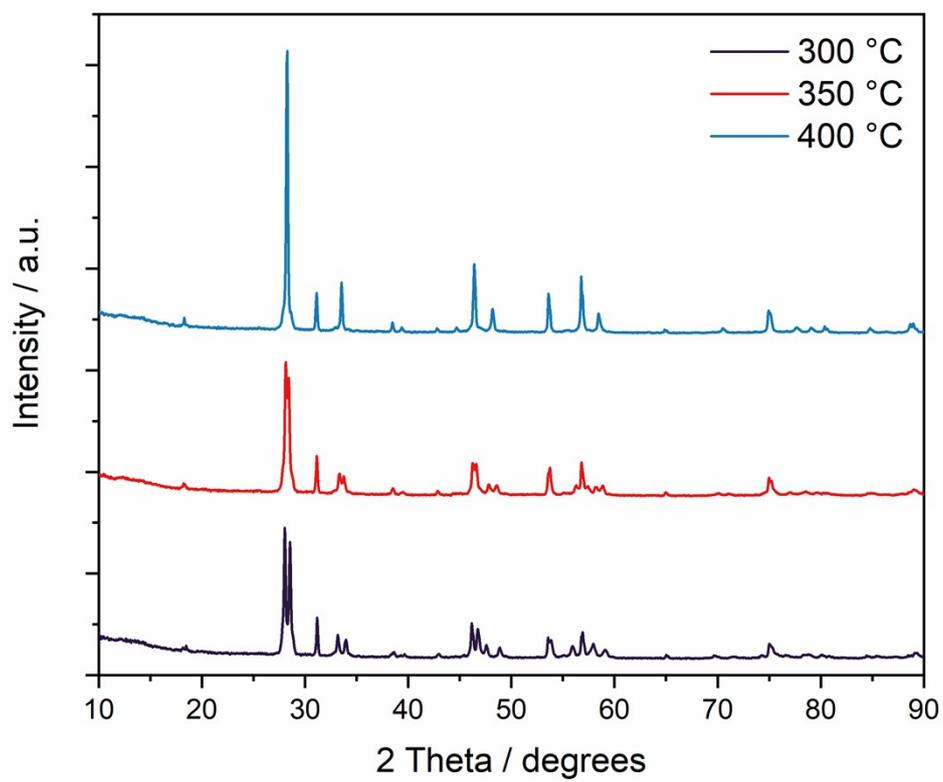


Figure S7. XRD patterns of La₆Gd₄ recorded at 300 °C, 350 °C and 400 °C, respectively.

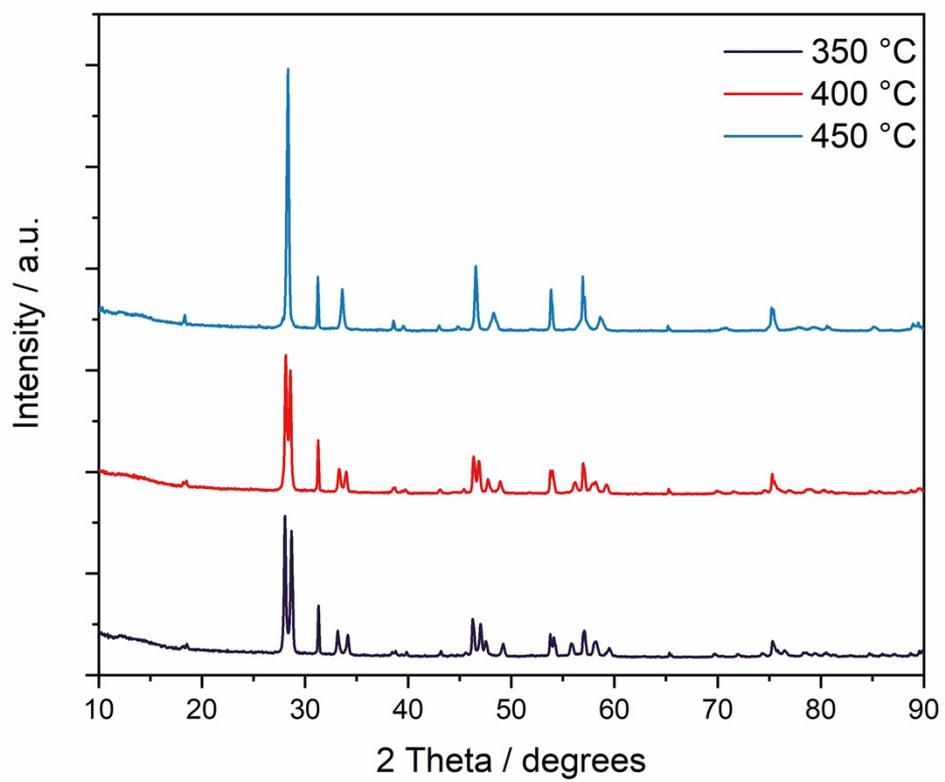


Figure S8. XRD patterns of La₅Gd₅ recorded at 350 °C, 400 °C and 450 °C, respectively.

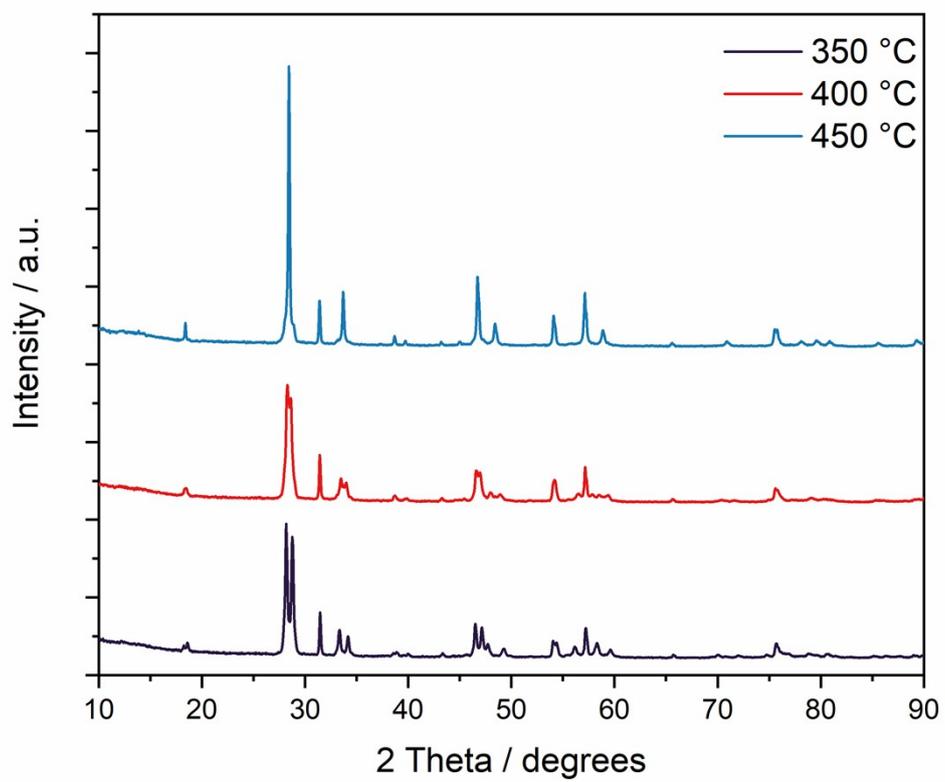


Figure S9. XRD patterns of La₄Gd₆ recorded at 350 °C, 400 °C and 450 °C, respectively.

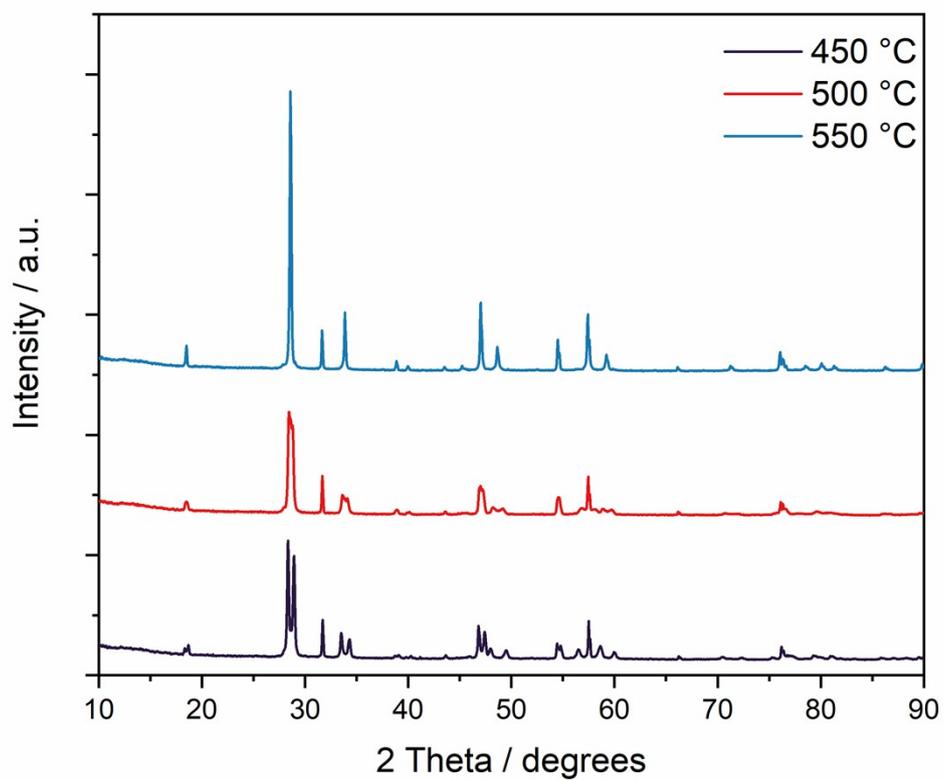


Figure S10. XRD patterns of La₂Gd₈ recorded at 450 °C, 500 °C and 550 °C, respectively.

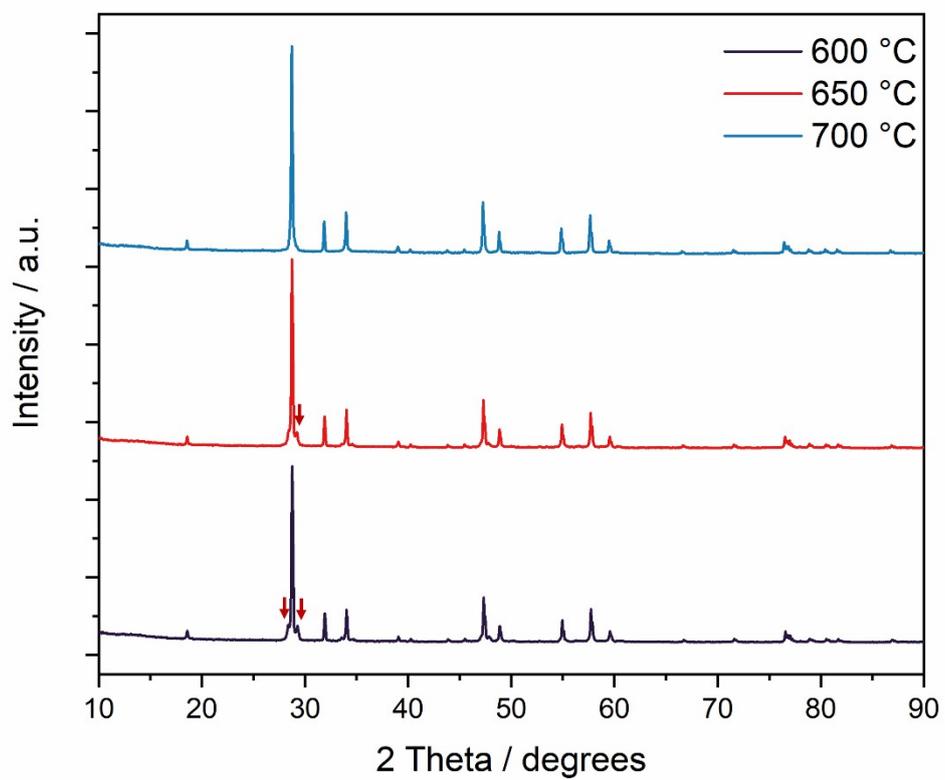


Figure S11. XRD patterns of GNM10 recorded at 600 °C, 650 °C and 700 °C, respectively. The peaks from monoclinic phase are marked by the arrows.

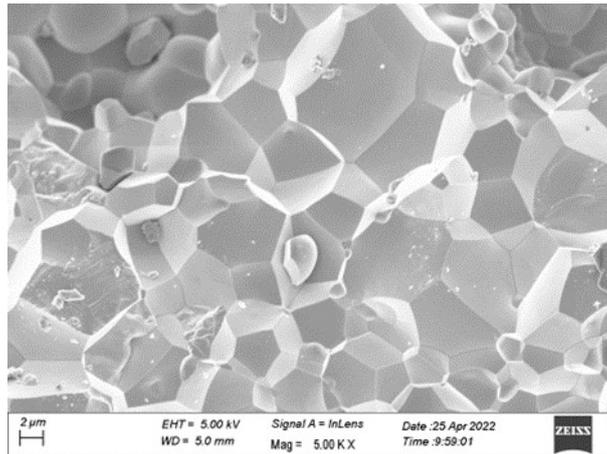


Figure S12. Microstructure of cross section of LNM10.

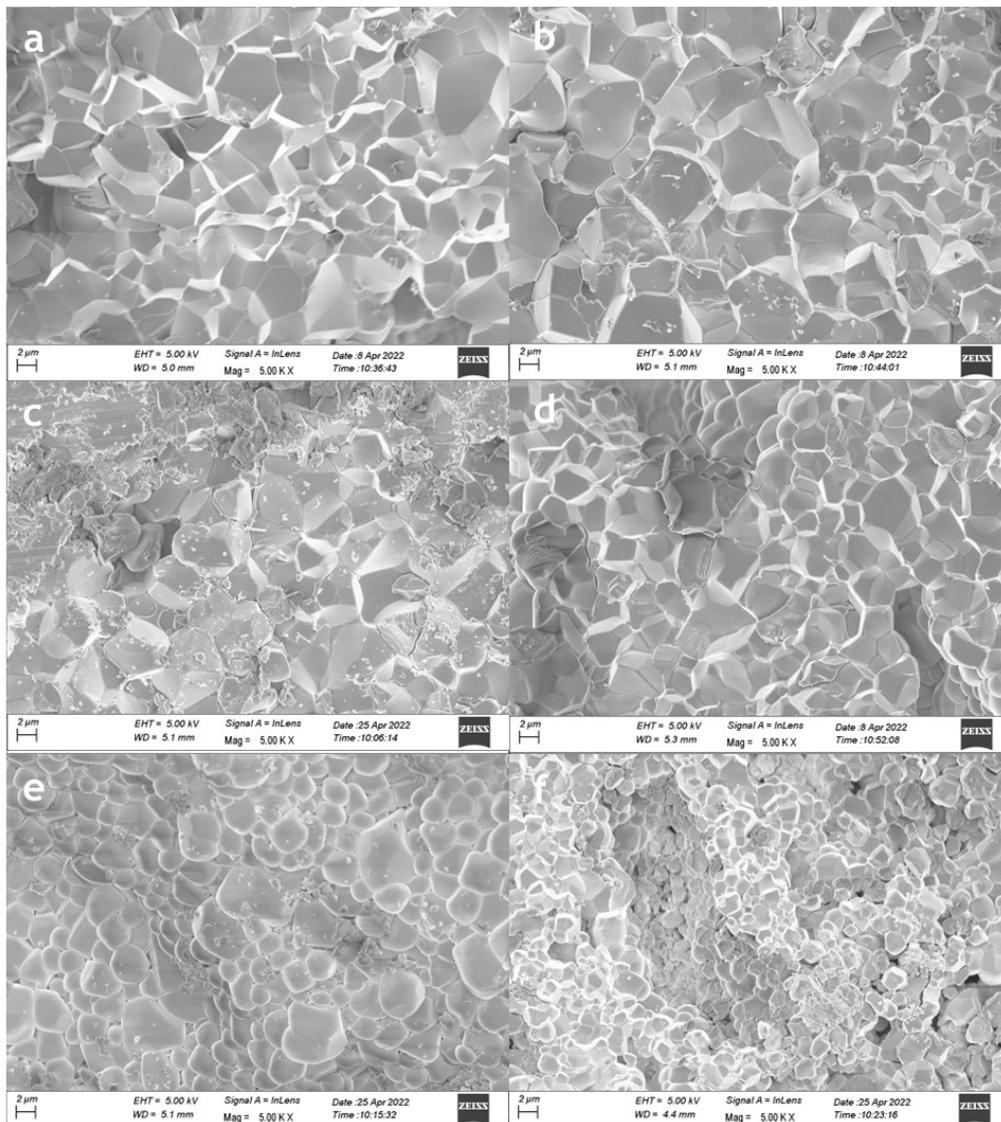


Figure S13. Microstructure of cross section of a) La₈Gd₂, b) La₆Gd₄, c) La₅Gd₅, d) La₄Gd₆, e) La₂Gd₈ and f) GNM10.

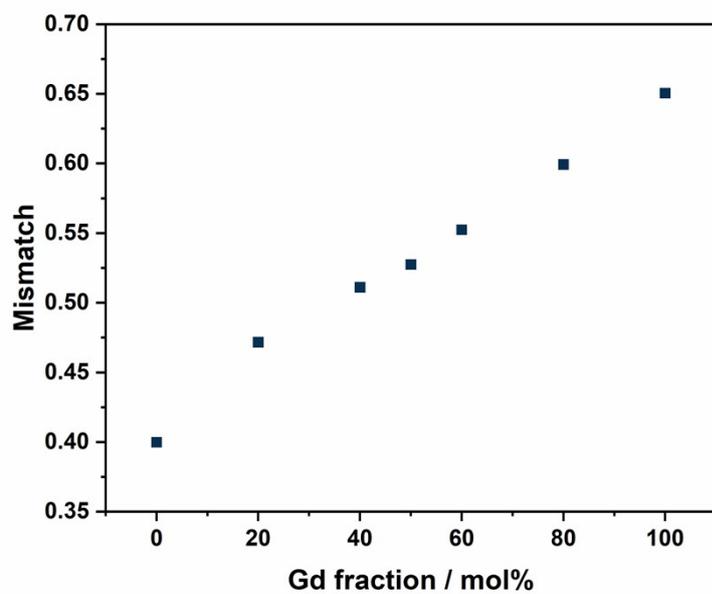


Figure S14. BVS results of $\text{La}_{1-x}\text{Gd}_x\text{Nb}_{0.9}\text{Mo}_{0.1}\text{O}_{4.05}$ series on La and Gd sites.

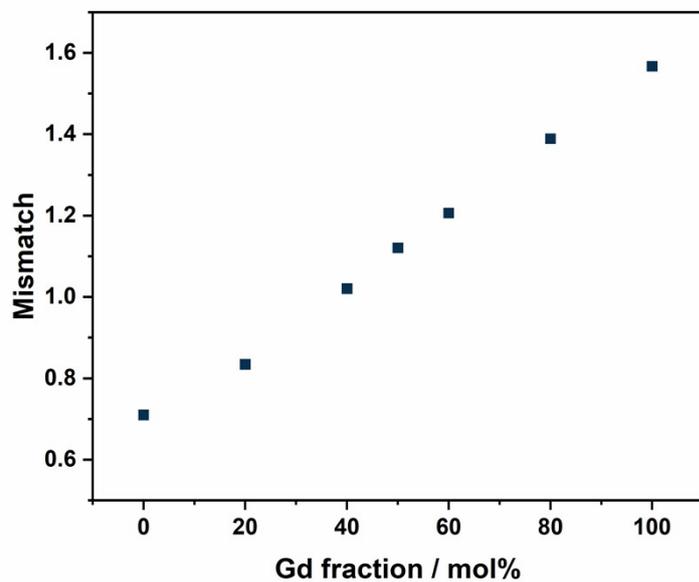


Figure S15. BVS results of $\text{La}_{1-x}\text{Gd}_x\text{Nb}_{0.9}\text{Mo}_{0.1}\text{O}_{4.05}$ series on Nb site.

Table S1. Refined structural parameters of all samples from Rietveld refinements against XRD data collected at 25 °C.

	LNm10	La8Gd2	La6Gd4	La5Gd5	La4Gd6	La2Gd8	GNM10
Space group	I12/a1						
a (Å)	5.3940(2)	5.4023(3)	5.4489(4)	5.4402(6)	5.4185(6)	5.3906(3)	5.3513(9)
b (Å)	11.6543(5)	11.5269(5)	11.3912(7)	11.3375(9)	11.2881(1)	11.1923(5)	11.1073(5)
c (Å)	5.3067(3)	5.2770(3)	5.1957(4)	5.1751(6)	5.1721(6)	5.1434(2)	5.1322(8)
β (°)	91.233(2)	91.600(2)	93.178(3)	93.420(5)	93.405(4)	93.713(2)	93.563(6)
V (Å ³)	333.531(9)	328.494(4)	322.003(4)	318.630(9)	315.796(4)	309.678(4)	304.468(1)
R _{wp} (%)	3.89	4.88	4.20	6.78	5.50	3.35	7.50
χ^2	1.83	5.34	4.47	7.12	6.38	4.14	8.43

Table S2. Refined structural parameters of all samples from Rietveld refinements against XRD data collected at 900 °C.

	LNM10	La8Gd2	La6Gd4	La5Gd5	La4Gd6	La2Gd8	GNM10
Space group	I4 ₁ /a						
a (Å)	5.4042(4)	5.3853(5)	5.3556(5)	5.3400(4)	5.3286(6)	5.3007(2)	5.2732(6)
c (Å)	11.7868(6)	11.6814(7)	11.5615(8)	11.5030(6)	11.4497(9)	11.3474(2)	11.2439(9)
V (Å ³)	344.241(9)	338.785(4)	331.617(9)	328.019(8)	325.110(5)	318.842(3)	312.656(8)
R _{wp} (%)	10.14	9.45	8.03	8.32	7.11	8.44	5.59
χ ²	8.16	7.28	6.25	6.45	6.21	7.69	7.56

Table S3. Refined structural parameters of all samples from Rietveld refinements against XRD data collected at 750 °C.

	LNM10	La8Gd2	La6Gd4	La5Gd5	La4Gd6	La2Gd8	GNM10
Space group	I4 ₁ /a						
a (Å)	5.3910(2)	5.3779(2)	5.3495(2)	5.3342(3)	5.3222(3)	5.2952(3)	5.2696(4)
c (Å)	11.7630(3)	11.6534(3)	11.5362(3)	11.4776(6)	11.4238(4)	11.3225(4)	11.2260(6)
V (Å ³)	341.874(9)	337.047(9)	330.134(2)	326.594(2)	323.598(7)	317.479(5)	311.742(4)
R _{wp} (%)	4.82	4.63	3.82	7.98	3.89	8.44	5.59
χ ²	2.37	5.06	4.19	8.67	4.76	7.69	7.56

