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SUPPLEMENTARY

to

Chemical lattice strain in nonstoichiometric oxides: an overview

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Oxide	Temperatures, °C	$^{\delta}$ range	$\beta = \varepsilon_{chem} / \Delta \delta$	Source	
		0.02-0.20	0.092	1	
CeO _{2–δ}	900	0.02-0.10	0.101	2	
		0.12-0.18	0.073		
$Ce_{0.9}Pr_{0.1}O_{2-\delta}$	650-900	0.01-0.06	0.087	3	
	800	0.05-0.10	0.084	_ 4	
Ce _{0.8} PI _{0.2} O _{2-δ}	800	0.10-0.15	0.108		
	700-900	0.00-0.14	0.101	5	
$Ce_{0.9}Gd_{0.1}O_{2-\delta}$	700-900	0.01-0.07	0.132	6	
	800-900	0.08-0.14	0.078	6	
$Ce_{0.8}Gd_{0.2}O_{2-\delta}$	700-800	0.10-0.15	0.055	7, 8	
Ce _{0.9} Υ _{0.1} Ο _{2-δ}	700-1000	0.05-0.23	0.086	9	
$Ce_{0.8}Y_{0.2}O_{2-\delta}$	700-1000	0.10-0.25	0.075	9	
Ce _{0.8} Y _{0.2} O _{2-δ}	900	0.12-0.20	0.080	10	
Се _{0.9} Sm _{0.1} O _{2-б}	700-1000	0.05-0.18	0.088	9	
$Ce_{0.8}Sm_{0.2}O_{2-\delta}$	Ce _{0.8} Sm _{0.2} O _{2-δ} 700-1000		0.092	9	
$Ce_{0.5}Zr_{0.4}Pr_{0.1}O_{2-\delta}$	2e _{0.5} Zr _{0.4} Pr _{0.1} O _{2-δ} 700-900		0.046	5	
$Ce_{0.5}Zr_{0.5}O_{2-\delta}$	-	0.00-0.25	0.048	5	
$Ce_{0.8}Zr_{0.2}O_{2-\delta}$	700	0.06-0.15	0.055		
	800	0.05-0.15	0.044	11	
	900	0.05-0.15	0.062		

Oxide	$\Delta\delta$	$eta = arepsilon_{chem} / \Delta \delta$	Source
$La_{0.8}Sr_{0.2}CrO_{3-\delta}$	0.10	0.016	12
La _{0.76} Sr _{0.24} CrO _{3-δ}	0.12	0.020	12
$La_{0.7}Sr_{0.3}CrO_{3-\delta}$	0.15	0.023	12
$La_{0.9}Ca_{0.1}CrO_{3-\delta}$	0.09	0.021	13
La _{0.8} Ca _{0.2} CrO _{3-δ}	0.04	0.028	13
La _{0.7} Ca _{0.3} CrO _{3-δ}	0.10	0.036	12
$La_{0.8}Sr_{0.2}Cr_{0.97}V_{0.03}O_{3-\delta}$	0.07	0.027	13
$La_{0.7}Ca_{0.3}Cr_{0.9}Al_{0.1}O_{3-\delta}$	0.12	0.034	12
$La_{0.7}Ca_{0.3}Cr_{0.9}Ti_{0.1}O_{3-\delta}$	0.07	0.032	12
LaCr _{0.95} Mg _{0.05} O _{3-δ}	0.02	0.016	14
LaCr _{0.85} Mg _{0.15} O _{3-δ}	0.07	0.010	14

Oxide	Temperatures, °C $\Delta\delta$ $\beta = \varepsilon_{chem}/\Delta\delta$		Source	
	room temperature	0.22	0.012	15
	(annealed samples) 0.22 0.012		0.012	15
	400-600 0.15 0.033		0.033	16
Ba Sr Ca Ea O	700-950	0.17	0.019-0.021	17
Bd _{0.5} Sr _{0.5} CO _{0.8} Fe _{0.2} O _{3-δ}	600	0.09	0.026	18
	700	0.10	0.022	18
	800	0.11	0.019	18
	900	0.12	0.016	18
$SrCo_{0.8}Fe_{0.2}O_{3-\delta}$	700-950	0.19	0.026-0.032	17
$SrFe_{0.7}AI_{0.3}O_{3-\delta}$	750-950	0.07	0.046	19
$La_{0.8}Sr_{0.2}Fe_{0.7}Ga_{0.3}O_{3-\delta}$	900	0.04	0.039	20
SrSn _{0.65} Fe _{0.35} O _{3-δ}	700-1000	0.015	0.032-0.041	21
$SrTi_{0.65}Fe_{0.35}O_{3-\delta}$	700-1000	0.06	0.040-0.049	22
$La_{0.2}Sr_{0.8}Fe_{0.55}Ti_{0.45}O_{3-\delta}$	789-998	0.05	0.052	23
Nd _{0.7} Sr _{0.3} Fe _{0.7} Co _{0.3} O _{3-δ}	750-1000	0.05	0.046	24
$Nd_{0.6}Sr_{0.4}Fe_{0.7}Co_{0.3}O_{3-\delta}$	650-1000	0.10	0.041	24
Nd _{0.5} Sr _{0.5} Fe _{0.7} Co _{0.3} O _{3-δ}	550-1000	0.13	0.036	24
Nd _{0.3} Sr _{0.7} Fe _{0.7} Co _{0.3} O _{3-δ}	550-1000	0.17	0.040	24
$Nd_{0.4}Sr_{0.6}FeO_{3-\delta}$	650-1000	0.11	0.040	25
$Nd_{0.3}Sr_{0.7}FeO_{3-\delta}$	650-1000	0.12	0.041	25
$Nd_{0,2}Sr_{0,8}FeO_{3-\delta}$	650-1000	0.12	0.041	25
$Ba_{0.95}La_{0.05}FeO_{3-\delta}$	850-950	0.025	0.061-0.071	26
	750-900	0.2	0.0574	27
SrFeO _{3-δ}	room temperature	0.2	0.0107	27
	(annealed samples)	0.5	0.0197	
$La_{0.3}Sr_{0.7}FeO_{3-\delta}$	800	0.17	0.035	28
$La_{0.5}Sr_{0.5}FeO_{3-\delta}$	800	0.10	0.059	29
$La_{0.5}Sr_{0.5}FeO_{3-\delta}$	750-900	0.065	0.033	30
La Sr FoO	500-900	0.16	0.020	31
La _{0.6} Si _{0.4} FeO _{3-δ}	659-777	0.05	0.037	32
$La_{0.8}Sr_{0.2}FeO_{3-\delta}$	850-900	0.025	0.015	33
	600-800	0.13	0.022	34
$La_{0.6}Sr_{0.4}Fe_{0.8}Co_{0.2}O_{3-\delta}$	700-900	0.13	0.031	35
	700-890	0.15	0.032	36
$La_{0.6}Sr_{0.4}Fe_{0.6}Co_{0.4}O_{3-\delta}$	600-800	0.13	0.030	34
$La_{0.6}Sr_{0.4}Fe_{0.5}Co_{0.5}O_{3-\delta}$	500-900	0.17	0.018	37
$La_{0.6}Sr_{0.4}Fe_{0.4}Co_{0.6}O_{3-\delta}$	600-800	0.12	0.028	34
	600-800	0.14	0.024	34
$La_{0.6}Sr_{0.4}Fe_{0.2}CO_{0.8}O_{3-\delta}$	800	0.18	0.022	38
$La_{0.5}Sr_{0.5}Fe_{0.5}Co_{0.5}O_{3-\delta}$	800-1000	0.12	0.036-0.039	39
$La_{0,1}Sr_{0,9}Fe_{0,2}Co_{0,8}O_{3-\delta}$	900-1000	0.12	0.047	40
La _{0.3} Sr _{0.7} CoO _{3-δ}	901	0.13	0.035	41
$La_{0.5}Sr_{0.5}CoO_{3-\delta}$	800	0.12	0.035	39
	500-900	0.17	0.022	37
La _{0.6} Sr _{0.4} COU _{3-δ}	892	0.11	0.030	41
$La_{0.8}Sr_{0.2}CoO_{3-\delta}$	891	0.07	0.025	41
LaCoO _{3-δ}	950-1050	0.03	0.020	42
(La _{0.6} Sr _{0.4}) _{0.99} CoO _{3-δ}	900	0.05	0.027	43

Table S3. Chemical expansion coefficients for some perovskite-like complex oxides containing Fe or Co

(La _{0.3} Sr _{0.7}) _{0.99} Co _{0.9} Ni _{0.1} O _{3-δ}	900	0.04	0.033	43

Oxides					
Oxide	Temperatures, °C	δ range	$\beta_a = \varepsilon_{chem}(a)/\Delta\delta$	$\beta_c = \varepsilon_{chem}(c)/\Delta\delta$	Source
LaBaCo ₂ O _{6-δ}	717-853	0.27-0.54	0.037-0.039	0.011-0.017	44
	1000	0.76-0.84	0.026	-0.016	45, 46
PrBaCo₂O _{6−δ}	573-777	0.43-0.80	0.013	-0.005	47
	852	0.73-0.83	0.017	-0.008	
	900	0.55-0.96	0.002	-0.009	48, 49
	200-1000	0.37-0.81	0.006	-0.017	50 *
	573-777	0.49-0.86	0.010-0.011	-0.008	51
NdBaCo ₂ O _{6-δ}	852	0.71-0.90	0.008	-0.007	
2 0 0	200-1000	0.44-0.86	0.013	-7.04·10 ⁻⁵	50 **
	350	0.36-0.65	-	-0.005	52
GdBaCo ₂ O _{6–δ}	440	0.59-0.70	0.007	-0.011	53
	600-750	0.60-0.95	0.008	-0.009	54
PrBaFe ₂ O _{6-δ}		0.50-0.90	0.0094	-0.0323	55
NdBaFe ₂ O _{6-δ}		0.50-0.95	0.0088	-0.0354	56, 57
SmBaFe₂O _{6−δ}	RT	0.50-0.92	0.0080	-0.0385	57-59
EuBaFe ₂ O _{6-δ}		0.59-0.85	0.0084	-0.0381	60
GdBaFe ₂ O _{6-δ}	-	0.61-0.90	0.0078	-0.0415	61
PrBaFeMnO _{6-δ}	RT	0.00-1.00	0.022	-0.008	62
$PrBaMn_2O_{6-\delta}$	RT	0.00-1.00	0.022	2.00·10 ⁻⁴	
	711	0.83-1.00	0.011	0.016	63
Sr ₂ FeMoO _{6-δ}	RT	0.01-0.09	0.012	-0.016	64
$La_2NiO_{4+\delta}$	800	0.01-0.06	-0.028 ***	0.076 ***	65
La ₂ (Ni _{0.9} Cu _{0.1})O _{4+δ}	600-900	0.01-0.07	-0.051 ***	0.84 ***	66
La ₂ (Ni _{0.9} Co _{0.1})O _{4+δ}	600-900	0.09-0.16	-0.051 ***	0.62 ***	66
La ₂ (Ni _{0.9} Fe _{0.1})O _{4+δ}	600-900	0.10-0.16	-0.081 ***	0.70 ***	66

Table S4. Chemical expansion coefficients for some double perovskite oxides and Ruddlesden-Popper

* orthorhombic symmetry, $\beta_b = \varepsilon_c(b)/\Delta\delta = 0.006$

** orthorhombic symmetry, $\beta_b = \varepsilon_c(b)/\Delta \delta = 0.017$

*** please note that as the oxygen content for Ruddlesden-Popper phases is written as " $4+\delta$ " unlike " $x-\delta$ " for the other oxides, here negative β refers to expansion, and positive – to contraction upon reduction (oxygen loss)



Fig. S1. Chemical strain of GdBaCo₂O_{6- δ}:⁵²⁻⁵⁴ filled symbols – $\varepsilon_{chem}(a)$, empty symbols – $\varepsilon_{chem}(c)$



Fig. S2. Chemical strain of $PrBaCo_2O_{6-6}$:⁴⁷⁻⁵⁰ filled symbols – $\varepsilon_{chem}(a)$, empty symbols – $\varepsilon_{chem}(c)$, crosses – $\varepsilon_{chem}(b)$, lines are given to guide the eye only



Fig. S3. Chemical strain of NdBaCo₂O_{6- δ}:^{50, 51} filled symbols – $\varepsilon_{chem}(a)$, empty symbols – $\varepsilon_{chem}(c)$, crosses – $\varepsilon_{chem}(b)$, lines are given to guide the eye only



Fig. S4. Volumetric and average linear chemical strain of NdBaCo_2O_{6-\delta}{}^{50, \, 51, \, 67}



Fig. S5. Chemical strain of $PrBaM_2O_{6-\delta}$ (M = Fe,⁵⁵ Fe_{0.5}Cu_{0.5},^{68, 69} Fe_{0.5}Mn_{0.5},⁶² Mn⁶²): filled symbols and solid lines $-\varepsilon_{chem}(a)$,

empty symbols and dashed lines – $\varepsilon_{chem}(c)$

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