Supporting Information for

Structural properties and magnetic ground states of 100 binary *d*-metal oxides studied by hybrid density functional methods

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Table S1. Summary of the studied binary *d*-metal oxides.

d-metal	Oxide	ICSD code[a]	Polymorph/Mineral	Space group	Space group for magnetic ground state	Pearson symbol	Oxidation state of the metal	Band gap (DFT-PBE0/TZVP)	Magnetic ground state (DFT-PBE0/TZVP)[d]	*k*-mesh
Sc	Sc_2O_3	26942	Kangite (impure)	*Ia*-3 (206)		*cI*80	III	6.3	DM	4×4×4
Y	Y_2O_3	82420	Yttriaite-(Y)	*Ia*-3 (206)		*cI*80	III	6.5	DM	4×4×4
La	La_2O_3	641600	C-La_2O_3	*Ia*-3 (206)		*cI*80	III	5.8	DM	4×4×4
	La_2O_3	100204	A-La_2O_3	*P*-3*m*1 (164)		*hP*5	III	6.0	DM	12×12×6
Ti	TiO	196273	ε-TiO	*P*-62*m* (189)		*hP*6	II	-	DM	6×6×10[e]
	Ti_2O_3	9646	Tistarite	*R*-3*c* (167)	*R*3*c* (161)	*hR*10	III	2.7	AFM	8×8×8
	TiO_2	202240	Rutile	$P4_2/mnm$ (136)		*tP*6	IV	3.9	DM	8×8×12
	TiO_2	63711	Anatase	$I4_1/amd$ (141)		*tI*12	IV	4.1	DM	8×8×8
	TiO_2	36408	Brookite	*Pbca* (61)		*oP*24	IV	4.4	DM	4×8×8
	Ti_3O_5	50984	α-Ti_3O_5	*Cmcm* (63)	*Cm* (8)	*oS*32	III/IV	2.0	AFM	8×8×4
	Ti_3O_5	26492	β-Ti_3O_5	*C*2/*m* (12)	*Cm* (8)	*mS*32	III/IV	1.3	AFM	8×8×4
	Ti_3O_5	194464	γ-Ti_3O_5	*C*2/*c* (15)	*P*1 (1)	*mS*32	III/IV	2.3	AFM	8×8×6
	Ti_3O_5	194465	δ-Ti_3O_5	*P*2/*a* (13)	*P*-1 (2)	*mS*32	III/IV	2.4	AFM	8×6×4
	Ti_3O_5		λ-Ti_3O_5	*C*2/*m* (12)	*Cm* (8)	*mS*32	III/IV	1.7	AFM	8×8×4
Zr	ZrO_2	82543	Baddeleyite	$P2_1/c$ (14)		*mP*12	IV	5.8	DM	8×8×8
	ZrO_2	23928		$P4_2/nmc$ (137)		*tP*6	IV	6.1	DM	12×12×8
Hf	HfO_2	27313		$P2_1/c$ (14)		*mP*12	IV	6.6	DM	8×8×8
V	V_2O_3	201106	Corundum/Karelianite	*R*-3*c* (167)	*R*3*c* (161)	*hR*10	III	3.0	AFM	8×8×8
	V_2O_3	6286	Karelianite	*C*2/*c* (15)	*P*2/*c* (13)	*mS*20	III	2.8	AFM	8×8×6
	VO_2	74705	Paramontroseite	$P2_1/c$ (14)	$P2_1$ (4)	*mP*12	IV	3.0	AFM	8×8×8
	VO_2	–[b]		*C*2/*m* (12)	*Cm* (8)	*mS*12	IV	3.3	AFM	6×6×6
	VO_2	66665	Paramontroseite	$P4_2/mnm$ (136)	*Cmmm* (65)	*tP*6	IV	2.8	AFM	8×8×12
	V_2O_5	60767	α-V_2O_5/Shcherbinaite, Navajoite (trihydrate)	*Pmmn* (59)		*oP*14	V	4.0	DM	4×12×8
	V_2O_5	80594	γ-V_2O_5	*Pnma* (62)		*oP*28	V	4.1	DM	4×12×4
Nb	NbO	14338		*Pm*-3*m* (221)		*cP*6	II	-	DM	8×8×8
	NbO_2	75197	Distorted rutile	$I4_1/a$ (88)		*tI*96	IV	2.1	DM	4×4×4
	NbO_2	75198	Rutile	$P4_2/mnm$ (136)		*tP*6	IV	-	DM	8×8×12
	Nb_2O_5	71317	*z*-Nb_2O_5	*C*2/*c* (15)		*mS*28	V	4.6	DM	6×6×8
Ta	Ta_2O_5	–	β-Ta_2O_5/Tantite	*Pmna* (53)		*oP*14	V	4.6	DM	6×12×6
Cr	Cr_2O_3	167268	Eskolaite	*R*-3*c* (167)	*R*3*c* (161)	*hR*10	III	5.1	AFM	8×8×8
	CrO_2	202836		$P4_2/mnm$ (136)	$P4_2/mnm$ (136)	*tP*6	IV	-	FM	8×8×12
	CrO_3	16031		*Ama2* (40)		*oS*16	VI	4.3	DM	8×8×8
Mo	MoO_2	80830	Tugarinovite	$P2_1/c$ (14)	$P2_1$ (4)	*mP*12	IV	-	AFM	8×8×8
	MoO_3	166363	α-MoO_3/Molybdite	*Pnma* (62)		*oP*16	VI	4.2	DM	2×12×12
W	WO_2	8217	Distorted rutile	$P2_1/c$ (14)	$P2_1$ (4)	*mP*12	IV	0.4	AFM	8×8×8
	WO_3	84843	ε-WO_3	*Pc* (7)		*mP*16	VI	3.5	DM	8×8×6
	WO_3	80053	δ-WO_3	*P*-1 (2)		*aP*32	VI	3.4	DM	6×6×6
	WO_3	50727	γ-WO_3/Tungstite (hydride)	$P2_1/c$ (14)		*mP*32	VI	3.3	DM	6×6×6
	WO_3	50729	β-WO_3/Krasnogorite	*Pbcn* (60)		*oP*32	VI	3.3	DM	6×6×6

	WO_3	50732	α-WO_3	*P*4/*ncc* (130)		*tP*16	VI	2.1	DM	8×8×6
	WO_3	88367		*P*4/*nmm* (129)		*tP*8	VI	2.1	DM	8×8×8
	WO_3	32001		*P*6/*mmm* (191)		*hP*12	VI	2.0	DM	6×6×12
Mn	MnO	9864	Manganosite	*Fm*-3*m* (225)	*R*-3*m* (166)	*cF*8	II	3.9	AFM	8×8×8
	MnO	262928		$P6_3mc$ (186)	$Pmc2_1$ (26)	*hP*4	II	3.0	AFM	12×8×8
	Mn_2O_3	24342	Bixbyite	*Pbca* (61)	*Pbca* (61)	*oP*80	III	-	AFM	4×4×4
	Mn_2O_3	9091	Bixbyite	*Ia*-3 (206)	*Ia*-3 (206)	*cI*80	III	-	FM	4×4×4
	Mn_3O_4	109250	Hausmannite	$I4_1/amd$ (141)	*Imma* (74)	*tI*28	II/III	3.2	FiM	6×6×6
	MnO_2	73363	α-MnO_2/Hollandite	*I*4/*m* (87)	*C*2/*m* (12)	*tI*24	IV	3.4	AFM	6×6×4
	MnO_2	78331	γ/R-MnO_2/Ramsdellite	*Pnam* (62)	$Pmc2_1$ (26)	*oP*12	IV	3.5	AFM	12×8×4
	MnO_2	73716	β-MnO_2/Pyrolusite	*P*4/*mnm* (136)	*Cmmm (65)*	*tP*6	IV	2.1	AFM	8×8×12
	MnO_2	193445	λ-MnO_2	*Fd*-3*m* (227)	*Imma* (74)	*cF*48	IV	3.7	AFM	8×8×8
	Mn_2O_7	60821		$P2_1/c$ (14)		*mP*72	VII	3.9	DM	6×2×4 [e]
Tc	TcO_2	173151		$P2_1/c$ (14)	$P2_1$ (4)	*mP*12	IV	2.4	AFM	8×8×8
	Tc_2O_7	16226		*Pbca* (61)		*oP*36	VII	4.9	DM	2×6×8
Re	ReO_2	647349		$P2_1/c$ (14)	$P2_1$ (4)	*mP*12	IV	1.5	AFM	8×8×8
	ReO_2	24060		*Pbcn* (60)	$P2_12_12$ (18)	*oP*12	IV	1.6	AFM	8×8×8
	ReO_2	154021	Rutile	$P4_2/mnm$ (136)	*Cmmm* (65)	*tP*6	IV	1.6	AFM	8×8×12
	ReO_3	77679		*Pm*-3*m* (221)		*cP*4	VI	-	DM	12×12×12
	Re_2O_7	15217		$P2_12_12_1$ (19)		*oP*72	VII	4.8	DM	2×2×8
Fe	Fe_3O_4	85806	Magnetite	*Fd*-3*m* (227)	*Fd*-3*m* (227)	*cF*56	II/III	-	FiM	8×8×8
	Fe_3O_4	98088		*P*2/*c* (13)	*P*2/*c* (13)	*mP*56	II/III	1.6	FiM	8×8×2
	Fe_2O_3	40142	α-Fe_2O_3/Hematite	*R*-3*c* (167)	*R*-3 (148)	*hR*10	III	4.0	AFM	8×8×8
	Fe_2O_3	237290	β-Fe_2O_3	*Ia*-3 (206)	$I2_12_12_1$ (24)	*cI*80	III	3.3	AFM	4×4×4
	Fe_2O_3	415250	ε-Fe_2O_3	$Pna2_1$ (33)	$Pna2_1$ (33)	*oP*40	III	4.0, 3.8	FiM	8×4×4
Ru	RuO_2	15071		$P4_2/mnm$ (136)	*Cmmm* (65)	*tP*6	IV	-	AFM	8×8×12
	RuO_4	415303		*P*-43*n* (218)		*cP*40	VIII	4.2	DM	4×4×4
	RuO_4	415306		*C*2/*c* (15)		*mS*20	VIII	4.1	DM	8×8×4
Os	OsO_2	15070		$P4_2/mnm$ (136)		*tP*6	IV	-	DM	8×8×12
	OsO_4	63		*C*2/*c* (15)		*mS*20	VIII	5.1	DM	8×8×4
Co	CoO	9865		*Fm*3*m* (225)	*R*-3*m* (166)	*cF*8	II	4.5	AFM	8×8×8
	CoO	43458		$P6_3mc$ (186)	$Pmc2_1$ (26)	*hP*4	II	3.2	AFM	12×8×8
	Co_3O_4	63165		*Fd*-3*m* (227)	*F*-43*m* (216)	*cF*56	II/III	4.0	AFM	6×6×6
Rh	Rh_2O_3	108941	Corundum	*R*-3*c* (167)		*hR*10	III	3.2	DM	8×8×8
	Rh_2O_3	9206		*Pbca* (61)		*oP*40	III	3.0	DM	8×8×2 [e]
	RhO_2	28498	Rutile	$P4_2/mnm$ (136)	$P4_2/mnm$ (136)	*tP*6	IV	-	FM	8×8×12
Ir	IrO_2	84577	Rutile	$P4_2/mnm$ (136)	*Cmmm* (65)	*tP*6	IV	-	AFM	8×8×12
Ni	NiO	9866	Bunsenite	*Fm*3*m* (225)	*R*-3*m* (166)	*cF*8	II	5.2	AFM	8×8×8
Pd	PdO	24692	Palladinite	$P4_2/mmc$ (131)		*tP*4	II	1.4	DM	12×12×8
Pt	PtO	– [c]		$P4_2/mmc$ (131)		*tP*4	II	1.4	DM	12×12×8
	Pt_3O_4	43002		*Pm*-3*n* (223)		*cP*14	II/IV	-	DM	8×8×8
	PtO_2	24923	α-PtO	$P6_3mc$ (186)		*hP*6	IV	3.6	DM	12×12×4
	PtO_2	4415	β-PtO	*Pnnm* (58)		*oP*6	IV	2.5	DM	8×8×12
Cu	Cu_2O	52043	Cuprite	*Pn*-3*m* (224)		*cP*6	I	2.3	DM	8×8×8
	CuO	67850	Tenorite	*C*2/*c* (15)	$P2_1/c$ (14)	*mS*8	II	3.8	AFM	6×12×6
	Cu_4O_3	100566	Paramelaconite	$I4_1/amd$ (141)	*Imma* (74)	*tI*28	I/II	2.9	AFM	8×8×8

Ag	Ag_2O	174089		*Pn*-3*m* (224)		*cP*6	I	1.7	DM	8×8×8
	AgO	202055		$I4_1/a$ (88)		*tI*32	I/III	1.5	DM	6×6×6
	Ag_2O_3	1509692		*Fdd2* (43)		*oF*40	III	2.3	DM	8×8×8
	Ag_6O_2	26557		*P*-31*m* (162)		*hP*8	0/I	0.5	DM	8×8×8
	Ag_3O_4	202218		$P2_1/c$ (14)	$P2_1/c$ (14)	*mP*14	II/III	-	FM	12×4×8
Au	Au_2O_3	8014		*Fdd*2 (43)		*oF*40	III	2.9	DM	8×8×8
Zn	ZnO	26170	Zincite	$P6_3mc$ (186)		*hP*4	II	3.6	DM	12×12×8
	ZnO_2	60763		*Pa*-3 (205)		*cP*12	II	5.5	DM	8×8×8
Cd	CdO	29290	Monteponite	*Fm*-3*m* (225)		*cF*8	II	1.4	DM	12×12×12
	CdO_2	36151		*Pa*-3 (205)		*cP*12	II	3.8	DM	8×8×8
Hg	HgO	14124	Montroydite	*Pnma* (62)		*oP*8	II	2.9	DM	6×8×12
	HgO	639125		$P3_221$ (154)		*hP*6	II	2.8	DM	12×12×4
	HgO_2	48214	α-HgO_2	*C*2/*m* (12)		*mS*6	II	2.0	DM	12×12×12
	HgO_2	24774	β-HgO_2	*Pbca* (61)		*oP*12	II	2.0	DM	6×6×8

[a] Code in Inorganic Crystal Structure Database (ICSD)
[b] Code in Crystallography Open Database is 1530870
[c] Code in Crystallography Open Database is 4124669
[d] Diamagnetic (DM), ferromagnetic (FM), ferrimagnetic (FiM), and antiferromagnetic (AFM) spin configurations
[e] TOLINTEG 10 10 10 10 20 was used in the CRYSTAL calculations.

Table S2. Optimized lattice parameters of the studied binary *d*-metal oxides. Differences to experimental values are listed in parentheses.

d-metal	Oxide[a]	Pearson symbol	Lattice parameters[b]											
			DFT-PBE0/SVP						DFT-PBE0/TZVP					
			a (Å)	*b* (Å)	*c* (Å)	α (˚)	β (˚)	γ (˚)	*a* (Å)	*b* (Å)	*c* (Å)	α (˚)	β (˚)	γ (˚)
Sc	Sc_2O_3[1]	*cI*80	9.824 (–0.3%)						9.851 (0.0%)					
Y	Y_2O_3[2]	*cI*80	10.577 (–0.2%)						10.605 (0.1%)					
La	La_2O_3[3]	*cI*80	11.430 (0.9%)						11.452 (1.1%)					
	La_2O_3[4]	*hP*5	3.958 (0.5%)		6.177 (0.7%)				3.964 (0.7%)		6.187 (0.8%)			
Ti	TiO[5]	*hP*3	4.944 (–1.0%)		2.869 (–0.3%)				4.951 (–0.9%)		2.872 (–0.2%)			
	Ti_2O_3	*hR*10	5.224 (1.3%)		13.482 (–0.9%)				5.237 (1.6%)		13.488 (–0.9%)			
	TiO_2[6]	*tP*6	4.571 (–0.5%)		2.959 (0.0%)				4.584 (–0.2%)		2.964 (0.2%)			
	TiO_2[7]	*tI*12	3.750 (–0.9%)		9.704 (2.0%)				3.769 (–0.4%)		9.673 (1.7%)			
	TiO_2[8]	*oP*24	9.206 (0.3%)	5.446 (0.0%)	5.102 (–0.7%)				9.213 (0.4%)	5.454 (0.1%)	5.128 (–0.2%)			
	α-Ti_3O_5	*oS*32	9.992 (1.5%)	3.769 (–0.8%)	9.981 (–0.1%)		89.9 (–0.1%)		10.019 (1.8%)	3.776 (–0.6%)	10.004 (0.2%)		89.9 (–0.1%)	
	β-Ti_3O_5	*mS*32	9.942 (2.0%)	3.811 (0.2%)	9.510 (0.7%)		91.8 (–0.2%)		10.040 (3.0%)	3.825 (0.6%)	9.486 (0.5%)		91.9 (0.0)	
	γ-Ti_3O_5	*mS*32	5.161 (1.7%)	5.728 (1.2%)	7.037 (–2.0%)	109.1 (–0.5%)	90.7 (0.8%)	116.1 (–0.5%)	5.174 (2.0%)	5.736 (1.4%)	7.057 (–1.7%)	109.0 (–0.6%)	90.8 (0.8%)	116.1 (–0.4%)
	δ-Ti_3O_5	*mS*32	5.132 (1.4%)	7.087 (–1.7%)	10.045 (0.8%)	108.5 (–0.8%)	90.0 (0.0%)	90.0 (0.0%)	5.145 (1.7%)	7.108 (–1.4%)	10.064 (1.0%)	108.6 (–0.6%)	90.0 (0.0%)	90.0 (0.0%)
	λ-Ti_3O_5	*mS*32	9.883 (0.5%)	3.776 (–0.5%)	10.089 (1.0%)		89.7 (–1.4%)		9.913 (0.8%)	3.780 (–0.3%)	10.019 (1.3%)		89.6 (–1.5%)	
Zr	ZrO_2[9]	*mP*12	5.154 (0.2%)	5.231 (0.4%)	5.302 (–0.2%)		99.0 (–0.2%)		5.169 (0.5%)	5.226 (0.3%)	5.327 (0.3%)		99.0 (–0.2%)	
	ZrO_2[10]	*tP*6	3.599 (–1.1%)		5.157 (–2.1%)				3.602 (–1.0)		5.170 (–1.9%)			
Hf	HfO_2[11]	*mP*12	5.175 (1.2%)	5.205 (0.6%)	5.338 (0.8%)		99.1 (–0.1%)		5.127 (0.3%)	5.235 (1.2%)	5.244 (–1.0%)		98.4 (–0.7%)	
V	V_2O_3	*hR*10	5.046 (1.9%)		13.786 (–1.5%)				5.053 (2.0%)		13.821 (–1.3%)			
	V_2O_3	*mS*20	5.499 (–0.9%)	5.070 (1.4%)	7.295 (0.6%)		95.7 (–1.1%)		5.509 (–0.7%(	5.079 (1.5%)	7.309 (0.8%)		95.7 (–1.0%)	
	VO_2	*mP*12	5.376 (0.1%)	4.453 (0.0%)	5.357 (0.0%)		112.0 (0.0%)		5.372 (0.0%)	4.457 (0.1%)	5.361 (0.0%)		112.0 (0.1%)	

	VO_2	*mS*12	12.077 (0.4%)	3.754 (1.6%)	6.332 (–1.4%)		106.1 (0.0%)		12.094 (0.5%)	3.758 (1.8%)	6.347 (–1.1%)		106.2 (0.1%)	
	VO_2	*tP*6	6.232 (–3.2%)	6.232 (–3.2%)	2.998 (5.0%)				6.251 (–2.9%)	6.251 (–2.9%)	3.001 (5.1%)			
	V_2O_5[12]	*oP*14	11.450 (–0.5%)	3.546 (–0.5%)	4.478 (2.5%)				11.455 (–0.5%)	3.550 (–0.4%)	4.625 (5.9%)			
	V_2O_5[13]	*oP*28	10.062 (1.2%)	3.563 (-0.6%)	10.212 (1.7%)				10.115 (1.7%)	3.567 (–0.5%)	10.503 (4.6%)			
Nb	NbO[14]	*cP*6	4.202 (–0.2%)						4.209 (0.0%)					
	NbO_2[15]	*tI*96	13.787 (0.6%)		5.938 (–0.8%)				13.791 (0.6%)		5.956 (–0.5%)			
	NbO_2[15]	*tP*6	4.959 (2.3%)		2.869 (–5.4%)				4.962 (2.4%)		2.878 (–5.1%)			
	Nb_2O_5[16]	*mS*28	12.797 (0.4%)	4.897 (0.3%)	5.599 (0.7%)		105.1 (0.1%)		12.821 (0.6%)	4.911 (0.6%)	5.609 (0.9%)		104.8 (–0.2%)	
Ta	Ta_2O_5[17]	*oP*14	6.448 (0.4%)	3.770 (0.0%)	7.720 (0.2%)				6.441 (0.2%)	3.763 (–0.2%)	7.691 (–0.2%)			
Cr	Cr_2O_3	*hR*10	4.965 (0.2%)		13.541 (–0.4%)				4.976 (0.4%)		13.571 (–0.2%)			
	CrO_2	*tP*6	4.359 (–1.4%)		2.943 (0.9%)				4.368 (–1.2%)		2.952 (1.2%)			
	CrO_3	*oS*16	5.731 (–0.2%)	8.824 (3.1%)	4.781 (–0.2%)				5.748 (0.1%)	8.979 (4.9%)	4.925 (2.8%)			
Mo	MoO_2	*mP*12	5.552 (0.2%)	4.865 (0.2%)	5.638 (0.5%)		119.4 (0.0%)		5.557 (0.3%)	4.866 (0.2%)	5.660 (0.9%)		119.6 (0.1%)	
	MoO_3	*oP*16	14.228 (2.7%)	3.694 (–0.1%)	3.967 (0.1%)				14.477 (4.5%)	3.695 (0.0%)	3.972 (0.2%)			
W	WO_2	*mP*12	5.587 (0.4%)	4.953 (1.2%)	5.581 (0.3%)		118.5 (–1.6%)		5.554 (–0.2%)	4.927 (0.6%)	5.585 (0.4%)		118.5 (–1.6%)	
	WO_3[18]	*mP*16	5.415 (2.6%)	5.430 (5.3%)	7.771 (1.4%)		90.0 (–1.9%)		5.416 (2.6%)	5.444 (5.6%)	7.731 (0.9%)		90.4 (–1.5%)	
	WO_3[19]	*aP*32	7.520 (2.8%)	7.757 (3.1%)	7.866 (2.3%)	90.0 (1.3%)	90.0 (–1.0%)	90.0 (–1.1%)	7.485 (2.4%)	7.751 (3.0%)	7.870 (2.4%)	90.0 (1.3%)	90.0 (–1.0%)	90.0 (–1.0%)
	WO_3[20]	*mP*32	7.472 (2.0%)	7.741 (2.3%)	7.900 (2.2%)		90.0 (–0.5%)		7.437 (1.5%)	7.777 (2.8%)	7.904 (2.3%)		90.0 (–0.5%)	
	WO_3[20]	*oP*32	7.472 (1.8%)	7.741 (2.2%)	7.900 (2.0%)				7.439 (1.3%)	7.778 (2.7%)	7.903 (2.0%)			
	WO_3[20]	*tP*16	5.306 (0.6%)		8.010 (2.1%)				5.310 (0.6%)		8.041 (2.5%)			
	WO_3	*tP*8	5.341 (0.7%)		4.004 (1.7%)				5.314 (0.2%)		4.020 (2.2%)			
	WO_3[21]	*hP*12	7.444 (2.0%)		3.821 (–2.0%)				7.417 (1.6%)		3.809 (–2.3%)			
Mn	MnO	*cF*8	3.150 (0.2%)		15.162 (–1.6%)				3.159 (0.5%)		15.191 (–1.4%)			

	MnO	*hP*4	3.440 (2.0%)	5.800 (–0.7%)	5.317 (–1.3%)				3.430 (1.7%)	5.786 (–0.9%)	5.392 (0.1%)			
	Mn_2O_3	*oP*80	9.366 (–0.5%)	9.419 (0.0%)	9.469 (0.5%)				9.384 (–0.3%)	9.437 (0.2%)	9.493 (0.7%)			
	Mn_2O_3	*cI*80	9.436 (0.2%)						9.452 (0.4%)					
	Mn_3O_4	*tI*28	5.777 (0.3%)	5.788 (0.5%)	9.409 (–0.5%)				5.785 (0.4%)	5.796 (0.6%)	9.453 (–0.1%)			
	MnO_2	*tI*24	13.709 (–1.2%)	2.862 (0.5%)	9.698 (–1.2%)		135.0 (0.0%)		13.728 (–1.1%)	2.862 (0.5%)	9.705 (–1.1%)		135.0 (0.0%)	
	MnO_2	*oP*12	2.863 (0.5%)	4.508 (1.2%)	9.237 (–0.9%)				2.862 (0.5%)	4.543 (2.0%)	9.211 (–1.2%)			
	MnO_2	*tP*6	6.177 (–0.8%)	6.177 (–0.8%)	2.877 (0.0%)				6.187 (–0.7%)	6.187 (–0.7%)	2.879 (0.1%)			
	MnO_2	*cF*48	5.702 (0.0%)		8.031 (–0.4%)				5.702 (0.0%)		8.028 (–0.4%)			
	Mn_2O_7	*mP*72	6.926 (1.9%)	16.991 (1.8%)	9.434 (–0.2%)		100.5 (0.3%)		6.985 (2.8%)	17.504 (4.9%)	9.598 (1.5%)		100.2 (0.0%)	
Tc	TcO_2	*mP*12	5.561 (1.4%)	4.608 (–3.1%)	5.571 (0.9%)		111.6 (–5.2%)		5.565 (1.5%)	4.611 (–3.0%)	5.575 (1.0%)		111.6 (–5.2%)	
	Tc_2O_7	*oP*36	13.683 (–0.5%)	7.484 (0.6%)	5.694 (1.4%)				13.852 (0.7%)	7.600 (2.2%)	5.762 (2.6%)			
Re	ReO_2	*mP*12	5.576 (–0.1%)	4.872 (1.3%)	5.618 (0.7%)		118.3 (–2.1%)		5.554 (–0.5%)	4.864 (1.1%)	5.606 (0.5%)		118.1 (–2.3%)	
	ReO_2	*oP*12	4.599 (0.0%)	4.866 (1.2%)	5.695 (0.9%)				4.606 (0.1%)	4.836 (0.6%)	5.688 (0.8%)			
	ReO_2	*tP*6	6.548 (–3.5%)	6.548 (–3.5%)	3.207 (14.2%)				6.542 (–3.6%)	6.542 (–3.6%)	3.197 (13.9%)			
	ReO_3[22]	*cP*4	3.765 (0.4%)						3.758 (0.2%)					
	Re_2O_7[23]	*oP*72	12.642 (1.1%)	15.176 (–0.1%)	5.497 (0.9%)				12.693 (1.5%)	15.443 (1.6%)	5.531 (1.5%)			
Fe	Fe_3O_4	*cF*56	8.390 (–0.1%)						8.403 (0.0%)					
	Fe_3O_4	*mP*56	5.986 (0.7%)	5.946 (0.4%)	16.780 (0.0%)		90.0 (–0.3%)		5.983 (0.6%)	5.976 (0.9%)	16.810 (0.2%)		90.0 (–0.3%)	
	Fe_2O_3	*hR*10	5.053 (0.3%)		13.683 (–0.5%)				5.054 (0.4%)		13.725 (–0.2%)			
	Fe_2O_3	*cI*80	9.422 (0.2%)	9.393 (–0.1%)	9.436 (0.3%)				9.422 (0.2%)	9.393 (–0.1%)	9.437 (0.3%)			
	Fe_2O_3	*oP*40	5.095 (0.5%)	8.769 (0.4%)	9.514 (1.0%)				5.100 (0.6%)	8.793 (0.6%)	9.524 (1.1%)			
Ru	RuO_2	*tP*6	6.384 (0.5%)	6.384 (0.5%)	3.118 (0.4%)				6.384 (0.5%)	6.385 (0.5%)	3.122 (0.5%)			
	RuO_4	*cP*40	8.626 (1.4%)						8.761 (3.0%)					

	RuO_4	*mS*20	9.362 (0.6%)	4.505 (2.5%)	8.542 (1.0%)		116.6 (–0.2%)		9.562 (2.8%)	4.534 (3.1%)	8.673 (2.6%)		116.5 (–0.2%)	
Os	OsO_2[24]	*tP*6	4.479 (–0.5%)		3.209 (0.8%)				4.474 (–0.6%)		3.211 (0.9%)			
	OsO_4	*mS*20	9.229 (–1.6)	4.476 (–0.9%)	8.462 (–1.9%)		116.6 (0.0%)		9.514 (1.4%)	4.572 (1.3%)	8.632 (0.0%)		116.6 (–0.1%)	
Co	CoO	*cF*8	2.959 (–1.8%)		14.903 (0.9%)				3.021 (0.2%)		14.714 (–0.4%)			
	CoO	*hP*4	3.278 (2.1%)	5.650 (1.6%)	5.172 (–1.3%)				3.276 (2.0%)	5.650 (1.6%)	5.222 (–0.3%)			
	Co_3O_4	*cF*56	8.079 (–0.1%)						8.090 (0.1%)					
Rh	Rh_2O_3[25]	*hR*10	5.128 (0.0%)		13.903 (0.4%)				5.138 (0.2%)		13.862 (0.1%)			
	Rh_2O_3[26]	*oP*40	5.146 (0.0%)	5.454 (0.2%)	14.717 (0.1%)				5.153 (0.1%)	5.454 (0.2%)	14.726 (0.2%)			
	RhO_2	*tP*6	4.494 (0.2%)		3.097 (0.3%)				4.495 (0.2%)		3.104 (0.5%)			
Ir	IrO_2	*tP*6	6.367 (–0.1%)	6.367 (–0.1%)	3.187 (0.9%)				6.360 (–0.2%)	6.360 (–0.2%)	3.191 (1.0%)			
Ni	NiO	*cF*8	2.949 (–0.2%)		14.403 (–0.5%)				2.963 (0.3%)		14.482 (0.1%)			
Pd	PdO[27]	*tP*4	3.061 (1.0%)		5.327 (–0.1%)				3.071 (1.4%)		5.317 (–0.3%)			
Pt	PtO[28]	*tP*4	3.136 (1.9%)		5.284 (–1.0%)				3.137 (1.9%)		5.273 (–1.2%)			
	Pt_3O_4[29]	*cP*14	5.620 (0.6%)						5.612 (0.5%)					
	PtO_2[30]	*hP*6	3.133 (1.1%)		8.703 (4.6%)				3.119 (0.6%)		9.023 (8.4%)			
	PtO_2[31]	*oP*6	4.536 (1.1%)	4.524 (–0.2%)	3.162 (0.8%)				4.544 (1.2%)	4.486 (–1.0%)	3.158 (0.6%)			
Cu	Cu_2O[32]	*cP*6	4.296 (0.6%)						4.318 (1.1%)					
	CuO	*mS*8	7.638 (2.0%)	3.334 (–2.8%)	6.401 (0.5%)	90.0 (0.0%)	94.15 (–1.3%)	90.0 (0.0%)	7.565 (1.1%)	3.423 (–0.2%)	6.372 (0.1%)	90.0 (0.0%)	94.8 (–0.7%)	90.0 (0.0%)
	Cu_4O_3	*tI*28	5.817 (–0.3%)	5.817 (–0.3%)	10.028 (1.0%)				5.859 (0.4%)	5.859 (0.4%)	9.977 (0.5%)			
Ag	Ag_2O[33]	*cP*6	4.742 (0.1%)						4.771 (0.7%)					
	AgO[34]	*tI*32	6.864 (0.5%)		9.200 (0.9%)				6.875 (0.6%)		9.209 (1.0%)			
	Ag_2O_3[35]	*oF*40	12.848 (–0.2%)	10.522 (0.3%)	3.728 (1.8%)				12.872 (0.0%)	10.556 (0.6%)	3.713 (1.3%)			
	Ag_6O_2[36]	*hP*8	5.325 (0.1%)		4.945 (–0.1%)				5.356 (0.7%)		4.925 (–0.5%)			

	Ag_3O_4	*mP*14	3.621 (1.2%)	9.255 (0.5%)	5.709 (0.6%)		106.9 (0.7%)		3.621 (1.2%)	9.255 (0.5%)	5.709 (0.6%)		106.9 (0.7%)	
Au	Au_2O_3[37]	*oF*40	10.642 (1.2%)	12.917 (0.4%)	3.883 (1.2%)				10.611 (0.9%)	12.923 (0.4%)	3.858 (0.5%)			
Zn	ZnO[38]	*hP*4	3.256 (0.2%)		5.183 (–0.5%)				3.267 (0.5%)		5.207 (0.0%)			
	ZnO_2[39]	*cP*12	4.872 (0.0%)						4.894 (0.5%)					
Cd	CdO[40]	*cF*8	4.691 (–0.1%)						4.688 (–0.1%)					
	CdO_2[41]	*cP*12	5.298 (–0.3%)						5.301 (–0.2%)					
Hg	HgO[42]	*oP*8	6.676 (1.0%)	5.300 (–4.0%)	3.462 (–1.7%)				6.702 (1.3%)	5.536 (0.3%)	3.551 (0.8%)			
	HgO[43]	*hP*6	3.515 (–1.6%)		8.566 (–1.2%)				3.610 (1.1%)		8.704 (0.4%)			
	HgO_2	*mS*6	4.571 (2.3%)	4.734 (–13.3%)	4.070 (15.7%)		111.7 (3.0%)		6.076 (35.9%)	4.066 (-25.5)	4.592 (30.5%)		127.1 (17.2%)	
	HgO_2	*oP*12	5.445 (–10.4%)	5.449 (–9.3%)	5.434 (13.2%)				5.471 (–10.0%)	5.472 (–9.0%)	5.465 (13.8%)			

[a] Literature citations are given here for the oxides that are not discussed in detail in the main paper.
[b] Non-magnetic experimental lattice parameters have been transformed so that they correspond to the unit cell used in the spin-polarized calculations. Differences to the experimental values are reported for the magnetic unit cell.

Table S3. Energy comparisons of different magnetic configurations for the paramagnetic binary *d*-metal oxides (DFT-PBE0/SVP level of theory).

Oxide	Pearson symbol	Magnetic configuration[b]	Relative energy (kJ mol^{-1} per atom)
Ti_2O_3[a]	*hR*10	DM	6.8
		FM	12.4
		AFM	**0.0**
α-Ti_3O_5[a]	*oS*32	DM	9.0
		FM	2.0
		FiM	2.3
		AFM	**0.0**
γ-Ti_3O_5[a]	*mS*32	DM	9.7
		FM	3.7
		FiM	3.4
		AFM	**0.0**
δ-Ti_3O_5[a]	*mS*32	DM	8.7
		FM	0.4
		FiM	0.1
		AFM	**0.0**
VO_2	*mP*12	DM	14.9
		FM	14.0
		AFM	**0.0**
VO_2	*mS*12	DM	26.4
		FM	7.0
		AFM	**0.0**
VO_2	*tP*6	DM	28.4
		FM	18.8
		AFM	**0.0**
NbO_2	*tP*6	**DM**	**0.0**
		FM	1.8
		AFM	0.0
	*tI*96	**DM**	**0.0**
		FM	5.9
		AFM	8.3
MoO_2	*mP*12	DM	3.5
		FM	3.7
		AFM	**0.0**
Mn_2O_3	*cI*80	DM	132.5
		FM	**0.0**
		FiM	2.2
TcO_2	*mP*12	DM	28.1
		FM	28.2
		AFM	**0.0**
ReO_2	*mP*12	DM	16.5
		FM	38.8
		AFM	**0.0**
ReO_2	*oP*12	DM	7.4
		FM	8.6
		AFM	**0.0**
ReO_2	*tP*6	DM	25.0
		FM	5.1
		AFM	**0.0**
RuO_2	*tP*6	DM	11.5
		FM	16.5
		AFM	**0.0**
RhO_2	*tP*6	DM	11.6
		FM	**0.0**
		AFM	1.9
IrO_2	*tP*6	DM	7.2
		AFM	**0.0**
		FM	0.1
Ag_3O_4	*mP*14	DM	2.8
		FM	**0.0**
		FiM	2.7
		AFM	2.7

[a] Magnetic ground state of the structure is not known from the experiment.
[b] Diamagnetic (DM), ferromagnetic (FM), ferrimagnetic (FiM), or antiferromagnetic (AFM) configuration.

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