Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Table S1 Dataset 1 containing metal oxides and their corresponding descriptor values, division set, and toxicity data.

Serial No.	Metal oxide	ΔH^c_f	χc	1/Log LC_{50}	Set
1	TiO_2	-1492	4.91	1.76	Training
2	Al_2O_3	-600	3.44	1.85	Training
3	ZrO_2	-638.1	4.95	2.02	Training
4	Fe_2O_3	-378.5	4.21	2.05	Training
5	SiO_2	-618.3	3.81	2.12	Test
6	Y_2O_3	-135.3	3.35	2.21	Test
7	V_2O_3	-139.5	3.24	2.24	Test
8	Cr_2O_3	-235.3	4.36	2.3	Test
9	Sb_2O_3	-206.7	4.46	2.31	Test
10	NiO	68	4.47	2.49	Test
11	Bi_2O_3	-148.5	5.34	2.5	Test
12	WO_3	-715.4	6.73	2.56	Test
13	Mn_2O_3	-96.3	5	2.64	Training
14	SnO_2	-266.6	4.57	2.67	Training
15	CoO	-786.8	7.44	2.83	Training
16	La_2O_3	-157.7	6.45	2.87	Training
17	In_2O_3	-52.1	6.78	2.92	Test
18	ZnO	-449.4	8.33	3.32	Training

Table 2S Dataset 2 containing metal oxides and their corresponding descriptor values, division set, and toxicity data.

Sl. No.	**Metal oxide**	ΔH_{Me+}	Me^{+}	**1/Log EC_{50}**	**Division set**
1	TiO_2	1575.73	4.0	1.74	Test
2	SnO_2	1717.32	4.0	2.01	Training
3	ZrO_2	1357.66	4.0	2.15	Test
4	SiO_2	1686.38	4.0	2.2	Test
5	Fe_2O_3	1408.29	3.0	2.29	Training
6	Al_2O_3	1187.83	3.0	2.49	Training
7	Cr_2O_3	1268.70	3.0	2.51	Test
8	Sb_2O_3	1233.06	3.0	2.64	Training
9	In_2O_3	1271.13	3.0	2.81	Training
10	Bi_2O_3	1137.40	3.0	2.82	Training
11	La_2O_3	1017.22	3.0	2.87	Test
12	Y_2O_3	837.15	3.0	2.87	Test
13	V_2O_3	1097.73	3.0	3.14	Training
14	CuO	706.25	2.0	3.2	Test
15	NiO	596.70	2.0	3.45	Test
16	ZnO	662.44	2.0	3.45	Test
17	CoO	601.80	2.0	3.51	Training

Table 3S Dataset 3 containing metal oxides and their corresponding descriptor values, division set, and toxicity data.

Sl. Nos.	MeOx	*LZELEHHO*	ΔH_{Me+}	1/Log EC_{50}	Division Set
1	Al_2O_3	0.21	1187.83	2.42	Test
2	Bi_2O_3	0.18	1137.40	3.55	Training
3	Cr_2O_3	0.20	1268.70	2.06	Training
4	CuO	0.18	706.25	4.24	Training
5	Fe_2O_3	0.17	1408.29	2.40	Test
6	In_2O_3	0.20	1271.13	2.83	Test
7	La_2O_3	0.12	1017.22	4.96	Training
8	NiO	0.18	596.70	3.79	Training
9	Sb_2O_3	0.17	1233.06	3.12	Training
10	SiO_2	0.24	1686.38	2.54	Test
11	SnO_2	0.22	1717.32	2.53	Test
12	TiO_2	0.19	1575.73	2.14	Training
13	V_2O_3	0.17	1097.73	3.48	Test
14	Y_2O_3	0.13	837.15	5.79	Test
15	ZnO	0.13	662.44	5.80	Training
16	ZrO_2	0.18	1357.66	2.58	Test

Table S4 Computed metrics in different values of sigma (sigma optimization table)

Sigma value	Dataset 1			Dataset 2			Dataset 3		
	Q^2_{F1}	Q^2_{F2}	$RMSE_P$	Q^2_{F1}	Q^2_{F2}	$RMSE_P$	Q^2_{F1}	Q^2_{F2}	$RMSE_P$
σ = 0.25	0.41	0.39	0.18	0.89	0.89	0.19	0.85	0.80	0.48
σ = 0.50	0.71	0.70	0.12	**0.91**	**0.91**	**0.17**	0.92	0.89	0.36
σ = 0.75	**0.87**	**0.86**	**0.08**	0.90	0.90	0.18	**0.92**	**0.90**	**0.35**
σ = 1.00	0.85	0.85	0.09	0.86	0.86	0.21	0.87	0.83	0.45
σ = 1.50	0.65	0.64	0.14	0.64	0.64	0.34	0.70	0.59	0.69
σ = 2.00	0.46	0.45	0.17	0.46	0.46	0.42	0.52	0.35	0.87

Table S5 Computed metrics in different values of gamma (gamma optimization table)

Gamma value	Dataset 1			Dataset 2			Dataset 3		
	Q^2_{F1}	Q^2_{F2}	$RMSE_P$	Q^2_{F1}	Q^2_{F2}	$RMSE_P$	Q^2_{F1}	Q^2_{F2}	$RMSE_P$
γ = 0.25	0.36	0.34	0.19	0.40	0.40	0.44	0.42	0.22	0.95
γ = 0.50	0.60	0.59	0.15	0.67	0.67	0.33	0.67	0.56	0.72
γ = 0.75	0.73	0.72	0.12	0.81	0.81	0.25	0.81	0.74	0.55
γ = 1.00	**0.79**	**0.79**	**0.11**	0.87	0.87	0.21	0.87	0.83	0.45
γ = 1.50	0.79	0.79	0.11	0.90	0.90	0.18	**0.91**	**0.88**	**0.38**
γ = 2.00	0.73	0.72	0.12	**0.91**	**0.91**	**0.17**	0.91	0.87	0.38

Table S6 Optimization of the number of close training compound of Dataset 1

No. of C.T.C	Q^2_{F1}			Q^2_{F2}			$RMSE_P$		
	EUC	**GK**	**LK**	**EUC**	**GK**	**LK**	**EUC**	**GK**	**LK**
2	0.45	0.48	0.59	0.44	0.46	0.58	0.17	0.17	0.15
3	0.57	0.58	0.47	0.56	0.57	0.45	0.15	0.15	0.17
4	0.85	0.80	0.80	0.84	0.79	0.79	0.09	0.10	0.10
5	**0.90**	**0.87**	**0.82**	**0.90**	**0.87**	**0.81**	**0.07**	**0.08**	**0.10**
6	0.78	0.87	0.86	0.78	0.86	0.85	0.11	0.08	0.09
7	0.73	0.86	0.80	0.72	0.85	0.80	0.12	0.09	0.10
8	0.63	0.86	0.78	0.62	0.86	0.77	0.14	0.09	0.11
9	0.63	0.87	0.79	0.62	0.86	0.79	0.14	0.08	0.11

C.T.C: close training compound; **EUC**: Euclidean distance similarity read-across; **GK**: Gaussian kernel function similarity read-across; **LK**: Laplacian kernel function similarity read-across.

Table S7 Optimization of the number of close training compound of Dataset 2

No. of C.T.C	Q^2_{F1}			Q^2_{F2}			$RMSE_P$		
	EUC	**GK**	**LK**	**EUC**	**GK**	**LK**	**EUC**	**GK**	**LK**
2	**0.91**	0.89	0.90	**0.91**	0.89	0.90	**0.17**	0.19	0.18
3	0.84	0.91	0.92	0.84	0.91	0.92	0.23	0.17	0.16
4	0.72	0.91	0.91	0.72	0.91	0.91	0.30	0.17	0.17
5	0.67	**0.92**	**0.92**	0.67	**0.92**	**0.92**	0.33	**0.16**	**0.16**
6	0.58	0.91	0.91	0.58	0.91	0.91	0.37	0.17	0.17
7	0.45	0.91	0.91	0.45	0.91	0.91	0.42	0.17	0.17
8	0.45	0.91	0.91	0.45	0.91	0.91	0.42	0.17	0.17

C.T.C: close training compound; **EUC**: Euclidean distance similarity read-across; **GK**: Gaussian kernel function similarity read-across; **LK**: Laplacian kernel function similarity read-across.

Table S8 Optimization of the number of close training compound of Dataset 3

No. of C.T.C	Q2F1			Q2F2			RMSEP		
	EUC	**GK**	**LK**	**EUC**	**GK**	**LK**	**EUC**	**GK**	**LK**
2	0.90	0.90	0.84	0.86	0.87	0.78	0.40	0.40	0.50
3	**0.91**	0.91	0.91	**0.88**	0.87	0.88	**0.37**	0.38	0.38
4	0.90	**0.93**	**0.93**	0.87	**0.91**	**0.90**	0.39	**0.33**	**0.34**
5	0.85	0.93	0.92	0.80	0.90	0.89	0.49	0.34	0.36
6	0.79	0.92	0.92	0.72	0.89	0.89	0.57	0.35	0.36
7	0.77	0.92	0.91	0.69	0.89	0.88	0.60	0.35	0.37
8	0.77	0.92	0.91	0.69	0.90	0.88	0.60	0.35	0.38

C.T.C: close training compound; **EUC**: Euclidean distance similarity read-across; **GK**: Gaussian kernel function similarity read-across; **LK**: Laplacian kernel function similarity read-across.

Table S9 Optimization of the distance and similarity threshold of Dataset 1

Threshold	Q^2_{F1}			Q^2_{F2}			$RMSE_P$		
	EUC	**GK**	**LK**	**EUC**	**GK**	**LK**	**EUC**	**GK**	**LK**
D=0.4, S=0.0	0.96	0.87	0.79	0.96	0.86	0.79	0.05	0.08	0.11
D=0.4, S=0.05	**0.96**	**0.87**	**0.83**	**0.96**	**0.86**	**0.82**	**0.05**	**0.09**	**0.10**
D=0.4, S=0.1	0.96	0.85	0.82	0.96	0.85	0.82	0.05	0.09	0.10
D=0.5, S=0.0	0.71	0.87	0.79	0.70	0.86	0.79	0.13	0.08	0.11
D=0.5, S=0.05	0.71	0.87	0.83	0.70	0.86	0.82	0.13	0.09	0.10
D=0.5, S=0.1	0.71	0.85	0.82	0.70	0.85	0.82	0.13	0.09	0.10
D=0.6, S=0.0	0.71	0.87	0.79	0.70	0.86	0.79	0.13	0.08	0.11
D=0.6, S=0.05	0.71	0.87	0.83	0.70	0.86	0.82	0.13	0.09	0.10
D=0.6, S=0.1	0.71	0.85	0.82	0.70	0.85	0.82	0.13	0.09	0.10

D: distance threshold; **S**: similarity threshold; **EUC**: Euclidean distance similarity read-across; **GK**: Gaussian kernel function similarity read-across; **LK**: Laplacian kernel function similarity read-across.

Table S10 Optimization of the distance and similarity threshold of Dataset 2

Threshold	Q^2_{F1}			Q^2_{F2}			$RMSE_P$		
	EUC	**GK**	**LK**	**EUC**	**GK**	**LK**	**EUC**	**GK**	**LK**
D=0.5, S=0	**0.59**	**0.91**	**0.91**	**0.59**	**0.91**	**0.91**	**0.37**	**0.17**	**0.17**
D=0.6, S=0	0.47	0.91	0.91	0.47	0.91	0.91	0.42	0.17	0.17
D=0.7, S=0	0.45	0.91	0.91	0.45	0.91	0.91	0.43	0.17	0.17
D=0.8, S=0	0.45	0.91	0.91	0.45	0.91	0.91	0.42	0.17	0.17
D=0.9, S=0	0.45	0.91	0.91	0.45	0.91	0.91	0.42	0.17	0.17
D=1, S=0	0.45	0.91	0.91	0.45	0.91	0.91	0.42	0.17	0.17

D: distance threshold; **S**: similarity threshold; **EUC**: Euclidean distance similarity read-across; **GK**: Gaussian kernel function similarity read-across; **LK**: Laplacian kernel function similarity read-across.

Table S11 Optimization of the distance and similarity threshold of Dataset 3

Threshold	Q^2_{F1}			Q^2_{F2}			$RMSE_P$		
	EUC	**GK**	**LK**	**EUC**	**GK**	**LK**	**EUC**	**GK**	**LK**
D=0.4, S=0.0	**0.96**	**0.92**	**0.91**	**0.95**	**0.90**	**0.88**	**0.23**	**0.35**	**0.38**
D=0.4, S=0.1	0.96	0.92	0.90	0.95	0.89	0.86	0.23	0.35	0.40
D=0.5, S=0.0	0.95	0.92	0.91	0.93	0.90	0.88	0.28	0.35	0.38
D=0.5, S=0.1	0.95	0.92	0.90	0.93	0.89	0.86	0.28	0.35	0.40
D=0.6, S=0.0	0.83	0.92	0.91	0.77	0.90	0.88	0.51	0.35	0.38
D=0.6, S=0.1	0.83	0.92	0.90	0.77	0.89	0.86	0.51	0.35	0.40
D=0.7, S=0.0	0.82	0.92	0.91	0.76	0.90	0.88	0.53	0.35	0.38
D=0.7, S=0.1	0.82	0.92	0.90	0.76	0.89	0.86	0.53	0.35	0.40

D: distance threshold; **S**: similarity threshold; **EUC**: Euclidean distance similarity read-across; **GK**: Gaussian kernel function similarity read-across; **LK**: Laplacian kernel function similarity read-across.