Electronic Supplementary Material (ESI) for Materials Advances.

Predicting and Accessing Metastable Phases

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Phonon dispersion

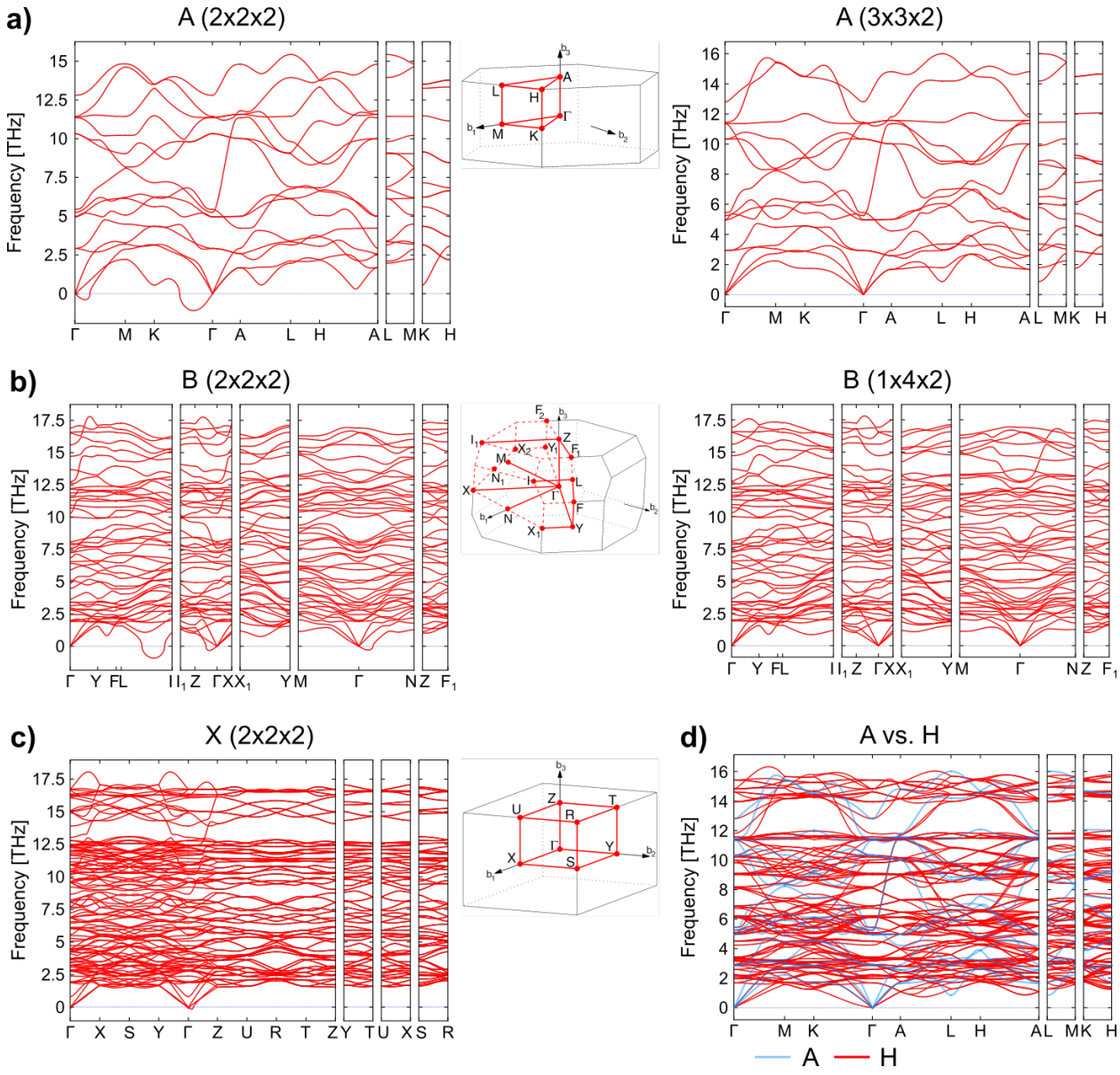

Figure S1. Phonon dispersion of: a) A, b) B, and c) X phase. The used k-point paths are shown in the middle. d) Comparison between the phonon dispersion of A (blue) and H phase (red). The "purple" bands in (d) emphasize the overlap in dispersion in the A and H phases.

Crystallographic Parameters

Table S1. Crystallographic parameters of the studied polymorphs for all studied oxides (chemistries).

Polymorph	Oxide	a [Å]	b [Å]	c [Å]	α [°]	β [°]	γ [°]
A	La_2O_3	3.9051	3.9051	6.0367	90.00	90.00	120.00
	Nd_2O_3	3.8243	3.8243	5.9555	90.00	90.00	120.00
	Sm_2O_3	3.7569	3.7569	5.8787	90.00	90.00	120.00
	Gd_2O_3	3.6922	3.6922	5.8053	90.00	90.00	120.00
	Dy_2O_3	3.6408	3.6408	5.7530	90.00	90.00	120.00
	Er_2O_3	3.5951	3.5951	5.7082	90.00	90.00	120.00
	Lu_2O_3	3.5282	3.5282	5.6442	90.00	90.00	120.00
B	La_2O_3	13.8371	3.9043	9.0648	90.00	102.49	90.00
	Nd_2O_3	14.2789	3.6693	8.9390	90.00	99.72	90.00
	Sm_2O_3	14.1025	3.5969	8.7972	90.00	99.84	90.00
	Gd_2O_3	13.9329	3.5277	8.6584	90.00	99.93	90.00
	Dy_2O_3	13.8088	3.4715	8.5484	90.00	100.03	90.00
	Er_2O_3	13.6948	3.4222	8.4512	90.00	100.10	90.00
	Lu_2O_3	13.5291	3.3511	8.3077	90.00	100.19	90.00
C	La_2O_3	11.2756	11.2756	11.2756	90.00	90.00	90.00
	Nd_2O_3	11.0516	11.0516	11.0516	90.00	90.00	90.00
	Sm_2O_3	10.8647	10.8647	10.8647	90.00	90.00	90.00
	Gd_2O_3	10.6845	10.6845	10.6845	90.00	90.00	90.00
	Dy_2O_3	10.5426	10.5426	10.5426	90.00	90.00	90.00
	Er_2O_3	10.4165	10.4165	10.4165	90.00	90.00	90.00
	Lu_2O_3	10.2322	10.2322	10.2322	90.00	90.00	90.00
H	La_2O_3	7.8107	7.8072	12.0711	90.00	90.01	119.99
	Nd_2O_3	7.6481	7.6480	12.0234	90.00	90.00	120.00
	Sm_2O_3	7.5150	7.5121	11.8660	90.00	90.01	120.00
	Gd_2O_3	7.3845	7.3831	11.7156	89.99	90.02	119.98
	Dy_2O_3	7.2822	7.2800	11.6072	89.99	90.02	119.98
	Er_2O_3	7.1912	7.1931	11.5096	90.01	89.98	120.02
	Lu_2O_3	7.0627	7.0556	11.3706	90.00	90.04	119.97
X	La_2O_3	8.7135	8.7135	8.8381	90.00	90.00	89.64
	Nd_2O_3	8.5456	8.5449	8.6884	90.00	90.00	89.30
	Sm_2O_3	8.4090	8.4089	8.5372	90.00	90.00	89.16
	Gd_2O_3	8.2771	8.2776	8.3915	90.00	90.00	89.04
	Dy_2O_3	8.1732	8.1730	8.2772	90.00	90.00	88.94
	Er_2O_3	8.0806	8.0807	8.1753	90.00	90.00	88.87
	Lu_2O_3	7.9434	7.9434	8.0294	90.00	90.00	88.75

Shifting Energies

Table S2. Parameters used to shift the total energies of the disordered phases (H and X), and the La_2O_3 A phase. The shifting parameters are in meV/atom.

Compound	A	H	X
La_2O_3	13.00	48.00	14.35
Nd_2O_3		53.75	31.15
Sm_2O_3		43.55	32.13
Gd_2O_3		45.50	34.23
Dy_2O_3		46.30	49.00
Er_2O_3		48.00	57.88
Lu_2O_3		50.00	63.75

Metastable Phase Diagrams

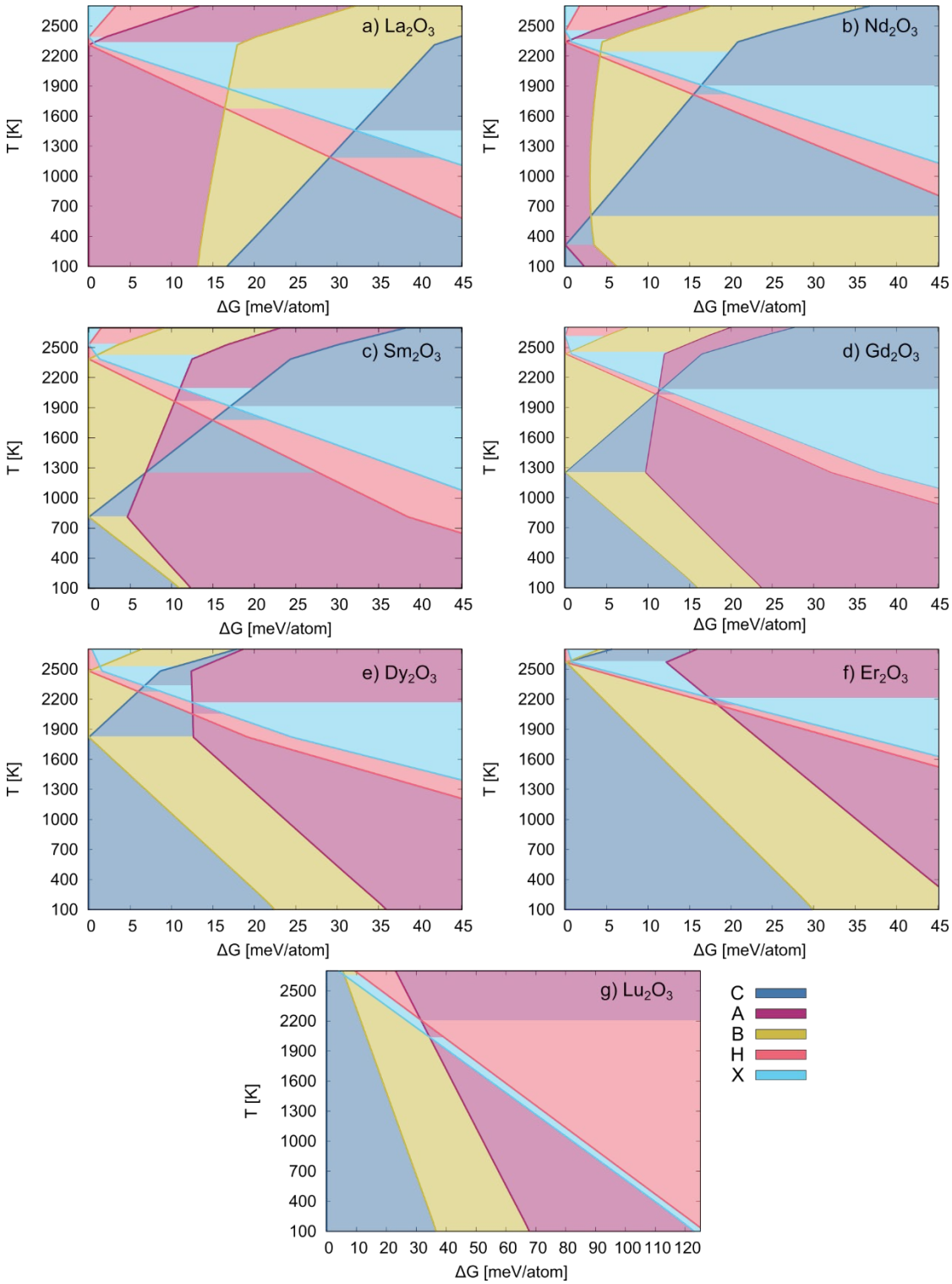

Figure S2. Metastable phase diagrams of: a) La_2O_3, b) Nd_2O_3, c) Sm_2O_3, d) Gd_2O_3, e) Dy_2O_3, f) Er_2O_3, and g) Lu_2O_3. The C, A, H, B and X phases are shown in blue, magenta, red, yellow and light-blue,

respectively. Note that the metastability threshold scale of Lu2O3 is up to 125 meV/atom so the X and H phase metastable regions are visible.