

Using Applied Pressure to Guide Materials Design: A Neutron Diffraction Study of $\text{La}_2\text{NiO}_{4+\delta}$ and $\text{Pr}_2\text{NiO}_{4+\delta}$

SUPPLEMENTARY INFORMATION

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The table below shows the determined structural parameters from the refinement of La_2NiO_4 and Pr_2NiO_4 . It contains the refined parameters from the Rietveld analysis: Lattice parameters (a , b & c), unit cell volume and the lanthanide and oxygen (2) z atom positions. The remaining structural parameters are fixed as defined in the main text. The quality of fit indicators are also given for the whole pattern including anvils and lead. High background from anvils results in the low χ^2 values in the Pr_2NiO_4 experiment as a result of an anvil with high preferred orientation.

La ₂ NiO ₄									
Pressure (GPa)	0.024	0.182	0.437	0.75	1.192	1.663	2.296	2.822	
Symmetry	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	
Space Group	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	
a (Å)	3.86209(13)	3.86151(15)	3.85900(17)	3.85669(17)	3.85314(17)	3.84935(17)	3.84486(18)	3.84010(21)	
b (Å)	3.86209(13)	3.86151(15)	3.85900(17)	3.85669(17)	3.85314(17)	3.84935(17)	3.84486(18)	3.84010(21)	
c (Å)	12.6908(8)	12.6852(10)	12.6774(11)	12.6661(11)	12.6542(11)	12.6367(11)	12.6217(12)	12.6059(14)	
Unit cell volume (Å ³)	189.294(15)	189.153(17)	188.790(19)	188.396(19)	187.874(19)	187.244(19)	186.586(20)	185.892(23)	
La z	0.3614(4)	0.3624(5)	0.3619(5)	0.3625(5)	0.3619(5)	0.3606(5)	0.3612(5)	0.3611(6)	
O2 z	0.1681(2)	0.1669(6)	0.1688(8)	0.1696(8)	0.1688(5)	0.1733(10)	0.1715(8)	0.1720(10)	
Z	2	2	2	2	2	2	2	2	
χ^2	2.3	1.9	2.4	2.4	1.9	1.8	1.9	1.3	
wRp	3.8	4.7	4.8	4.9	4.3	4.2	4.5	5.3	
Rp	4.2	5.8	6.3	6.1	4.3	4.5	4.6	5.5	
Pr ₂ NiO ₄									
Pressure (GPa)	0	0.022	0.063	0.128	0.266	0.671	1.197	1.677	2.234
Symmetry	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space Group	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>	<i>Fmmm</i>
a (Å)	5.3952(5)	5.3971(4)	5.3965(5)	5.3970(5)	5.3953(6)	5.3890(7)	5.3853(7)	5.3754(7)	5.3724(11)
b (Å)	5.4617(5)	5.4610(4)	5.4627(5)	5.4622(5)	5.4627(6)	5.4604(7)	5.4547(7)	5.4516(7)	5.4455(11)
c (Å)	12.4711(10)	12.4648(9)	12.4580(10)	12.4499(11)	12.4426(12)	12.4257(14)	12.4080(14)	12.3937(14)	12.3643
Unit cell volume (Å ³)	367.482(34)	367.379(30)	367.252(34)	367.01(4)	366.72(4)	365.64(5)	364.48(5)	363.19(5)	361.73(9)
La z	0.3574(5)	0.3585(4)	0.3595(5)	0.3590(5)	0.3617(7)	0.3577(7)	0.3584(7)	0.3594(7)	0.3615(9)
O2 z	0.1714(7)	0.1717(5)	0.1713(6)	0.1703	0.1692(6)	0.1715(8)	0.1703(8)	0.1705(7)	0.1728(9)
Z	4	4	4	4	4	4	4	4	4
χ^2	0.8	1.3	0.8	0.9	0.8	0.9	1.0	0.9	0.9
wRp	5.8	4.9	5.9	6.2	6.3	6.9	6.6	6.8	6.4
Rp	6.6	5.5	6.9	7.1	6.9	7.8	7.2	7.3	7.2

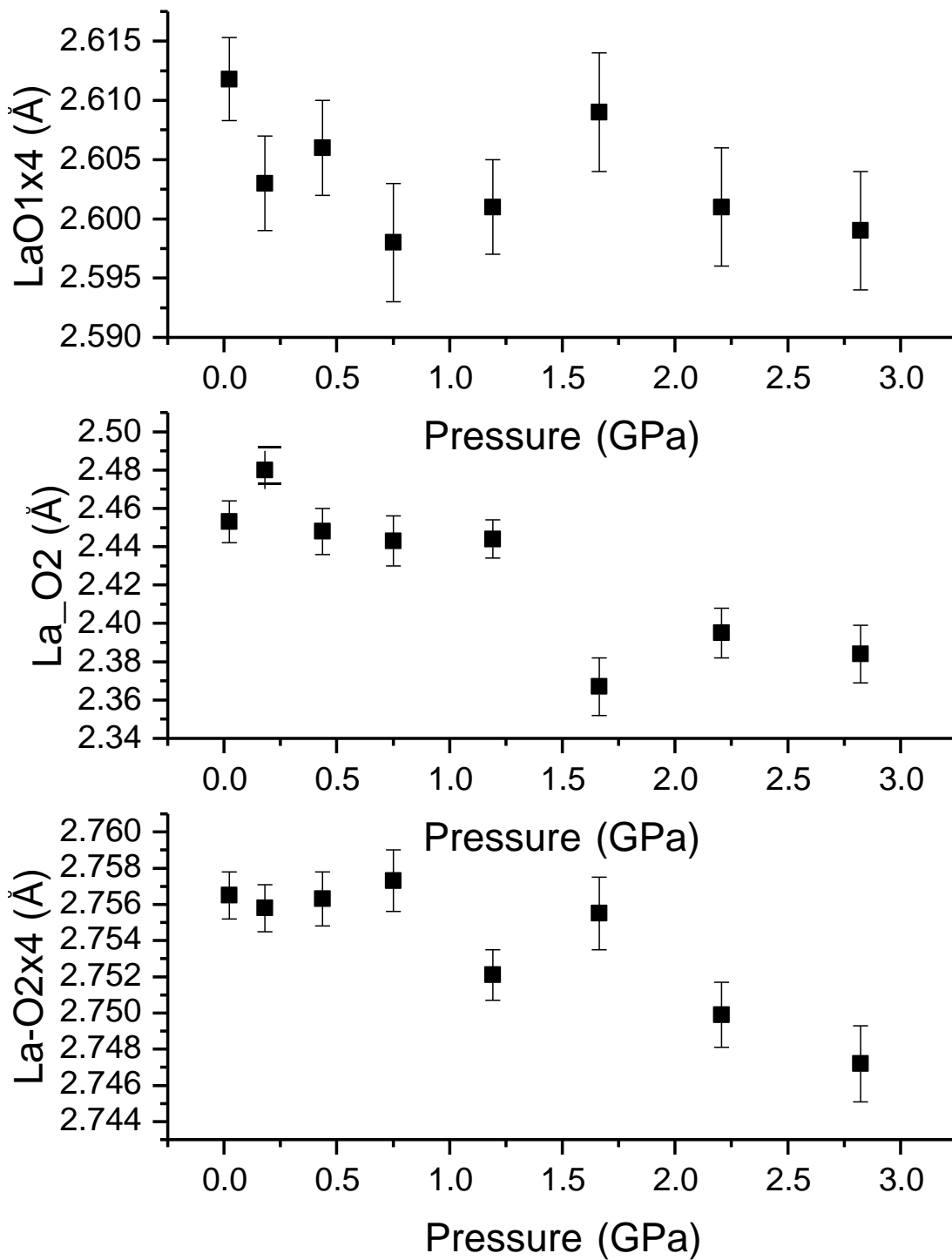


Figure S1: Variation in La-O bond distances with pressure of $\text{La}_2\text{NiO}_{4+\delta}$.

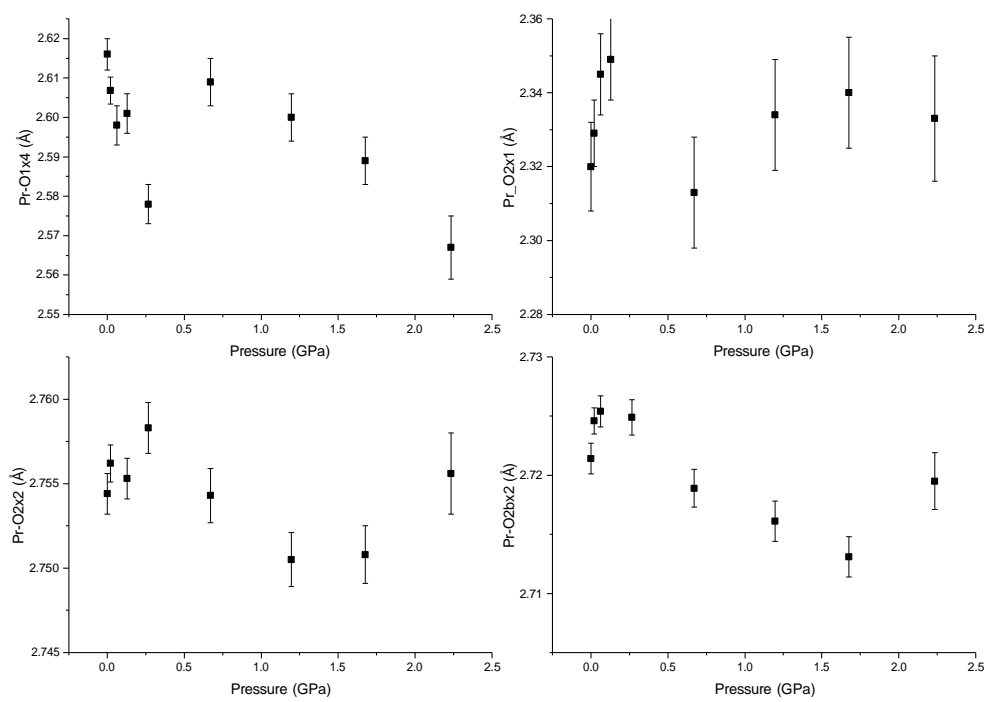


Figure S2: Variation in Pr–O bond distances with pressure of $\text{Pr}_2\text{NiO}_{4+\delta}$.

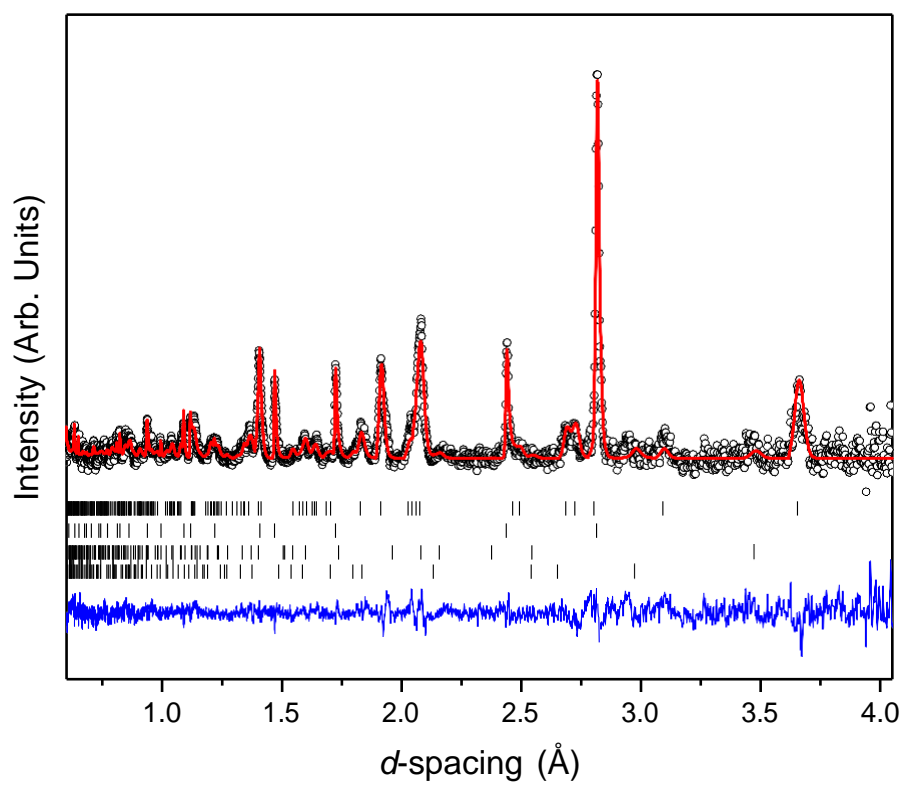


Figure S3: Diffraction pattern of $\text{Pr}_2\text{NiO}_{4+\delta}$ at 2.2 GPa.