Electronic Supplementary Material (ESI) for RSC Advances.

Table S1. Band gaps of metal oxide nanoparticles from literature and experiments

Metal oxide	α (°)	β(°)	γ(°)	a (Å)	b (Å)	c (Å)	Size (nm)	Eg (eV) (Exp.)	Reference
Al_2O_3	90	90	120	4.81	4.81	13.12	66.0	5.97	19
Al_2O_3	90	90	120	4.81	4.81	13.12	86.0	5.97	20
CeO_2	90	90	90	5.46	5.46	5.46	12.0	3.39	21
CeO_2	90	90	90	5.46	5.46	5.46	3.6	3.68	21
CeO_2	90	90	90	5.46	5.46	5.46	2.6	3.44	21
Cr_2O_3	90	90	120	4.58	4.58	14.72	35.1	3.78	22
Cr_2O_3	90	90	120	4.58	4.58	14.72	38.1	3.72	22
Cr_2O_3	90	90	120	4.58	4.58	14.72	40.3	3.67	22
Cr_2O_3	90	90	120	4.58	4.58	14.72	25.0	4.33	23
Cr_2O_3	90	90	120	4.58	4.58	14.72	28.0	4.11	23
Cr_2O_3	90	90	120	4.58	4.58	14.72	34.0	3.81	23
Cr_2O_3	90	90	120	4.58	4.58	14.72	35.0	3.78	23
Cr_2O_3	90	90	120	4.58	4.58	14.72	40.0	3.62	23
Cr_2O_3	90	90	120	4.58	4.58	14.72	45.0	3.54	23
Cu_2O	90	90	90	4.31	4.31	4.31	4.0	2.90	24
Cu_2O	90	90	90	4.31	4.31	4.31	9.0	2.50	24
Cu_2O	90	90	90	4.31	4.31	4.31	6.0	2.83	25
Cu_2O	90	90	90	4.31	4.31	4.31	20.0	2.04	24
Fe_2O_3	90	90	120	4.74	4.74	13.49	100.0	2.05	26
Fe_2O_3	90	90	120	4.74	4.74	13.49	100.0	2.12	26
Fe_2O_3	90	90	120	4.74	4.74	13.49	100.0	2.46	26
Fe_2O_3	90	90	120	4.74	4.74	13.49	100.0	2.88	26
Fe_3O_4	90	90	90	8.04	8.04	8.04	12.0	1.85	3
Ga_2O_3	90	103.7	90	12.50	3.10	5.92	2.5	5.10	27
Ga_2O_3	90	103.7	90	12.50	3.10	5.92	70.0	4.90	28
Ga_2O_3	90	103.7	90	12.50	3.10	5.92	60.0	4.80	29
HfO_2	90	99.216	90	5.14	5.19	5.31	17.0	6.07	30
In_2O_3	90	90	90	10.35	10.35	10.35	17.4	3.84	31
In_2O_3	90	90	90	10.35	10.35	10.35	16.6	3.86	31
La_2O_3	90	90	120	3.94	3.94	6.18	20.0	5.77	3
La_2O_3	90	90	120	3.94	3.94	6.18	40.0	4.20	32
MgO	90	90	90	4.25	4.25	4.25	7.0	4.27	33
Mn_2O_3	90	90	90	9.03	9.03	9.03	30.2	3.27	34
NiO	90	90	90	4.16	4.16	4.16	3.5	3.67	35
NiO	90	90	90	4.16	4.16	4.16	4.6	3.63	35
NiO	90	90	90	4.16	4.16	4.16	5.5	3.62	35
NiO	90	90	90	4.16	4.16	4.16	10.1	3.62	35
NiO	90	90	90	4.16	4.16	4.16	12.4	3.61	35
NiO	90	90	90	4.16	4.16	4.16	8.3	3.22	36
NiO	90	90	90	4.16	4.16	4.16	11.6	3.24	36

NiO	90	90	90	4.16	4.16	4.16	18.3	3.34	36
NiO	90	90	90	4.16	4.16	4.16	20.7	3.19	36
NiO	90	90	90	4.16	4.16	4.16	31.0	3.41	36
NiO	90	90	90	4.16	4.16	4.16	43.4	3.21	36
Sb_2O_3	90	90	90	5.18	16.61	5.51	11.8	4.49	3
SnO_2	90	90	90	4.83	4.83	3.24	4.5	4.20	37
SnO_2	90	90	90	4.83	4.83	3.24	4.0	4.10	38
SnO_2	90	90	90	4.83	4.83	3.24	5.0	4.21	39
SnO_2	90	90	90	4.83	4.83	3.24	5.2	4.20	40
SnO_2	90	90	90	4.83	4.83	3.24	3.7	4.33	40
SnO_2	90	90	90	4.83	4.83	3.24	62.4	4.00	3
SnO_2	90	90	90	4.83	4.83	3.24	12.8	3.40	41
SnO_2	90	90	90	4.83	4.83	3.24	29.1	3.16	41
SnO_2	90	90	90	4.83	4.83	3.24	37.0	3.35	40
SnO_2	90	90	90	4.83	4.83	3.24	8.0	4.26	42
SnO_2	90	90	90	4.83	4.83	3.24	15.0	4.00	42
SnO_2	90	90	90	4.83	4.83	3.24	17.0	3.90	42
TiO_2-a	90	90	90	3.82	3.82	9.70	5.0	3.18	exp.
TiO_2-a	90	90	90	3.82	3.82	9.70	25.0	3.23	exp.
TiO_2-a	90	90	90	3.82	3.82	9.70	40.0	3.21	exp.
TiO_2-a	90	90	90	3.82	3.82	9.70	12.6	3.33	3
TiO_2-a	90	90	90	3.82	3.82	9.70	9.8	3.21	43
TiO_2-a	90	90	90	3.82	3.82	9.70	16.0	3.25	43
TiO_2-a	90	90	90	3.82	3.82	9.70	3.9	3.26	43
TiO_2-a	90	90	90	3.82	3.82	9.70	10.6	3.26	43
TiO_2-a	90	90	90	3.82	3.82	9.70	16.9	3.25	43
TiO_2-a	90	90	90	3.82	3.82	9.70	9.3	3.25	43
TiO_2-a	90	90	90	3.82	3.82	9.70	5.0	3.22	43
TiO_2-a	90	90	90	3.82	3.82	9.70	7.9	3.25	43
TiO_2-a	90	90	90	3.82	3.82	9.70	9.2	3.28	43
TiO_2-a	90	90	90	3.82	3.82	9.70	18.0	3.24	43
TiO_2-a	90	90	90	3.82	3.82	9.70	12.3	3.25	43
TiO_2-a	90	90	90	3.82	3.82	9.70	7.8	3.24	43
TiO_2-a	90	90	90	3.82	3.82	9.70	7.4	3.24	43
TiO_2-a	90	90	90	3.82	3.82	9.70	17.0	3.23	43
TiO_2-a	90	90	90	3.82	3.82	9.70	12.4	3.25	43
TiO_2-a	90	90	90	3.82	3.82	9.70	16.7	3.27	43
TiO_2-b	90	90	90	9.28	5.52	5.19	7.9	3.48	44
TiO_2-b	90	90	90	9.28	5.52	5.19	18.9	3.11	45
TiO_2-r	90	90	90	4.66	4.66	2.97	40.0	3.00	exp.
TiO_2-r	90	90	90	4.66	4.66	2.97	100.0	3.00	exp.
WO_3	90	91.75	90	5.39	5.36	7.84	42.0	2.77	46
Y_2O_3	90	90	90	10.65	10.65	10.65	14.6	5.30	47
ZnO	90	90	120	3.29	3.29	5.31	22.6	3.31	3

ZnO	90	90	120	3.29	3.29	5.31	14.0	3.30	48
ZnO	90	90	120	3.29	3.29	5.31	20.0	3.25	48
ZnO	90	90	120	3.29	3.29	5.31	26.0	3.22	48
ZnO	90	90	120	3.29	3.29	5.31	50.0	3.11	exp.
ZnO	90	90	120	3.29	3.29	5.31	53.4	3.35	49
ZnO	90	90	120	3.29	3.29	5.31	43.4	3.19	50
ZrO_2	90	99.2	90	5.19	5.24	5.38	40.0	5.04	3

*exp.: Band gaps measured by UV-vis spectroscopic analysis in this study

Number of reference is corresponding to that in text

Table S2. Applicability domain characterization for developed nano-QSPR model

Outlier

Training Set													
Metal oxide	*BETA*-standardized	D^{-2}-standardized	H_F-standardized	*V2*-standardized	E_{Fermi}-standardized	*TFW*-standardized	R-standardized	E_T-standardized	*DENC*-standardized	*XCENC*-standardized	AVERAGE	STDEV	AVERAGE +1.28STDEV
Al_2O_3	0.3995	0.6402	2.8965	0.2238	0.7241	0.0561	0.0148	0.3893	0.1578	0.0139	0.5516	0.8167	1.5970
CeO_2-1	0.3995	0.4826	0.0280	0.0280	0.4048	0.1804	0.8010	0.5736	0.3484	0.4753	0.3722	0.2288	0.6650
CeO_2-2	0.3995	1.1771	0.0280	0.0280	0.4048	0.1804	0.8010	0.5736	0.3484	0.4753	0.4416	0.3333	0.8682
CeO_2-3	0.3995	2.8498	0.0280	0.0280	0.4048	0.1804	0.8010	0.5736	0.3484	0.4753	0.6089	0.7804	1.6077
Cr_2O_3-1	0.3995	0.6131	0.8364	0.3126	0.8111	0.6370	0.0148	1.3924	0.2193	0.1786	0.5415	0.3852	1.0345
Cu_2O-1	0.3995	0.8305	1.0666	0.4156	0.0039	0.7675	0.8010	1.9253	3.4123	1.4792	1.1101	0.9276	2.2975
Fe_3O_4-1	0.3995	0.4826	0.2296	1.0201	0.4074	0.9465	0.4203	3.7281	2.1972	1.6076	1.1439	1.0464	2.4834
Ga_2O_3-1	3.0522	0.6412	0.4689	0.8796	1.2124	0.8372	0.0148	0.3459	0.1090	0.2095	0.7771	0.8384	1.8502
Ga_2O_3-2	3.0522	3.1351	0.4689	0.8796	1.2124	0.8372	0.0148	0.3459	0.1090	0.2095	1.0265	1.0931	2.4256
HfO_2-1	1.9225	0.6462	1.8193	0.0755	0.3906	0.6409	0.8010	0.4266	0.7110	0.5899	0.8024	0.5685	1.5300
In_2O_3-1	0.3995	0.5650	0.4947	1.9048	0.5893	1.5153	0.0148	0.3224	0.4003	1.1509	0.7357	0.5632	1.4566
La_2O_3-1	0.3995	0.6205	0.9077	0.5582	0.7149	0.4778	0.0148	0.2401	0.8432	2.0528	0.6830	0.5233	1.3527
MgO-1	0.3995	0.1644	0.0202	0.4393	0.5084	0.9339	1.6417	1.3465	1.4933	1.0546	0.8002	0.5439	1.4963
Mn_2O_3-1	0.3995	0.6209	0.0129	1.3995	0.5045	0.7409	0.0148	1.1922	0.3090	0.4396	0.5634	0.4294	1.1130
NiO-1	0.3995	1.2828	1.0837	0.4727	1.5137	1.6062	1.6417	0.4772	0.4885	0.3975	0.9363	0.5125	1.5923
NiO-2	0.3995	0.4703	1.0837	0.4727	1.5137	1.6062	1.6417	0.4772	0.4885	0.3975	0.8551	0.5155	1.5149
NiO-4	0.3995	0.4151	1.0837	0.4727	1.5137	1.6062	1.6417	0.4772	0.4885	0.3975	0.8496	0.5199	1.5150
NiO-5	0.3995	0.4930	1.0837	0.4727	1.5137	1.6062	1.6417	0.4772	0.4885	0.3975	0.8574	0.5138	1.5151
NiO-6	0.3995	0.5979	1.0837	0.4727	1.5137	1.6062	1.6417	0.4772	0.4885	0.3975	0.8678	0.5073	1.5172

Sb_2O_3-1	0.3995	0.4770	0.9059	4.3114	0.0178	1.8456	0.0148	0.6620	1.3169	0.8049	1.0756	1.2023	2.6145
SnO_2-1	0.3995	0.5205	0.7629	0.2157	0.2892	0.8889	0.8010	0.4689	0.6904	1.8074	0.6844	0.4305	1.2354
SnO_2-3	0.3995	0.2987	0.7629	0.2157	0.2892	0.8889	0.8010	0.4689	0.6904	1.8074	0.6623	0.4439	1.2304
SnO_2-5	0.3995	1.0798	0.7629	0.2157	0.2892	0.8889	0.8010	0.4689	0.6904	1.8074	0.7404	0.4417	1.3058
SnO_2-6	0.3995	0.6205	0.7629	0.2157	0.2892	0.8889	0.8010	0.4689	0.6904	1.8074	0.6944	0.4277	1.2419
TiO_2-a-1	0.3995	0.5678	0.2672	0.6028	1.6847	0.6854	0.8010	0.4793	0.6452	0.3098	0.6443	0.3818	1.1329
TiO_2-b-1	0.3995	0.2680	0.8859	0.0483	1.4179	0.4829	0.8010	0.4753	0.7877	0.3097	0.5876	0.3733	1.0654
TiO_2-r-1	0.3995	0.6419	0.6315	0.2799	1.1793	0.3855	0.8010	0.4882	0.8533	0.3087	0.5969	0.2700	0.9425
WO_3-1	0.0414	0.6334	0.2382	0.0103	1.7081	0.8903	1.6169	0.5189	0.6150	0.0057	0.6278	0.5908	1.3840
ZnO-1	0.3995	0.6275	1.1849	0.8082	1.5343	0.8892	1.6417	1.3457	1.5188	0.8894	1.0839	0.4013	1.5976
ZrO_2-1	1.9185	0.6320	1.7784	0.0560	0.6278	0.5906	0.8010	0.5188	0.2860	1.2868	0.8496	0.5847	1.5981

Validation Set

NAME	*BETA*- standardized	D^{-2}- standardized	H_F- standardized	*V2*- standardized	E_{Fermi}- standardized	*TFW*- standardized	*R*- standardized	E_T- standardized	*DENC*- standardized	*XCENC*- standardized	AVER-AGE	STDEV	AVERAGE +1.28STDEV
Cr_2O_3-2	0.3995	0.6306	0.8364	0.3126	0.8111	0.6370	0.0148	1.3924	0.2193	0.1786	0.5432	0.3855	1.0367
Cu_2O-2	0.3995	0.3550	1.0666	0.4156	0.0039	0.7675	0.8010	1.9253	3.4123	1.4792	1.0626	0.9526	2.2819
Cu_2O-3	0.3995	0.0098	1.0666	0.4156	0.0039	0.7675	0.8010	1.9253	3.4123	1.4792	1.0281	0.9834	2.2868
Cu_2O-4	0.3995	0.5877	1.0666	0.4156	0.0039	0.7675	0.8010	1.9253	3.4123	1.4792	1.0859	0.9377	2.2862
Fe_2O_3-1	0.3995	0.6444	0.0916	0.2514	0.3448	1.1364	0.0148	2.0181	0.6478	1.0160	0.6565	0.5720	1.3887
NiO-3	0.3995	0.1346	1.0837	0.4727	1.5137	1.6062	1.6417	0.4772	0.4885	0.3975	0.8215	0.5493	1.5246
SnO_2-2	0.3995	0.8305	0.7629	0.2157	0.2892	0.8889	0.8010	0.4689	0.6904	1.8074	0.7154	0.4287	1.2642
SnO_2-4	0.3995	0.2274	0.7629	0.2157	0.2892	0.8889	0.8010	0.4689	0.6904	1.8074	0.6551	0.4502	1.2313
TiO_2-b-2	0.3995	0.5806	0.8859	0.0483	1.4179	0.4829	0.8010	0.4753	0.7877	0.3097	0.6189	0.3580	1.0771
Y_2O_3-1	0.3995	0.5359	4.3427	2.0225	1.2205	0.1735	0.0148	0.2606	2.1465	2.4678	1.3584	1.3126	3.0385

Table S3. Band gaps calculated by empirical equation

Metal oxide	α (°)	β (°)	γ (°)	a (Å)	b (Å)	c (Å)	*Size* (nm)	E_{g1} (eV)	E_{g2} (eV)
Al_2O_3	90	90	120	4.81	4.81	13.12	76.0	4.99	9.61
CeO_2	90	90	90	5.46	5.46	5.46	12.0	1.87	4.46
CeO_2	90	90	90	5.46	5.46	5.46	3.6	1.87	4.46
CeO_2	90	90	90	5.46	5.46	5.46	2.6	1.87	4.46
Cr_2O_3	90	90	120	4.58	4.58	14.72	26.5	2.75	3.77
Cu_2O	90	90	90	4.31	4.31	4.31	4.0	0.67	1.8
Fe_3O_4	90	90	90	8.04	8.04	8.04	12.0	1.59	2.68
Ga_2O_3	90	103.7	90	12.50	3.10	5.92	65.0	2.35	4.86
Ga_2O_3	90	103.7	90	12.50	3.10	5.92	2.5	2.35	4.86
HfO_2	90	99.216	90	5.14	5.19	5.31	200.0	3.82	7.16
In_2O_3	90	90	90	10.35	10.35	10.35	17.0	2.37	4.03
La_2O_3	90	90	120	3.94	3.94	6.18	30.0	2.82	9.5
MgO	90	90	90	4.25	4.25	4.25	7.0	1.86	6.68
Mn_2O_3	90	90	90	9.03	9.03	9.03	30.2	1.82	3.08
NiO	90	90	90	4.16	4.16	4.16	3.5	0.66	2.37
NiO	90	90	90	4.16	4.16	4.16	4.6	0.66	2.37
NiO	90	90	90	4.16	4.16	4.16	10.1	0.66	2.37
NiO	90	90	90	4.16	4.16	4.16	12.4	0.66	2.37
NiO	90	90	90	4.16	4.16	4.16	22.0	0.66	2.37
Sb_2O_3	90	90	90	5.18	16.61	5.51	11.8	2.82	2.6
SnO_2	90	90	90	4.83	4.83	3.24	4.5	1.00	3.76
SnO_2	90	90	90	4.83	4.83	3.24	5.0	1.00	3.76
SnO_2	90	90	90	4.83	4.83	3.24	3.7	1.00	3.76
SnO_2	90	90	90	4.83	4.83	3.24	30.0	1.00	3.76
TiO_2-a	90	90	90	3.82	3.82	9.70	17.3	2.13	——
TiO_2-b	90	90	90	9.28	5.52	5.19	7.9	2.80	4.99
TiO_2-r	90	90	90	4.66	4.66	2.97	70.0	1.15	——
WO_3	90	91.75	90	5.39	5.36	7.84	42.0	1.58	2.68
ZnO	90	90	120	3.29	3.29	5.31	35.0	0.55	3.41
ZrO_2	90	99.2	90	5.19	5.24	5.38	40.0	3.77	8.38

*E_{g1} values were computed according to empirical equation using computed heat of formation.

*E_{g2} values were computed according to empirical equation using experimental heat of formation.

Table S4. Comparison of computed and experimental values for heat of formation

Name	$\Delta H_{exp.}$ (cal/mol)	ΔH_{cal} (cal/mol)
Al_2O_3	399090	265782
CeO_2	233000	114800
Cr_2O_3	269700	63573
Cu_2O	39840	-26726
Fe_2O_3	196500	112108
Fe_3O_4	267125	124930
Ga_2O_3	260550	112344
HfO_2	266910	181544
In_2O_3	222500	114771
La_2O3	458000	211066
MgO	143840	57091
Mn_2O_3	229053	121907
NiO	58400	28623
Sb_2O_3	133400	149498
SnO_2	138800	-40043
TiO_2-a	363260	102261
TiO_2-b	218000	139569
WO_3	200840	92490
Y_2O_3	455001	382593
ZnO	83170	-41090
ZrO_2	288200	179955

*ΔH_{exp}: Experimental heat of formation of unit cell.

*$\Delta H_{cal:}$ Computed heat of formation of unit cell.

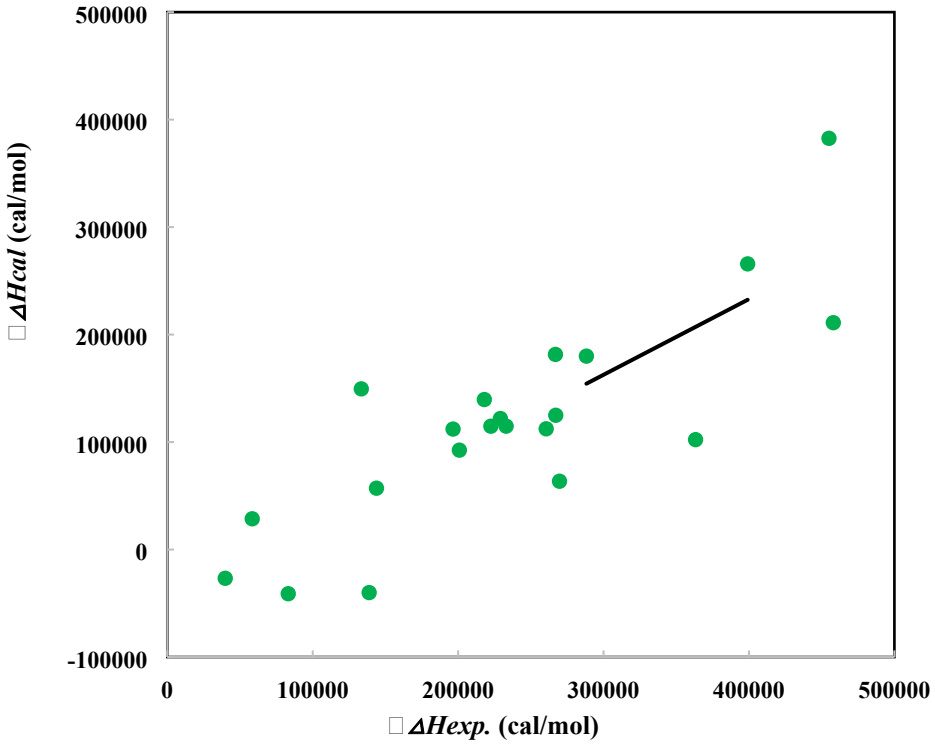

Figure S1. Relationship between computed and experimental values for heat of formation

References:

[1] Portier, J., Campet, G., Kwon, C. W., Etourneau, J., Subramanian, M. A. Relationships between optical band gap and thermodynamic properties of binary oxides. International Journal of Inorganic Materials, 2001, 3(7), 1091-1094.

[2] Appendix-Standard Thermodynamic Properties of Chemical Substance. 2000, CRC Handbook of Chemistry and Physicis, CRC PRESS LLC.

Table S5. Standard error of regression coefficients of the QSPR model

Descriptors	Coefficient	Standard error
H_F	0.553	0.211
BETA	0.0806	0.050
D^{-2}	1.09	6.51
V2	-0.0159	0.0917
E_{Fermi}	0.180	0.096
TFW	-2.23	1.43
R	0.803	0.611
E_T	0.00469	0.0009
DENC	-0.000305	0.00147
XCENC	-0.00403	0.00498