Supplementary Materials

Integrating Density Functional Theory with Machine Learning for Enhanced Band Gap Prediction in Metal Oxides

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Convergence Test:

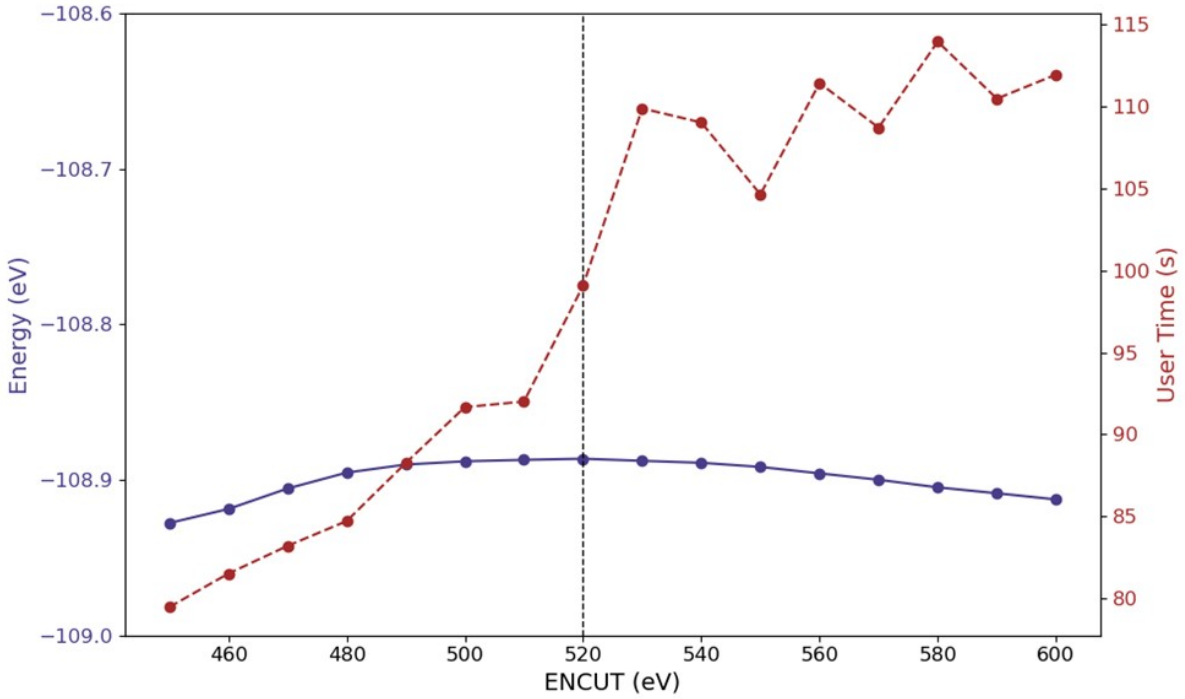

Figure S1. Convergence of Total Energy with Respect to Plane-Wave Cutoff Energy for c-ZnO.

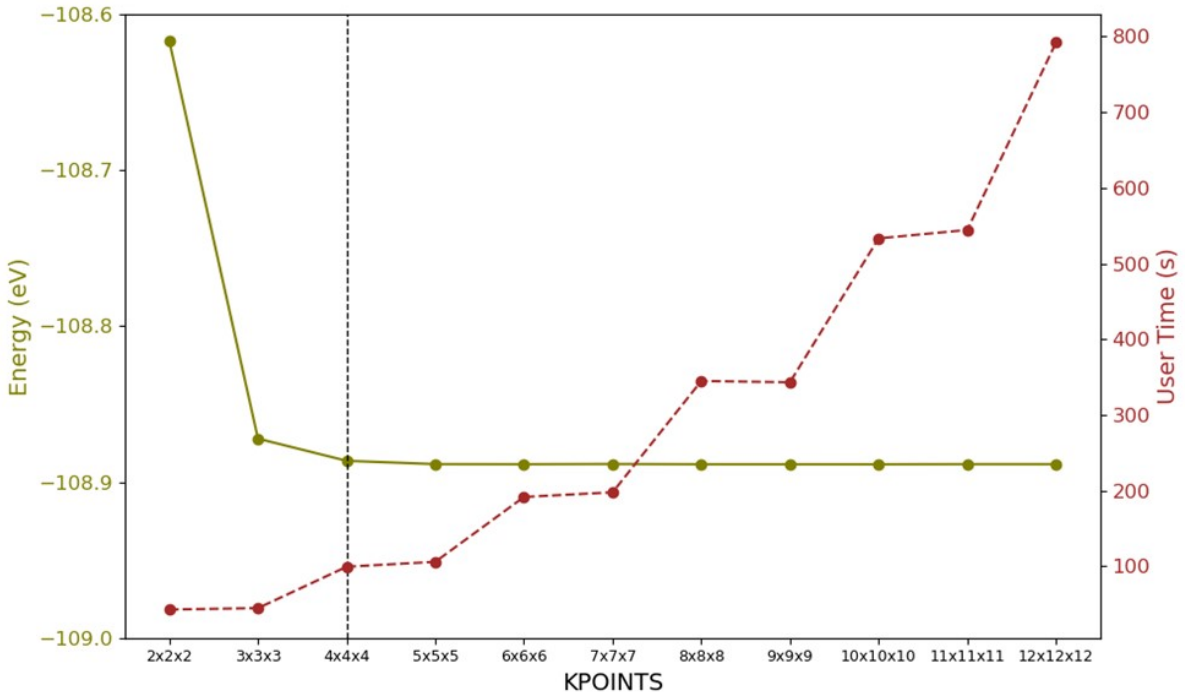

Figure S2. Convergence of Total Energy with Respect to K-Point Sampling for c-ZnO.

Rutile TiO_2:

rPBE:

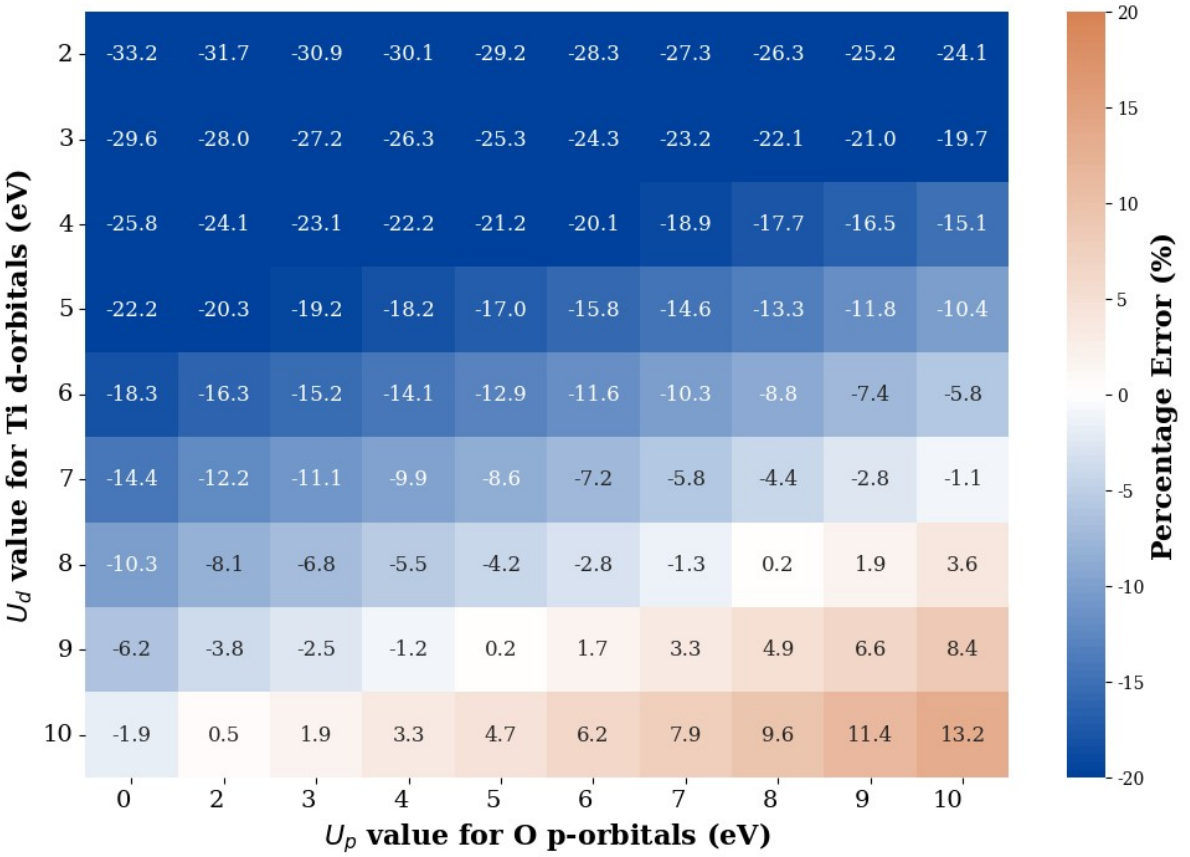

Figure S3. Heatmap of rPBE predicted band gap for rutile TiO_2 as a function of the U_d and U_p parameters.

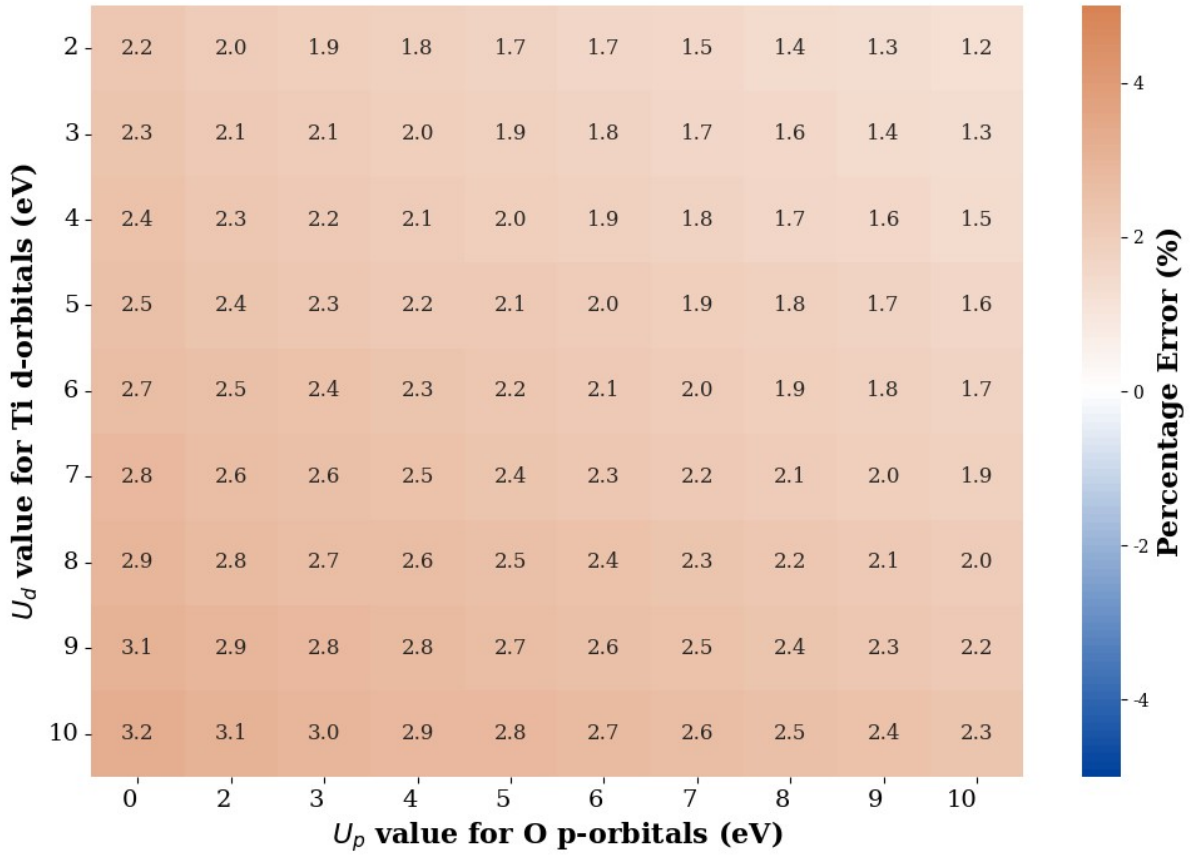

Figure S4. Heatmap of rPBE predicted lattice constant (a = b) for rutile TiO_2 as a function of the U_d and U_p parameters.

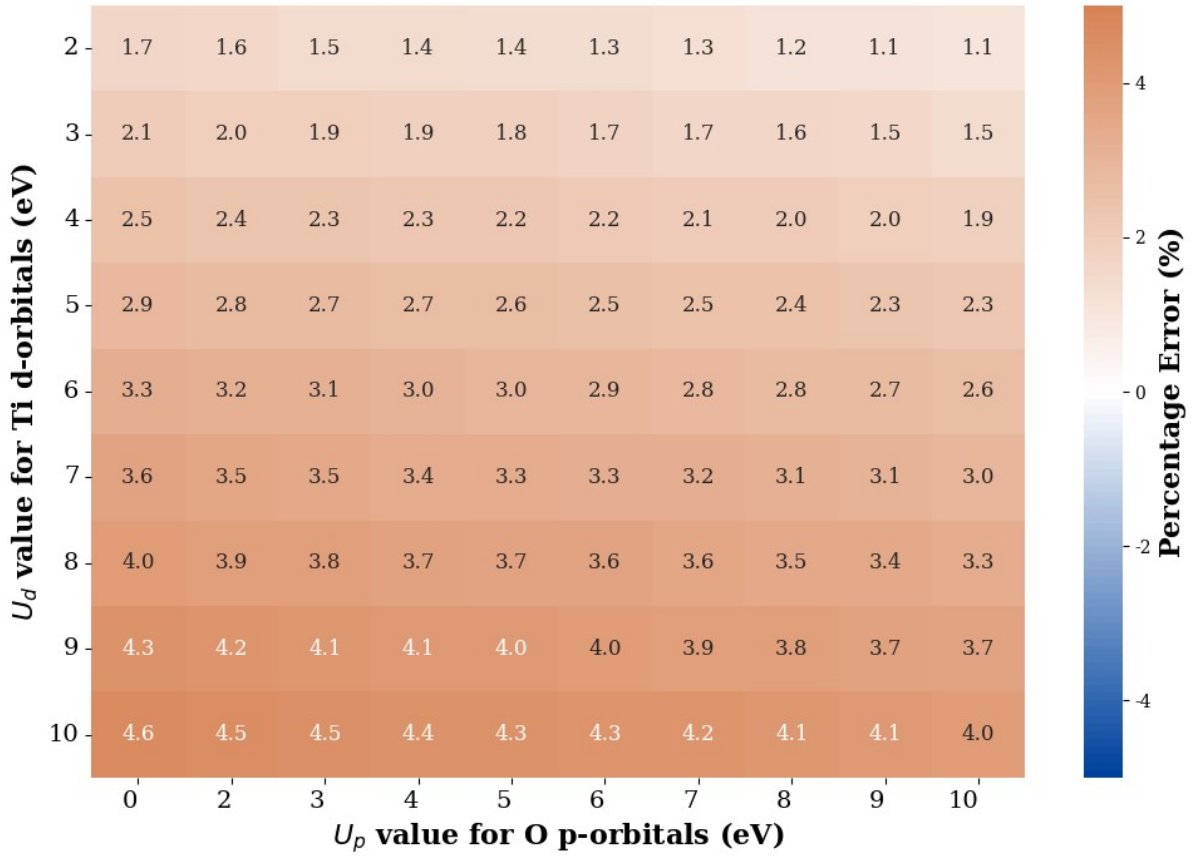

Figure S5. Heatmap of rPBE predicted lattice constant (c) for rutile TiO_2 as a function of the U_d and U_p parameters.

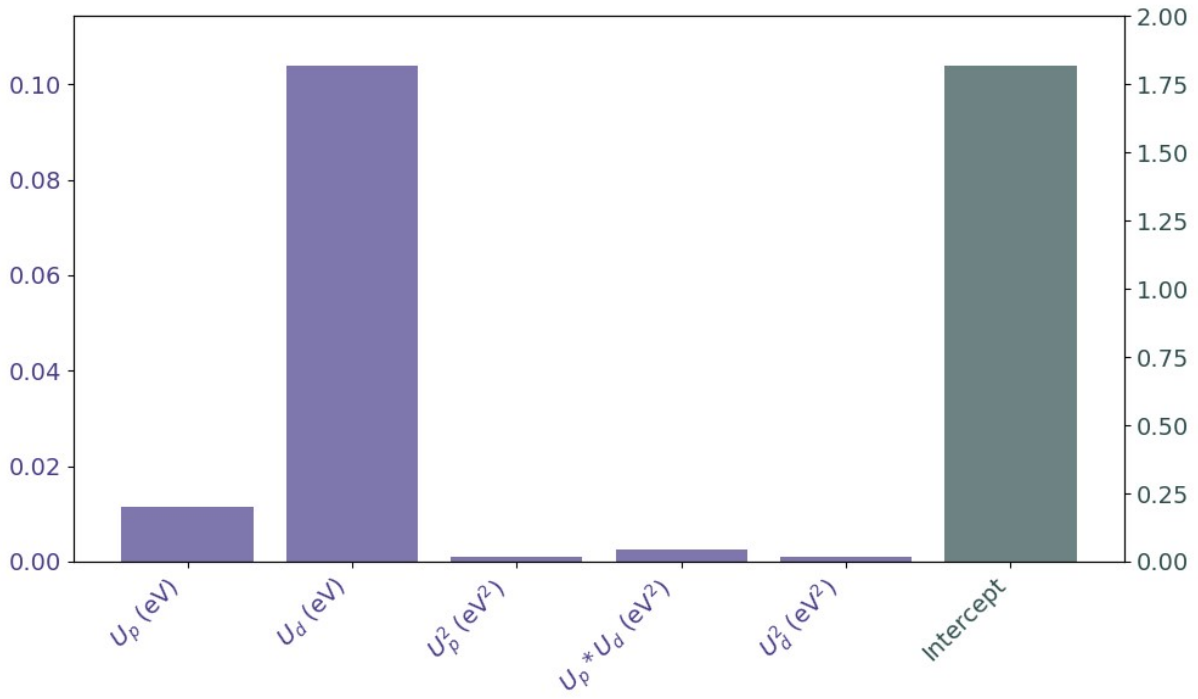

Figure S6. Feature importance of the PR model for predicting the rPBE band gap of rutile TiO_2. Lighter shades indicate features with negative contributions.

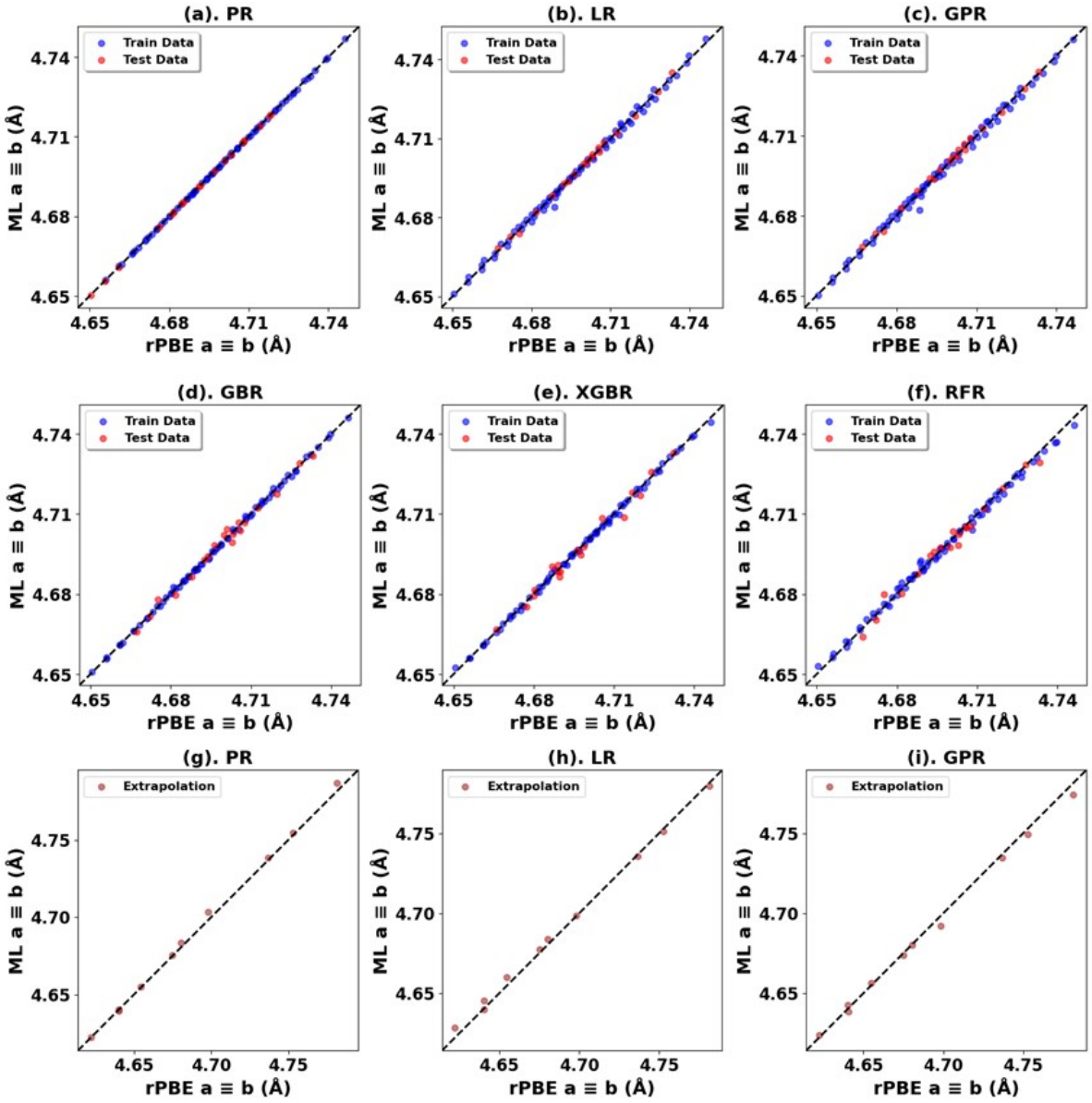

Figure S7. (a) - (f) Performance of models for rPBE lattice parameter (a = b) prediction of rutile TiO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S1. Comparative performance of models for rPBE lattice constant (a = b) prediction in rutile TiO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Rutile TiO_2	*PR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	LR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	GPR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	GBR	0.00	0.00	0.00	0.99	0.00	0.02	0.02	0.82

	XGBR	0.00	0.00	0.00	0.97	0.00	0.02	0.02	0.81
	RFR	0.00	0.00	0.00	0.97	0.00	0.02	0.02	0.80

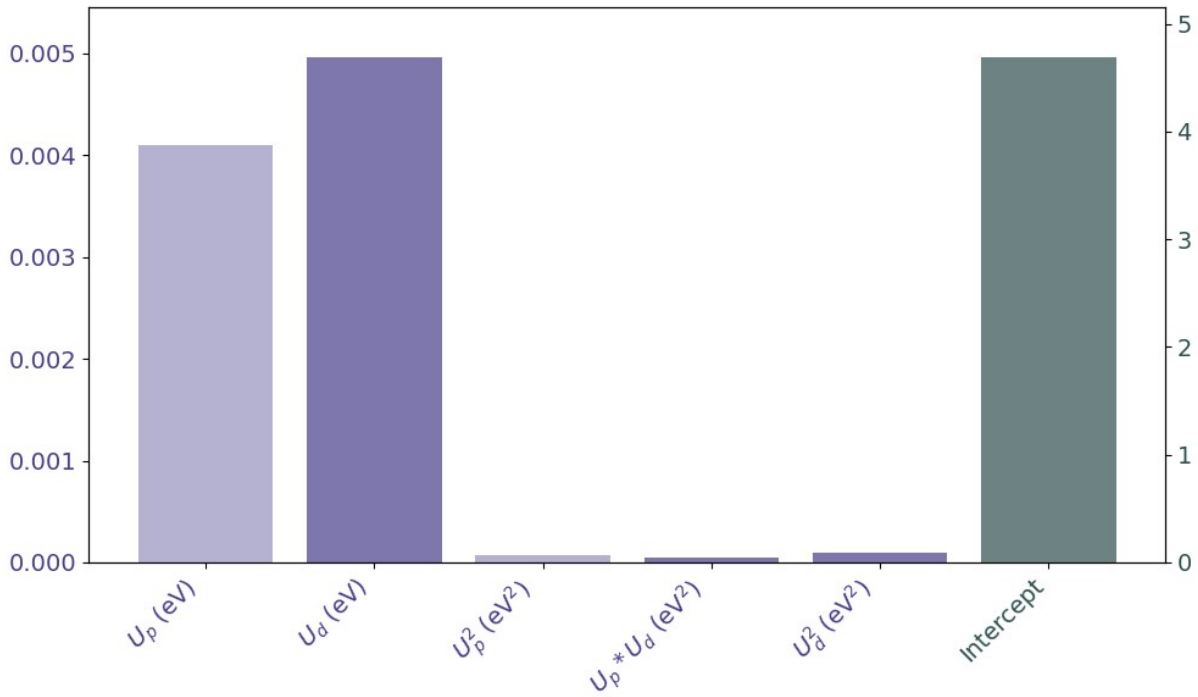

Figure S8. Feature importance of the PR model for predicting the rPBE lattice constant (a = b) of rutile TiO_2. Lighter shades indicate features with negative contributions.

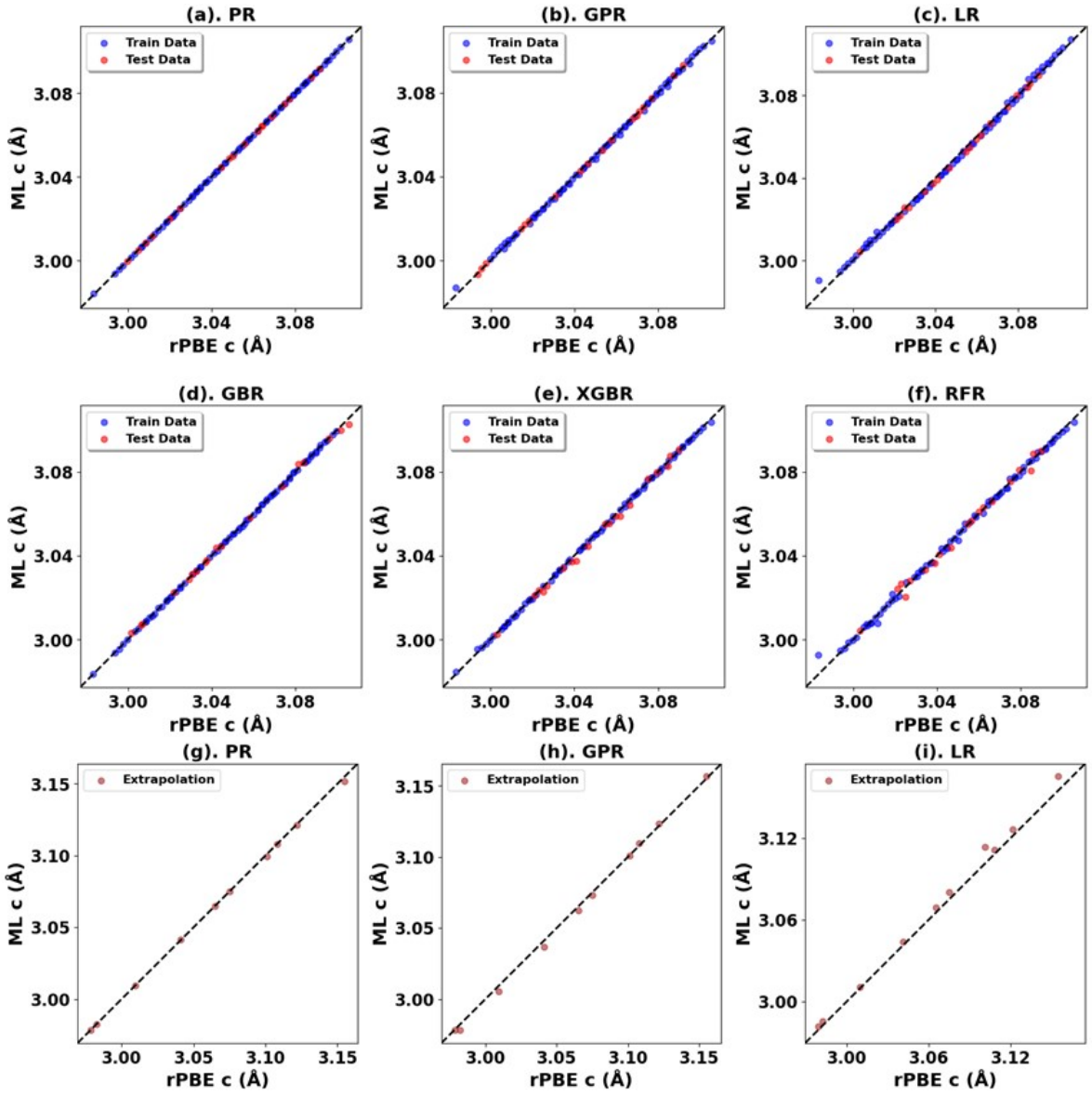

Figure S9. (a) - (f) Performance of models for rPBE lattice parameter (c) prediction of rutile TiO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S2. Comparative performance of models for rPBE lattice constant (c) prediction in rutile TiO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Rutile TiO_2	PR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	GPR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	LR	0.00	0.00	0.00	1.00	0.00	0.01	0.00	0.99
	GBR	0.00	0.00	0.00	0.99	0.00	0.02	0.02	0.88

	XGBR	0.00	0.00	0.00	0.99	0.00	0.02	0.02	0.87
	RFR	0.00	0.00	0.00	0.99	0.00	0.02	0.02	0.87

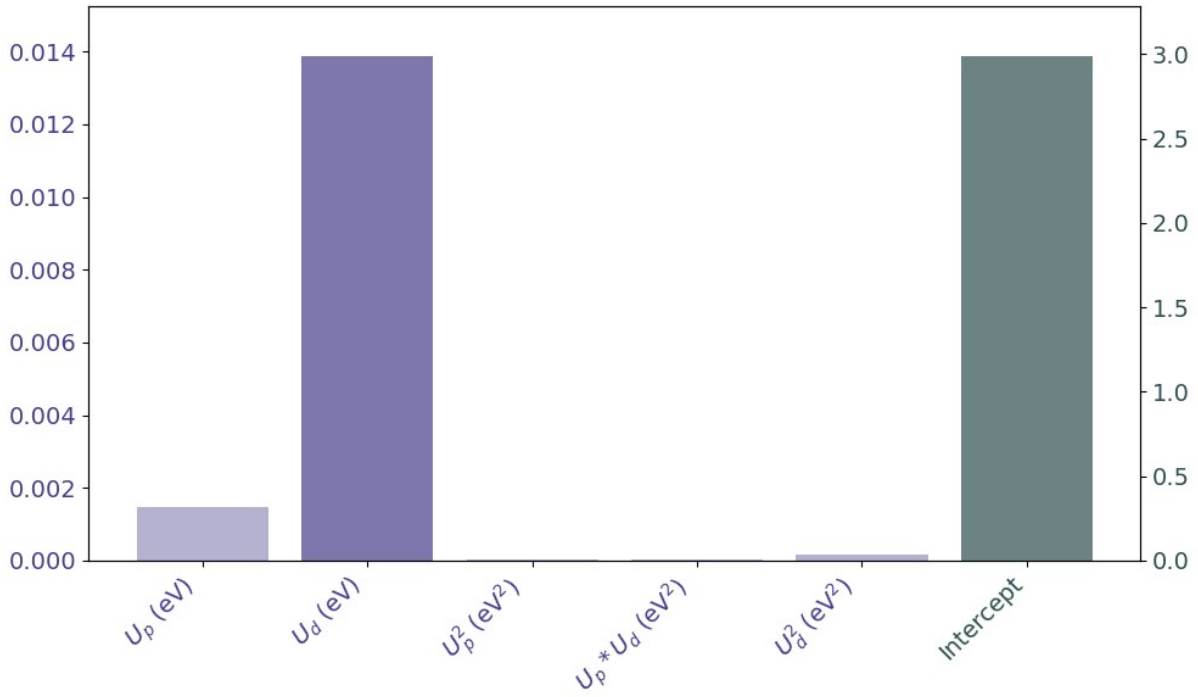

Figure S10. Feature importance of the PR model for predicting the rPBE lattice constant (c) of rutile TiO_2. Lighter shades indicate features with negative contributions.

Table S3. Influence of U_d and U_p on rutile TiO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)	% Deviation in a = b	% Deviation in c	% Deviation in E_g	% Deviation in c/a
0	0	4.6886	2.9834	1.838	2.07	0.73	-39.34	-1.31
2	0	4.6976	3.0117	2.023	2.26	1.68	-33.23	-0.56
2	2	4.6892	3.0085	2.068	2.08	1.58	-31.75	-0.49
2	3	4.6846	3.0067	2.093	1.98	1.52	-30.92	-0.45
2	4	4.6801	3.0050	2.118	1.88	1.46	-30.10	-0.41
2	5	4.6753	3.0032	2.145	1.78	1.40	-29.21	-0.37
2	6	4.6710	3.0015	2.173	1.68	1.34	-28.28	-0.34
2	7	4.6660	2.9996	2.202	1.57	1.28	-27.33	-0.29
2	8	4.6610	2.9977	2.233	1.47	1.21	-26.30	-0.25
2	9	4.6559	2.9958	2.266	1.35	1.15	-25.21	-0.20
2	10	4.6506	2.9937	2.301	1.24	1.08	-24.06	-0.16
3	0	4.7028	3.0250	2.132	2.38	2.13	-29.64	-0.24
3	2	4.6944	3.0217	2.181	2.19	2.02	-28.02	-0.17
3	3	4.6900	3.0200	2.207	2.10	1.96	-27.16	-0.13
3	4	4.6855	3.0182	2.234	2.00	1.90	-26.27	-0.09

3	5	4.6809	3.0164	2.263	1.90	1.84	-25.31	-0.05
3	6	4.6761	3.0145	2.294	1.79	1.78	-24.29	-0.01
3	7	4.6713	3.0126	2.326	1.69	1.71	-23.23	0.02
3	8	4.6661	3.0104	2.36	1.58	1.64	-22.11	0.06
3	9	4.6610	3.0084	2.395	1.47	1.57	-20.96	0.11
3	10	4.6561	3.0064	2.433	1.36	1.51	-19.70	0.15
4	0	4.7080	3.0377	2.247	2.49	2.56	-25.84	0.07
4	2	4.6999	3.0345	2.3	2.31	2.45	-24.09	0.14
4	3	4.6955	3.0327	2.329	2.22	2.39	-23.14	0.17
4	4	4.6911	3.0309	2.358	2.12	2.33	-22.18	0.21
4	5	4.6865	3.0290	2.389	2.02	2.27	-21.16	0.24
4	6	4.6818	3.0271	2.422	1.92	2.20	-20.07	0.28
4	7	4.6771	3.0251	2.456	1.82	2.14	-18.94	0.32
4	8	4.6721	3.0229	2.493	1.71	2.06	-17.72	0.35
4	9	4.6672	3.0209	2.531	1.60	2.00	-16.47	0.39
4	10	4.6621	3.0187	2.572	1.49	1.92	-15.12	0.43
5	0	4.7138	3.0501	2.358	2.61	2.98	-22.18	0.36
5	2	4.7055	3.0466	2.416	2.43	2.86	-20.26	0.42
5	3	4.7013	3.0448	2.447	2.34	2.80	-19.24	0.45
5	4	4.6969	3.0429	2.48	2.25	2.74	-18.15	0.48
5	5	4.6924	3.0409	2.514	2.15	2.67	-17.03	0.51
5	6	4.6878	3.0389	2.55	2.05	2.60	-15.84	0.54
5	7	4.6831	3.0369	2.588	1.95	2.54	-14.59	0.58
5	8	4.6783	3.0348	2.628	1.84	2.47	-13.27	0.61
5	9	4.6734	3.0327	2.671	1.73	2.39	-11.85	0.65
5	10	4.6684	3.0307	2.715	1.63	2.32	-10.40	0.69
6	0	4.7199	3.0620	2.474	2.75	3.38	-18.35	0.62
6	2	4.7118	3.0584	2.536	2.57	3.26	-16.30	0.67
6	3	4.7076	3.0566	2.569	2.48	3.20	-15.21	0.70
6	4	4.7033	3.0546	2.604	2.39	3.13	-14.06	0.73
6	5	4.6988	3.0527	2.64	2.29	3.07	-12.87	0.76
6	6	4.6943	3.0506	2.678	2.19	3.00	-11.62	0.79
6	7	4.6896	3.0486	2.719	2.09	2.93	-10.26	0.82
6	8	4.6848	3.0464	2.762	1.98	2.86	-8.84	0.86
6	9	4.6801	3.0444	2.806	1.88	2.79	-7.39	0.89
6	10	4.6750	3.0422	2.854	1.77	2.71	-5.81	0.93
7	0	4.7265	3.0735	2.594	2.89	3.77	-14.39	0.86
7	2	4.7184	3.0699	2.659	2.71	3.65	-12.24	0.91
7	3	4.7142	3.0680	2.694	2.62	3.58	-11.09	0.94
7	4	4.7098	3.0660	2.731	2.53	3.52	-9.87	0.97
7	5	4.7055	3.0640	2.77	2.43	3.45	-8.58	0.99
7	6	4.7010	3.0620	2.811	2.34	3.38	-7.23	1.02
7	7	4.6964	3.0599	2.853	2.24	3.31	-5.84	1.05
7	8	4.6917	3.0577	2.898	2.13	3.24	-4.36	1.08
7	9	4.6869	3.0557	2.946	2.03	3.17	-2.77	1.12
7	10	4.6819	3.0534	2.996	1.92	3.09	-1.12	1.15

8	0	4.7333	3.0847	2.717	3.04	4.15	-10.33	1.08
8	2	4.7252	3.0810	2.786	2.86	4.02	-8.05	1.13
8	3	4.7211	3.0791	2.823	2.77	3.96	-6.83	1.16
8	4	4.7168	3.0771	2.862	2.68	3.89	-5.54	1.18
8	5	4.7124	3.0751	2.902	2.58	3.83	-4.22	1.21
8	6	4.7079	3.0730	2.945	2.49	3.75	-2.81	1.24
8	7	4.7033	3.0708	2.99	2.39	3.68	-1.32	1.27
8	8	4.6988	3.0689	3.037	2.29	3.61	0.23	1.30
8	9	4.6938	3.0664	3.087	2.18	3.53	1.88	1.32
8	10	4.6890	3.0644	3.14	2.07	3.46	3.63	1.36
9	0	4.7398	3.0951	2.843	3.18	4.50	-6.17	1.28
9	2	4.7323	3.0917	2.914	3.02	4.39	-3.83	1.33
9	3	4.7282	3.0898	2.954	2.93	4.32	-2.51	1.36
9	4	4.7239	3.0879	2.994	2.83	4.26	-1.19	1.38
9	5	4.7196	3.0858	3.037	2.74	4.19	0.23	1.41
9	6	4.7151	3.0837	3.082	2.64	4.12	1.72	1.44
9	7	4.7105	3.0815	3.129	2.54	4.04	3.27	1.46
9	8	4.7058	3.0794	3.178	2.44	3.97	4.88	1.49
9	9	4.7010	3.0771	3.231	2.34	3.89	6.63	1.52
9	10	4.6961	3.0747	3.286	2.23	3.81	8.45	1.55
10	0	4.7463	3.1055	2.972	3.32	4.85	-1.91	1.48
10	2	4.7390	3.1017	3.046	3.16	4.72	0.53	1.51
10	3	4.7350	3.0998	3.087	3.08	4.66	1.88	1.54
10	4	4.7308	3.0978	3.129	2.98	4.59	3.27	1.56
10	5	4.7269	3.0962	3.172	2.90	4.54	4.69	1.59
10	6	4.7224	3.0941	3.219	2.80	4.47	6.24	1.62
10	7	4.7179	3.0919	3.268	2.70	4.39	7.85	1.64
10	8	4.7132	3.0897	3.32	2.60	4.32	9.57	1.67
10	9	4.7084	3.0874	3.374	2.50	4.24	11.35	1.70
10	10	4.7035	3.0851	3.431	2.39	4.16	13.23	1.73

Table S4. Influence of U_d and U_p on rutile TiO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)
1	11	4.6404	2.9786	2.21
2	15	4.6221	2.9823	2.509

4	14	4.6403	3.0093	2.762
7	15	4.6547	3.0412	3.295
9	14	4.6750	3.0651	3.539
10	14	4.6803	3.0750	3.697
11	4	4.7368	3.1080	3.265
12	2	4.7528	3.1218	3.31
13	15	4.6983	3.1012	4.232
15	0	4.7816	3.1551	3.616

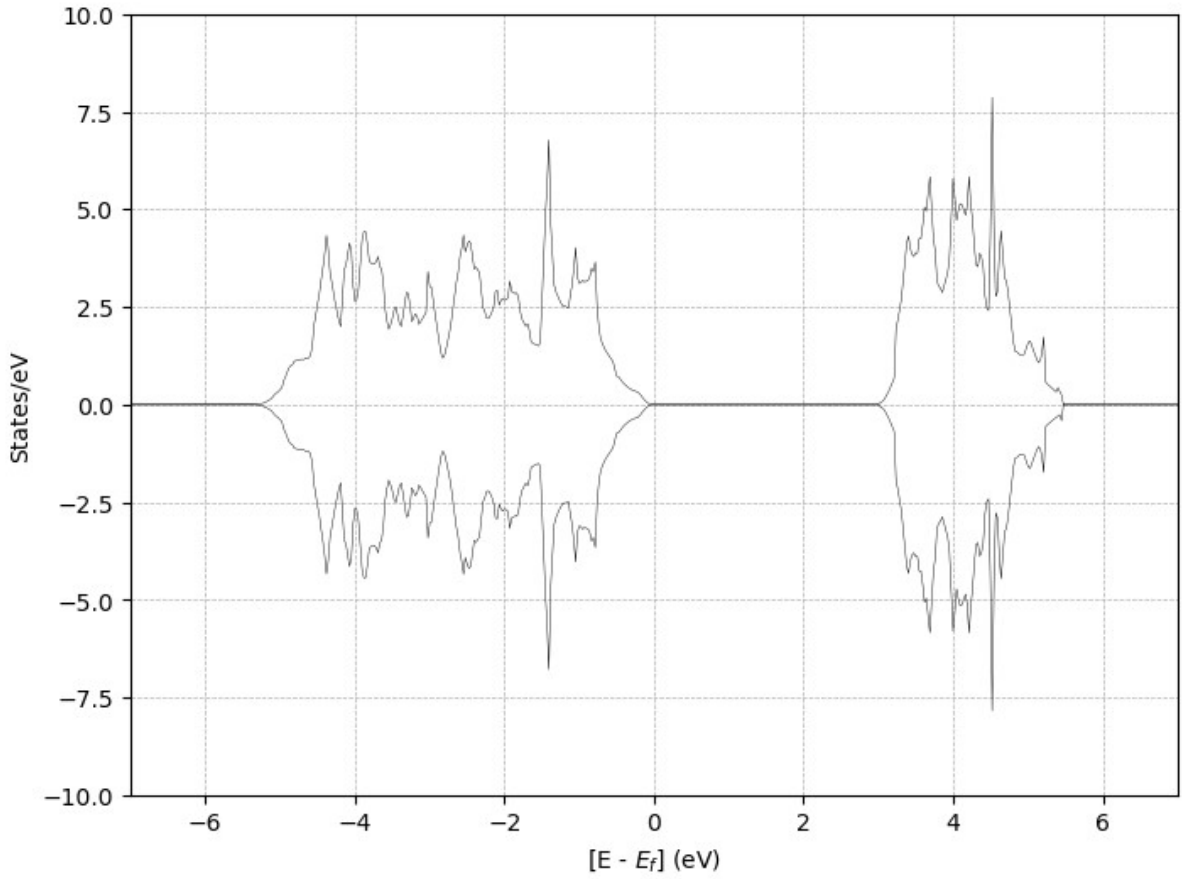

Figure S11. DOS for rutile TiO_2 with rPBE functional: U_p = 8 eV, U_d = 8 eV

PBE:

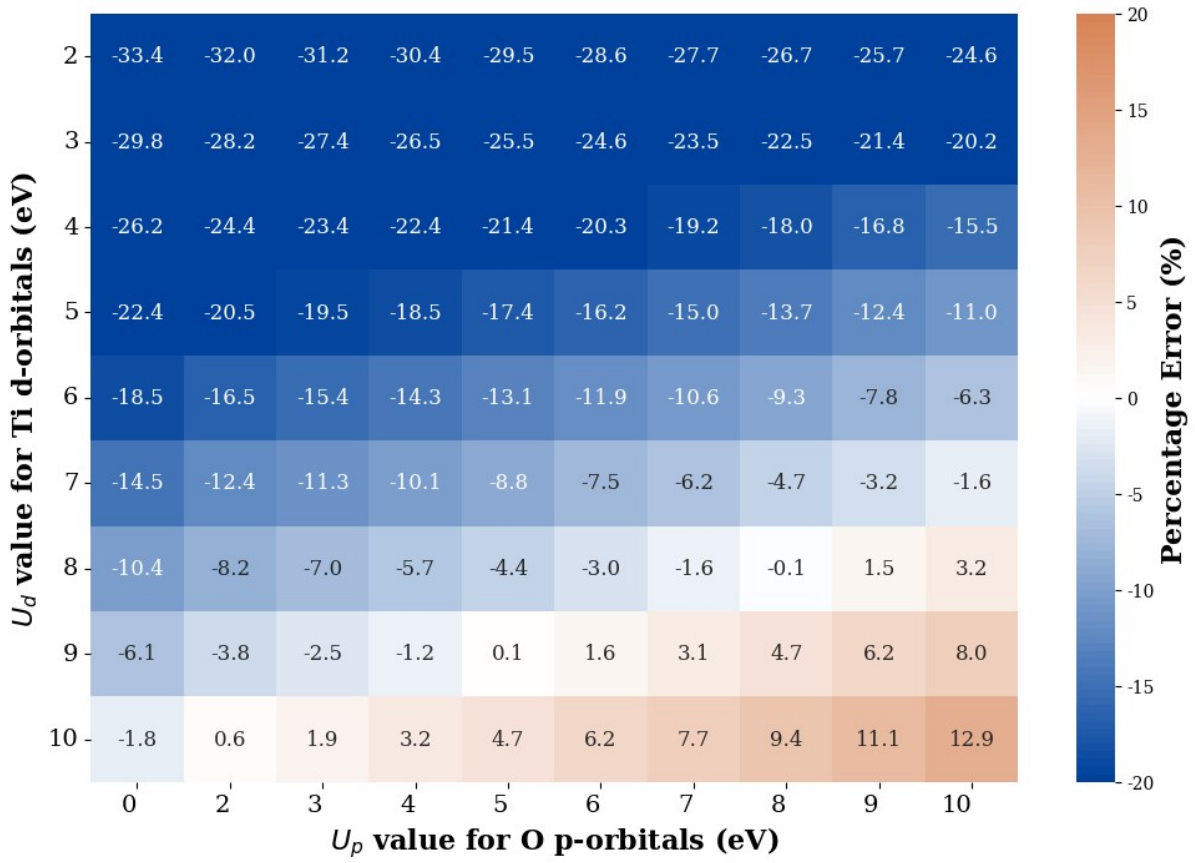

Figure S12. Heatmap of PBE predicted band gap for rutile TiO_2 as a function of the U_d and U_p parameters.

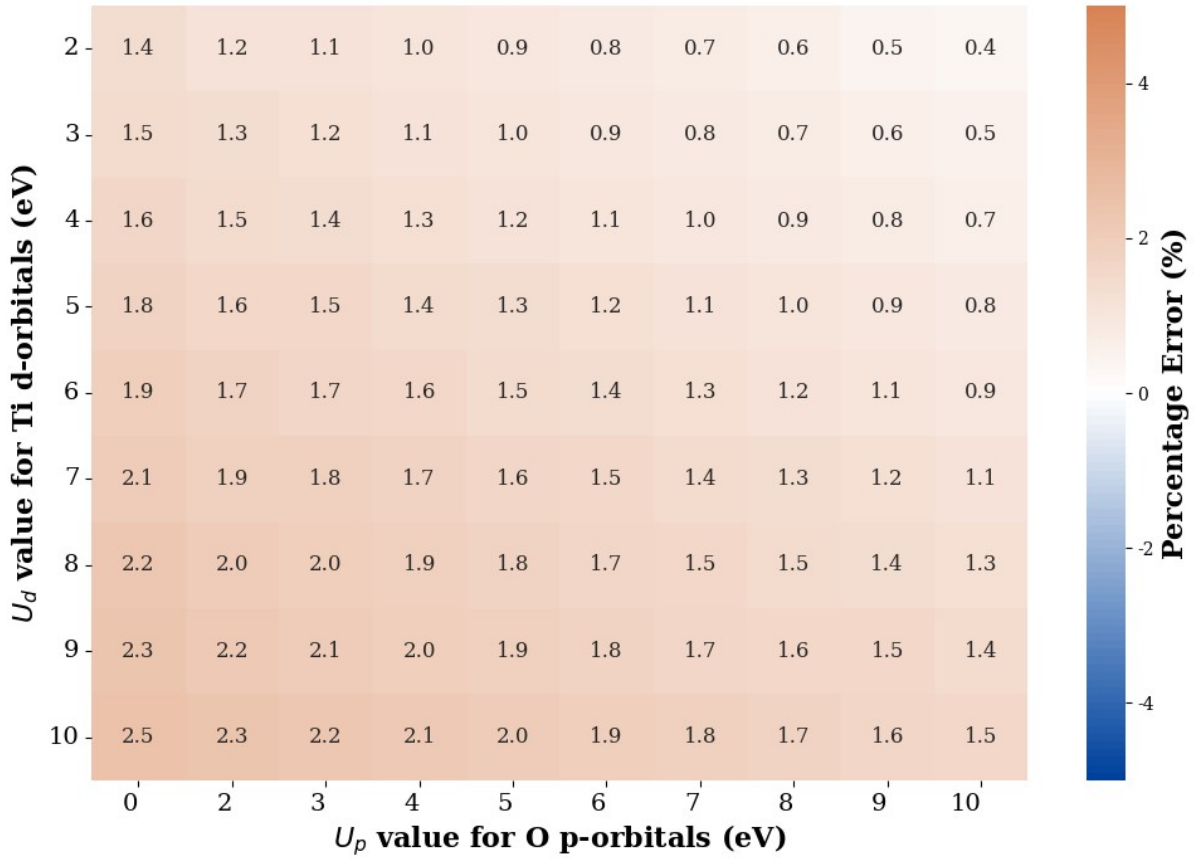

Figure S13. Heatmap of PBE predicted lattice constant (a = b) for rutile TiO_2 as a function of the U_d and U_p parameters.

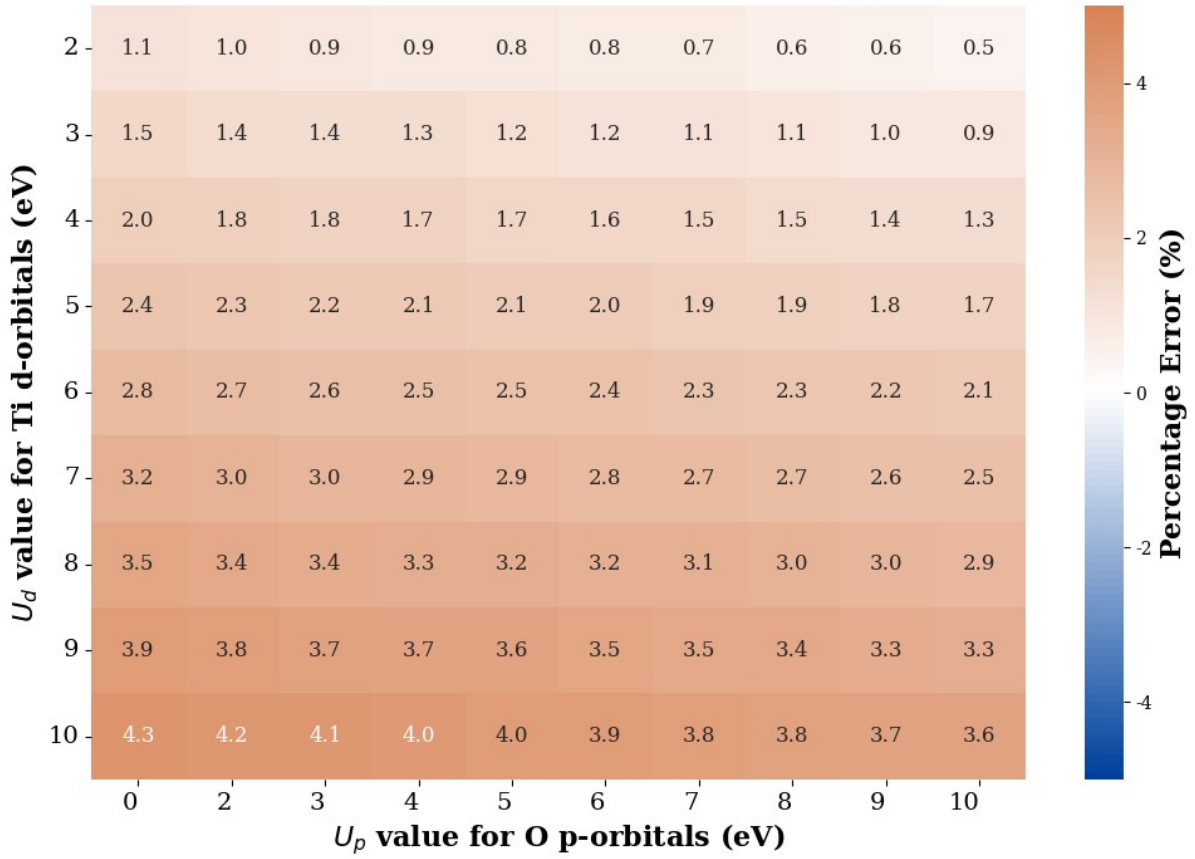

Figure S14. Heatmap of PBE predicted lattice constant (c) for rutile TiO_2 as a function of the U_d and U_p parameters.

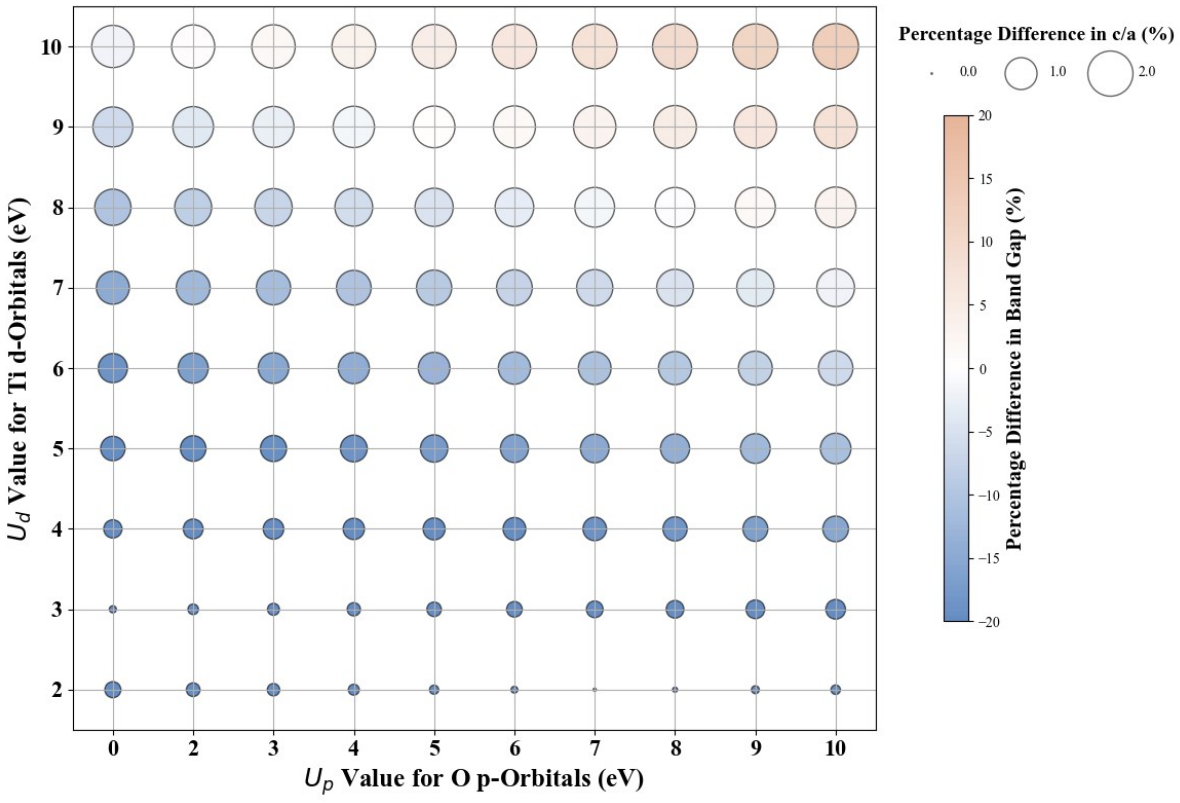

Figure S15. Effect of Hubbard U values on PBE band gap and lattice parameters of rutile TiO_2.

Table S5. Influence of U_d and U_p on rutile TiO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)	% Deviation in a = b	% Deviation in c	% Deviation in E_g	% Deviation in c/a
0	0	4.6459	2.9677	1.826	1.14	0.20	-39.74	-0.93
2	0	4.6566	2.9947	2.017	1.37	1.11	-33.43	-0.25
2	2	4.6482	2.9914	2.061	1.19	1.00	-31.98	-0.18
2	3	4.6442	2.9898	2.085	1.10	0.95	-31.19	-0.15
2	4	4.6399	2.9881	2.109	1.01	0.89	-30.40	-0.12
2	5	4.6355	2.9863	2.135	0.91	0.83	-29.54	-0.08
2	6	4.6309	2.9844	2.162	0.81	0.76	-28.65	-0.05
2	7	4.6263	2.9825	2.191	0.71	0.70	-27.69	-0.01
2	8	4.6216	2.9805	2.221	0.61	0.63	-26.70	0.03
2	9	4.6166	2.9784	2.252	0.50	0.56	-25.68	0.06
2	10	4.6118	2.9761	2.284	0.39	0.48	-24.62	0.09
3	0	4.6625	3.0077	2.127	1.50	1.55	-29.80	0.05
3	2	4.6541	3.0041	2.176	1.32	1.43	-28.18	0.11
3	3	4.6499	3.0023	2.201	1.22	1.37	-27.36	0.14
3	4	4.6457	3.0005	2.228	1.13	1.31	-26.47	0.17
3	5	4.6413	2.9987	2.256	1.04	1.25	-25.54	0.21
3	6	4.6369	2.9968	2.286	0.94	1.18	-24.55	0.24
3	7	4.6324	2.9950	2.317	0.84	1.12	-23.53	0.28
3	8	4.6278	2.9930	2.349	0.74	1.05	-22.48	0.31
3	9	4.6228	2.9909	2.383	0.63	0.98	-21.35	0.35
3	10	4.6179	2.9889	2.419	0.53	0.91	-20.17	0.38
4	0	4.6687	3.0201	2.237	1.63	1.97	-26.17	0.33
4	2	4.6606	3.0166	2.291	1.46	1.85	-24.39	0.39
4	3	4.6565	3.0148	2.32	1.37	1.79	-23.43	0.42
4	4	4.6523	3.0130	2.35	1.27	1.73	-22.44	0.45
4	5	4.6476	3.0109	2.382	1.17	1.66	-21.39	0.48
4	6	4.6431	3.0090	2.415	1.08	1.59	-20.30	0.51
4	7	4.6385	3.0071	2.449	0.98	1.53	-19.17	0.55
4	8	4.6340	3.0051	2.484	0.88	1.46	-18.02	0.58
4	9	4.6292	3.0030	2.521	0.77	1.39	-16.80	0.61
4	10	4.6242	3.0009	2.56	0.66	1.32	-15.51	0.65
5	0	4.6751	3.0321	2.351	1.77	2.37	-22.41	0.59
5	2	4.6671	3.0287	2.408	1.60	2.26	-20.53	0.65
5	3	4.6630	3.0269	2.439	1.51	2.20	-19.50	0.68
5	4	4.6588	3.0251	2.47	1.42	2.14	-18.48	0.71
5	5	4.6544	3.0232	2.504	1.32	2.07	-17.36	0.74
5	6	4.6499	3.0213	2.539	1.22	2.01	-16.20	0.77
5	7	4.6452	3.0192	2.576	1.12	1.94	-14.98	0.81

5	8	4.6403	3.0169	2.615	1.01	1.86	-13.70	0.84
5	9	4.6355	3.0148	2.655	0.91	1.79	-12.38	0.87
5	10	4.6306	3.0131	2.698	0.80	1.73	-10.96	0.92
6	0	4.6818	3.0440	2.469	1.92	2.77	-18.51	0.84
6	2	4.6738	3.0405	2.53	1.74	2.66	-16.50	0.90
6	3	4.6697	3.0386	2.562	1.65	2.59	-15.45	0.92
6	4	4.6654	3.0368	2.596	1.56	2.53	-14.32	0.96
6	5	4.6611	3.0349	2.632	1.47	2.47	-13.14	0.99
6	6	4.6567	3.0331	2.669	1.37	2.41	-11.91	1.02
6	7	4.6520	3.0310	2.708	1.27	2.34	-10.63	1.06
6	8	4.6472	3.0287	2.749	1.17	2.26	-9.27	1.08
6	9	4.6423	3.0270	2.793	1.06	2.20	-7.82	1.13
6	10	4.6371	3.0247	2.839	0.94	2.12	-6.30	1.17
7	0	4.6886	3.0555	2.591	2.07	3.16	-14.49	1.07
7	2	4.6807	3.0520	2.655	1.89	3.05	-12.38	1.13
7	3	4.6766	3.0502	2.689	1.80	2.98	-11.25	1.16
7	4	4.6724	3.0483	2.725	1.71	2.92	-10.07	1.19
7	5	4.6681	3.0466	2.762	1.62	2.86	-8.84	1.22
7	6	4.6635	3.0446	2.802	1.52	2.80	-7.52	1.26
7	7	4.6589	3.0426	2.843	1.42	2.73	-6.17	1.29
7	8	4.6541	3.0405	2.887	1.32	2.66	-4.72	1.33
7	9	4.6492	3.0385	2.933	1.21	2.59	-3.20	1.36
7	10	4.6442	3.0364	2.981	1.10	2.52	-1.62	1.40
8	0	4.6957	3.0668	2.716	2.22	3.55	-10.36	1.30
8	2	4.6878	3.0632	2.783	2.05	3.42	-8.15	1.35
8	3	4.6837	3.0614	2.819	1.96	3.36	-6.96	1.38
8	4	4.6795	3.0595	2.857	1.87	3.30	-5.71	1.40
8	5	4.6751	3.0575	2.896	1.77	3.23	-4.42	1.43
8	6	4.6706	3.0556	2.938	1.67	3.17	-3.04	1.47
8	7	4.6639	3.0537	2.983	1.53	3.10	-1.55	1.55
8	8	4.6613	3.0518	3.027	1.47	3.04	-0.10	1.54
8	9	4.6564	3.0497	3.075	1.37	2.97	1.49	1.58
8	10	4.6514	3.0475	3.126	1.26	2.89	3.17	1.62
9	0	4.7006	3.0783	2.845	2.33	3.93	-6.11	1.57
9	2	4.6926	3.0747	2.916	2.15	3.81	-3.76	1.62
9	3	4.6885	3.0728	2.954	2.06	3.75	-2.51	1.65
9	4	4.6843	3.0709	2.993	1.97	3.68	-1.22	1.68
9	5	4.6800	3.0690	3.034	1.88	3.62	0.13	1.71
9	6	4.6753	3.0668	3.078	1.78	3.54	1.58	1.74
9	7	4.6710	3.0648	3.123	1.68	3.48	3.07	1.77
9	8	4.6664	3.0627	3.171	1.58	3.41	4.65	1.80
9	9	4.6637	3.0604	3.219	1.52	3.33	6.24	1.78
9	10	4.6587	3.0583	3.272	1.42	3.26	7.99	1.82
10	0	4.7081	3.0888	2.974	2.49	4.29	-1.85	1.75
10	2	4.6997	3.0855	3.048	2.31	4.18	0.59	1.83
10	3	4.6956	3.0836	3.087	2.22	4.11	1.88	1.85

10	4	4.6914	3.0816	3.128	2.13	4.05	3.23	1.88
10	5	4.6870	3.0796	3.171	2.03	3.98	4.65	1.91
10	6	4.6826	3.0776	3.217	1.93	3.91	6.17	1.94
10	7	4.6780	3.0755	3.264	1.84	3.84	7.72	1.97
10	8	4.6735	3.0733	3.314	1.74	3.77	9.37	1.99
10	9	4.6692	3.0710	3.366	1.64	3.69	11.09	2.01
10	10	4.6638	3.0688	3.421	1.53	3.61	12.90	2.05

Table S6. Influence of U_d and U_p on rutile TiO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)
1	11	4.6009	2.9619	2.189
2	15	4.5837	2.9665	2.482
4	14	4.6036	2.9915	2.737
7	15	4.6167	3.0250	3.277
9	14	4.6371	3.0490	3.529
10	14	4.6449	3.0595	3.685
11	4	4.6985	3.0920	3.283
12	2	4.7141	3.1060	3.333
13	15	4.6614	3.0860	4.227
15	0	4.7444	3.1407	3.645

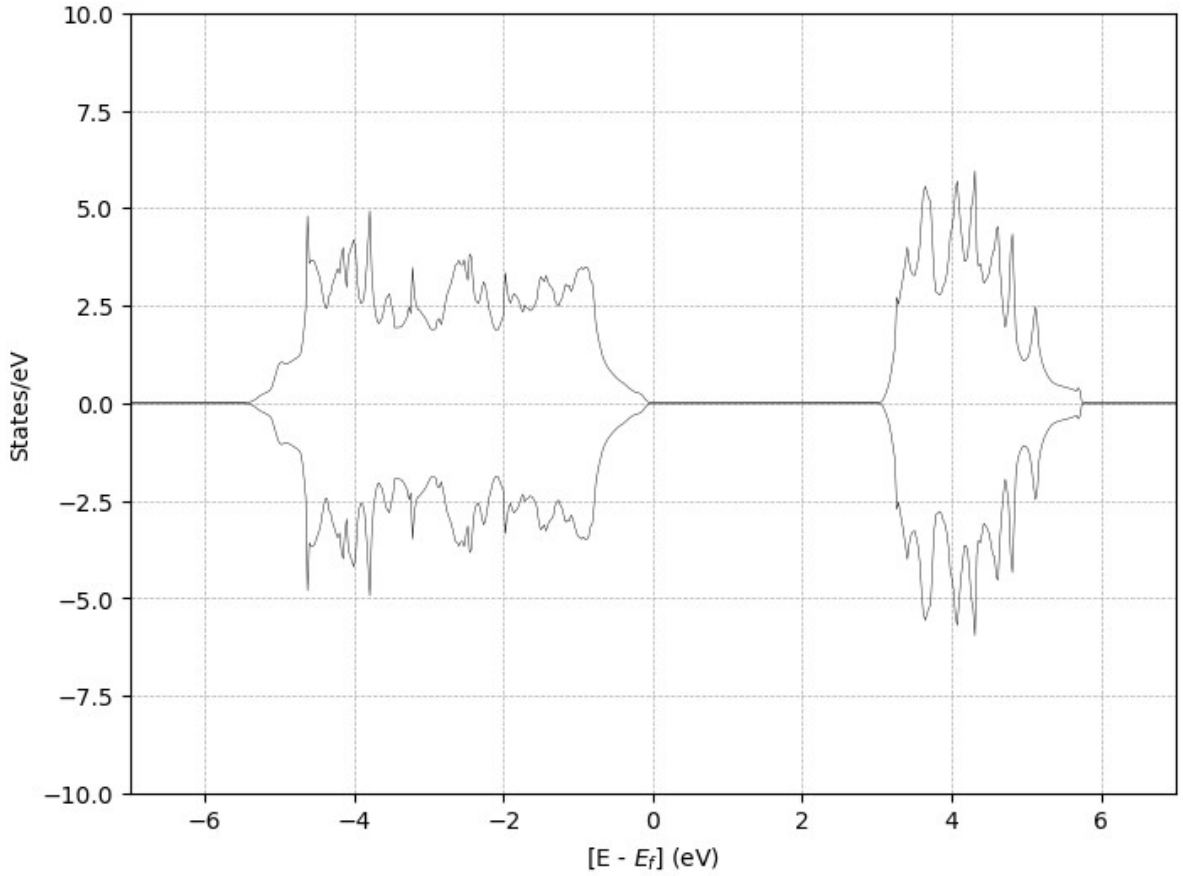

Figure S16. DOS for rutile TiO_2 with PBE functional: U_p = 8 eV, U_d = 8 eV

Anatase TiO_2:

rPBE:

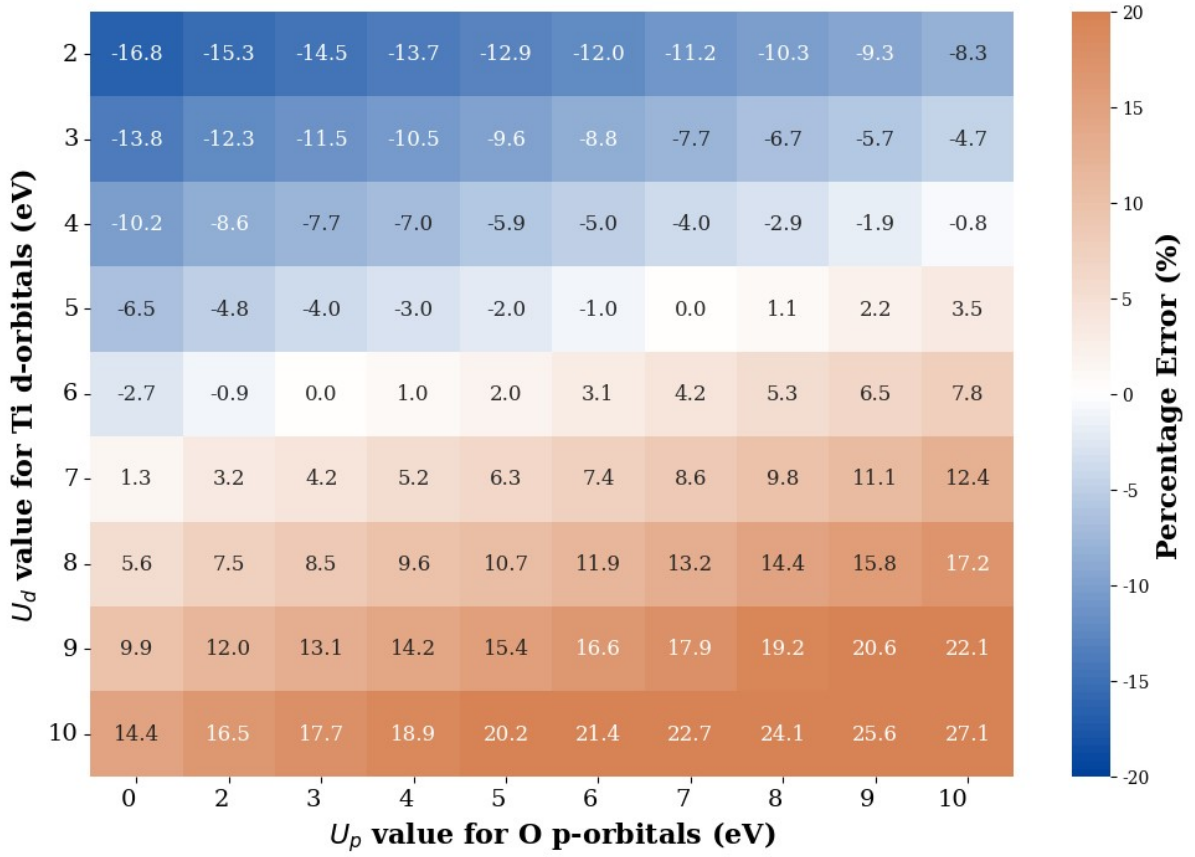

Figure S17. Heatmap of rPBE predicted band gap for anatase TiO_2 as a function of the U_d and U_p parameters.

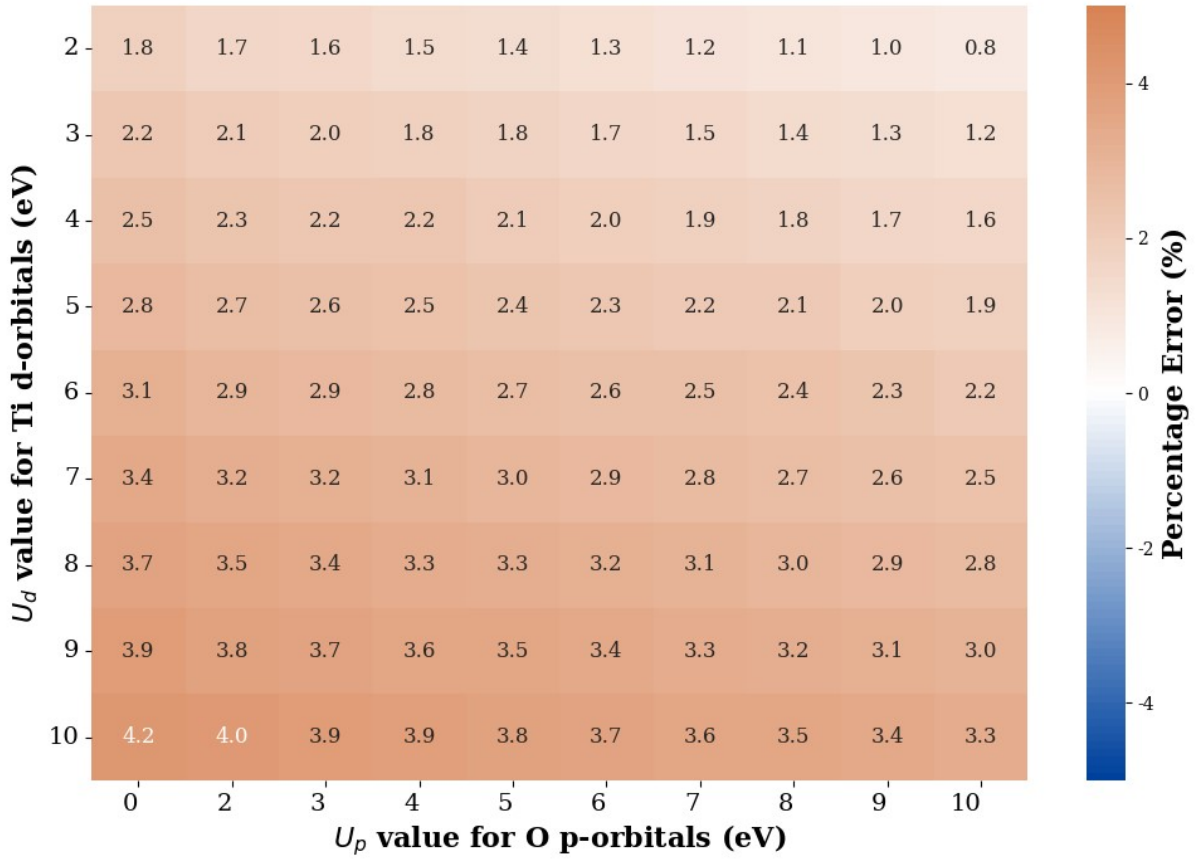

Figure S18. Heatmap of rPBE predicted lattice constant (a = b) for rutile TiO_2 as a function of the U_d and U_p parameters.

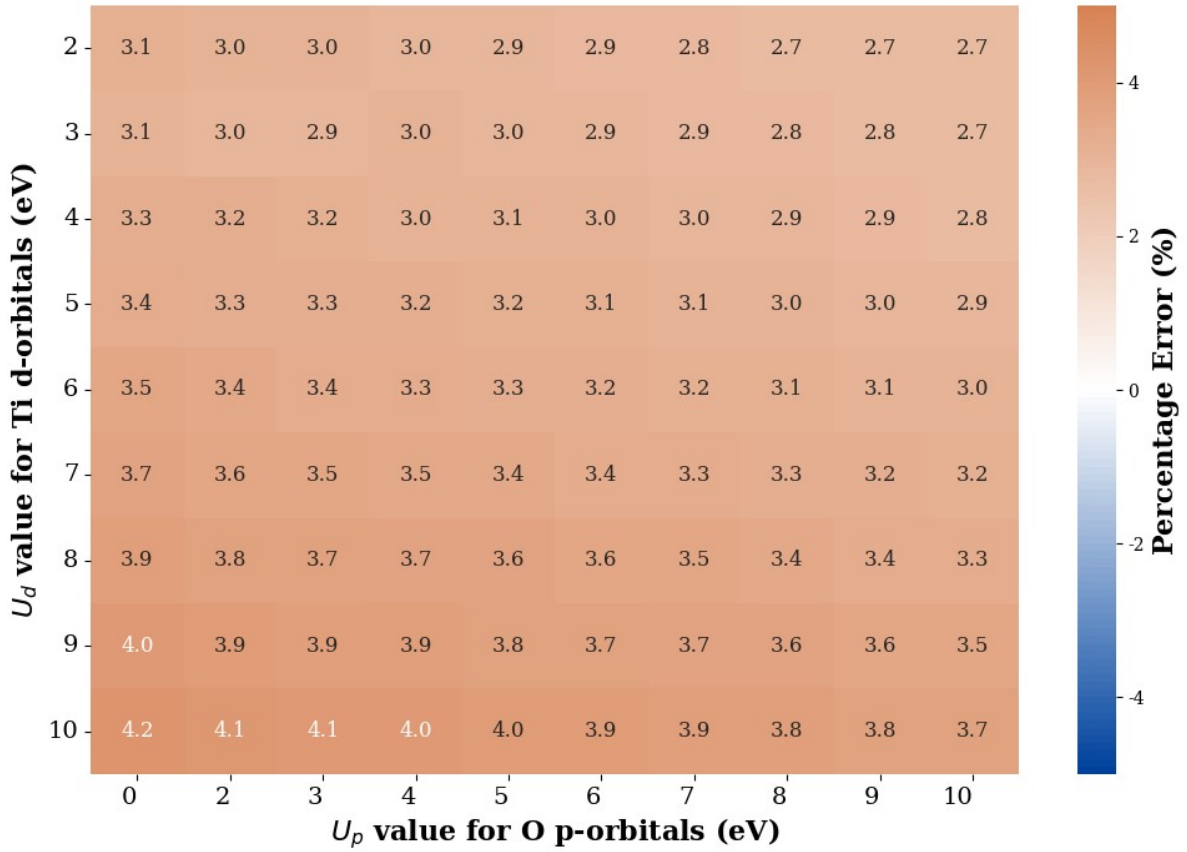

Figure S19. Heatmap of rPBE predicted lattice constant (c) for anatase TiO_2 as a function of the U_d and U_p parameters.

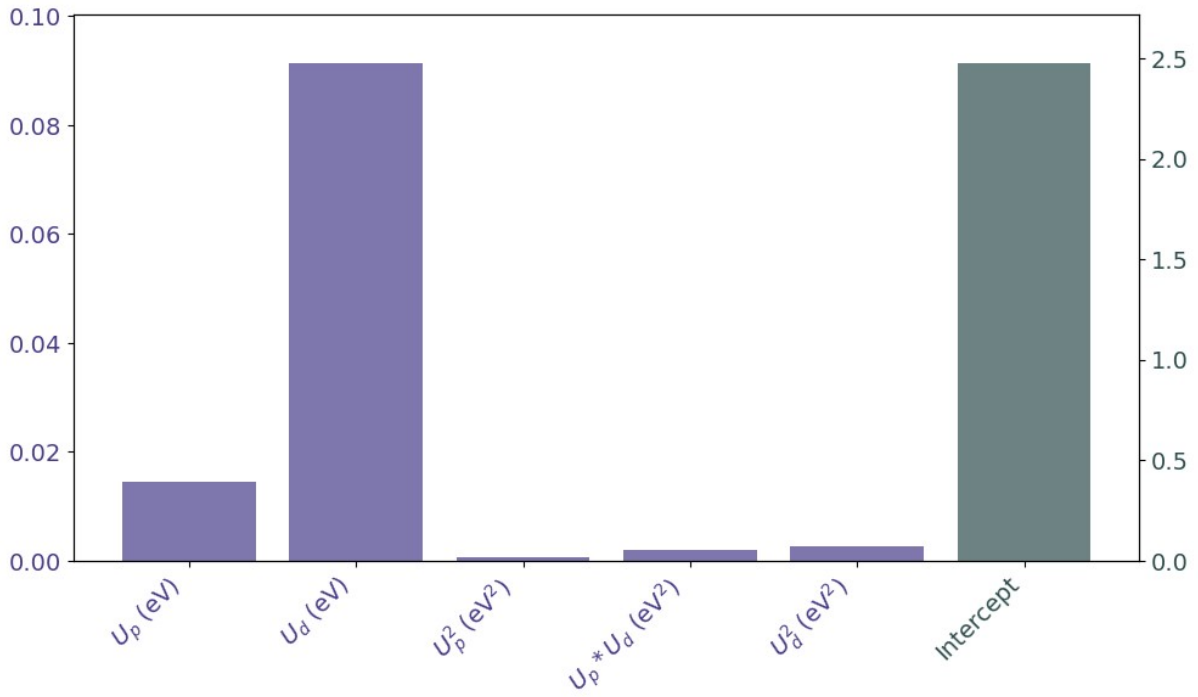

Figure S20. Feature importance of the PR model for predicting the rPBE band gap of anatase TiO_2.

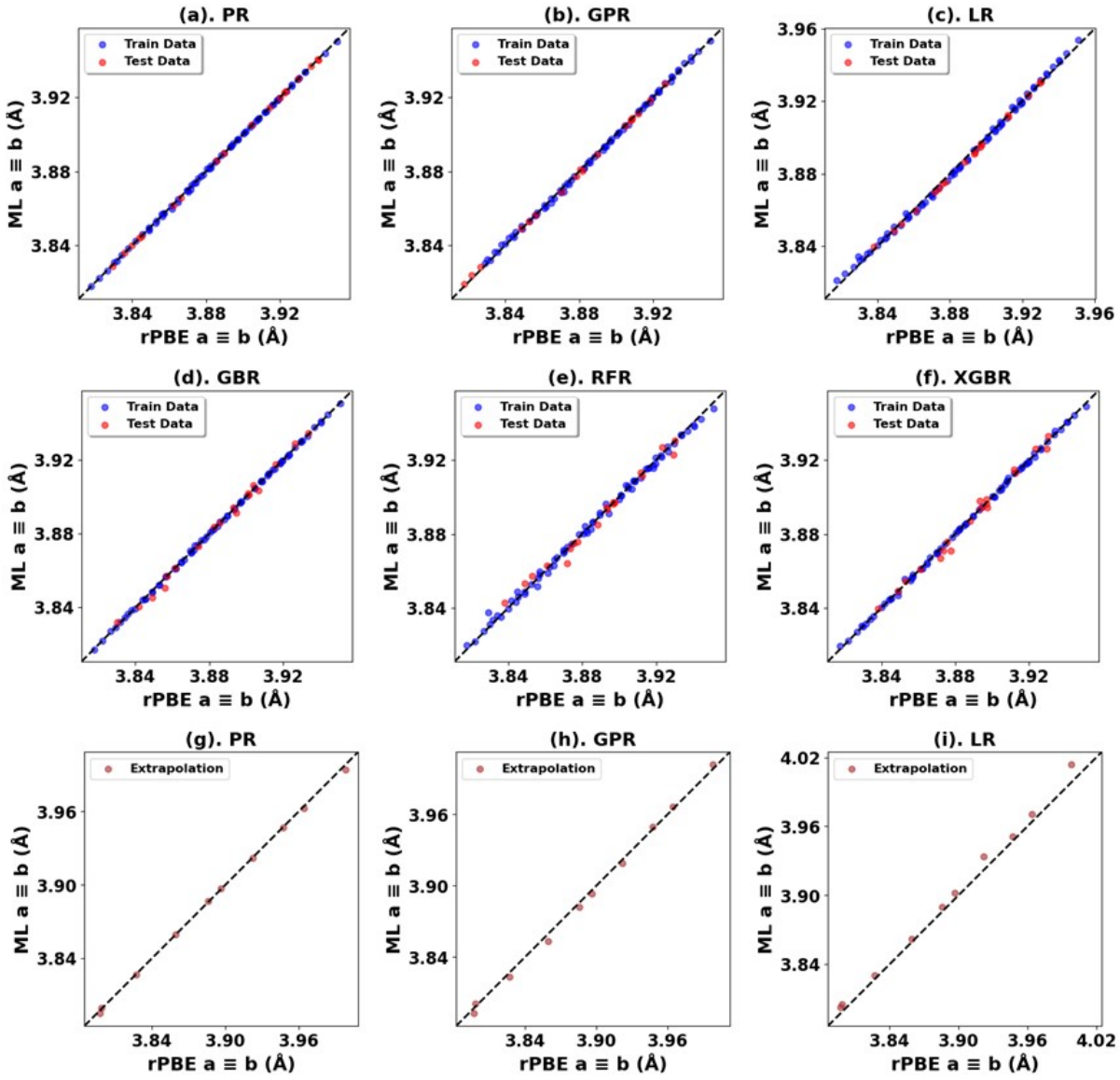

Figure S21. (a) - (f) Performance of models for rPBE lattice parameter (a = b) prediction of anatase TiO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S7. Comparative performance of models for rPBE lattice constant (a = b) prediction in anatase TiO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Anatase TiO_2	*PR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	GPR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	LR	0.00	0.00	0.00	1.00	0.00	0.01	0.01	0.99
	GBR	0.00	0.00	0.00	0.99	0.00	0.02	0.02	0.89
	XGBR	0.00	0.00	0.00	0.98	0.00	0.02	0.02	0.88

	RFR	0.00	0.00	0.00	0.98	0.00	0.02	0.02	0.87

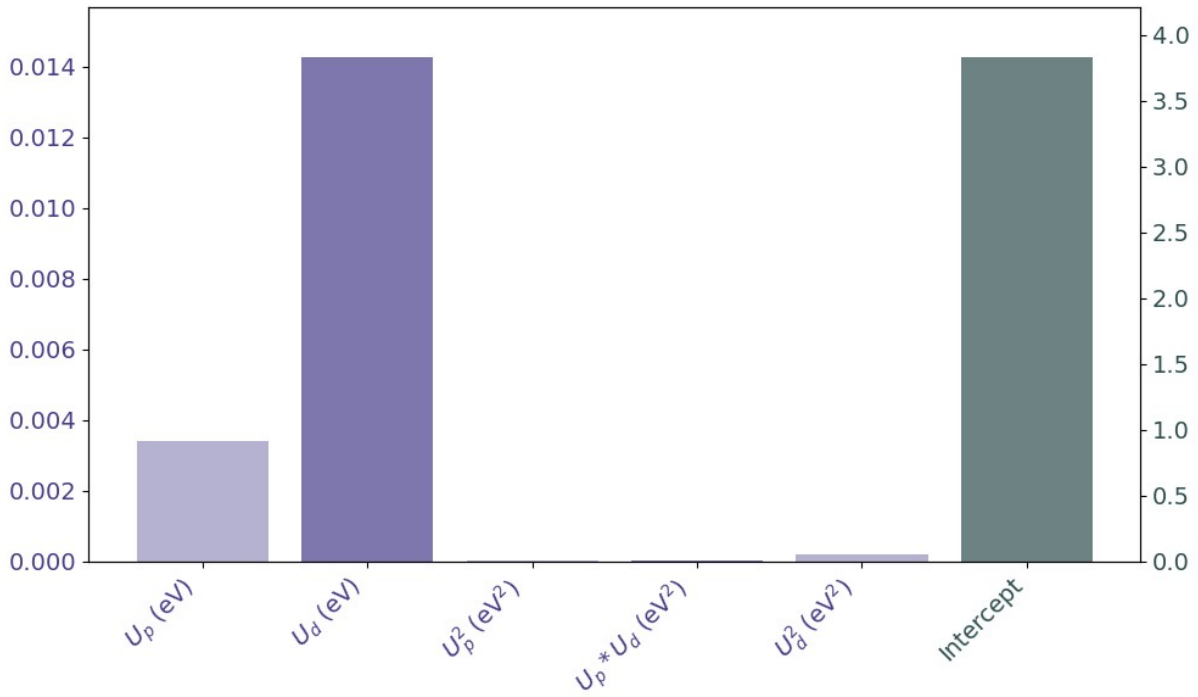

Figure S22. Feature importance of the PR model for predicting the rPBE lattice constant (a = b) of anatase TiO_2. Lighter shades indicate features with negative contributions.

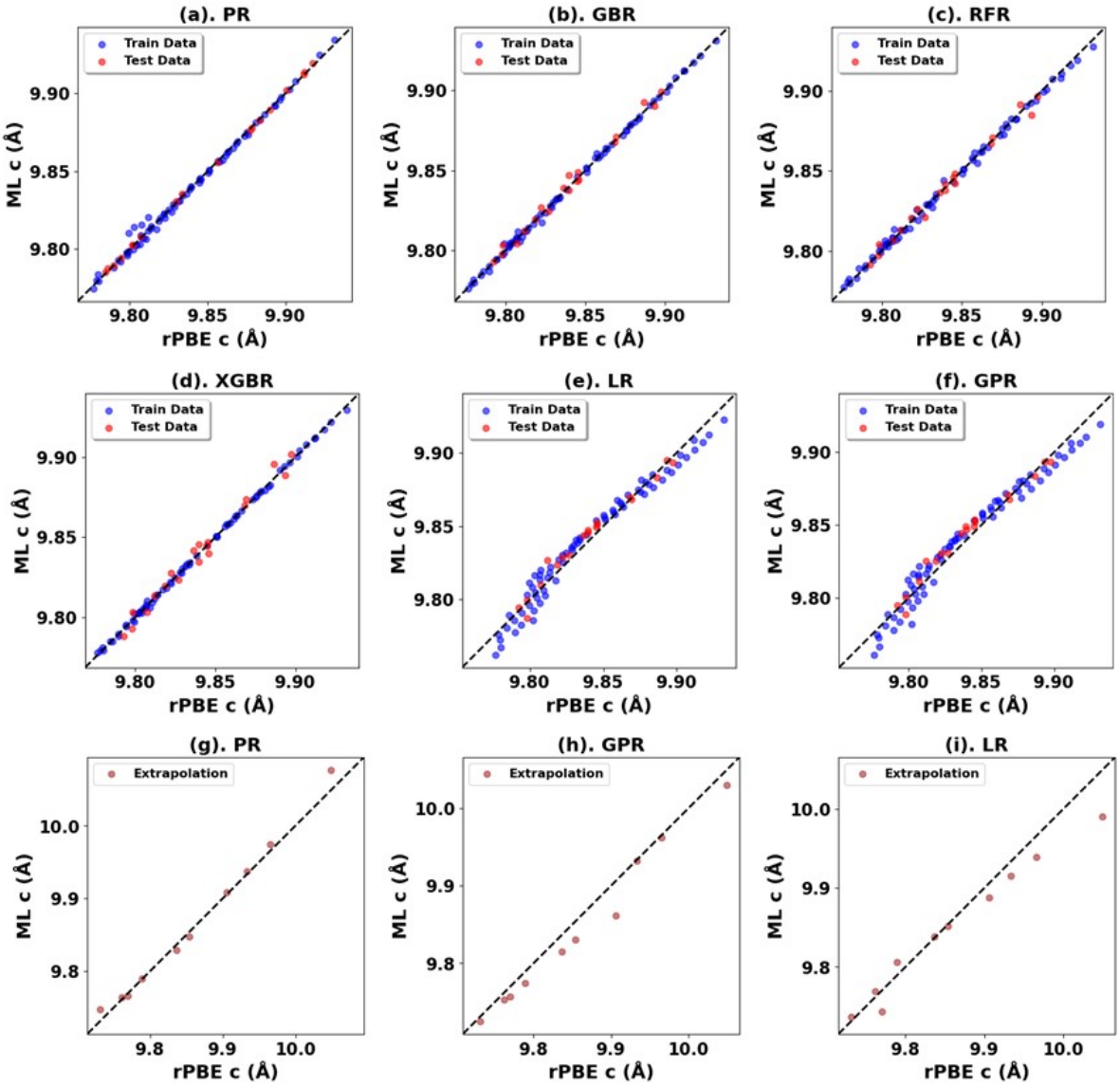

Figure S23. (a) - (f) Performance of models for rPBE lattice parameter (c) prediction of anatase TiO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S8. Comparative performance of models for rPBE lattice constant (c) prediction in anatase TiO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Anatase TiO_2	*PR	0.00	0.00	0.00	0.99	0.00	0.01	0.01	0.99
	GPR	0.00	0.01	0.01	0.95	0.00	0.02	0.02	0.96
	LR	0.00	0.01	0.01	0.96	0.00	0.02	0.02	0.94
	GBR	0.00	0.00	0.00	0.99	0.00	0.05	0.04	0.77
	XGBR	0.00	0.01	0.00	0.98	0.00	0.05	0.04	0.76

	RFR	0.00	0.01	0.00	0.98	0.00	0.05	0.04	0.75

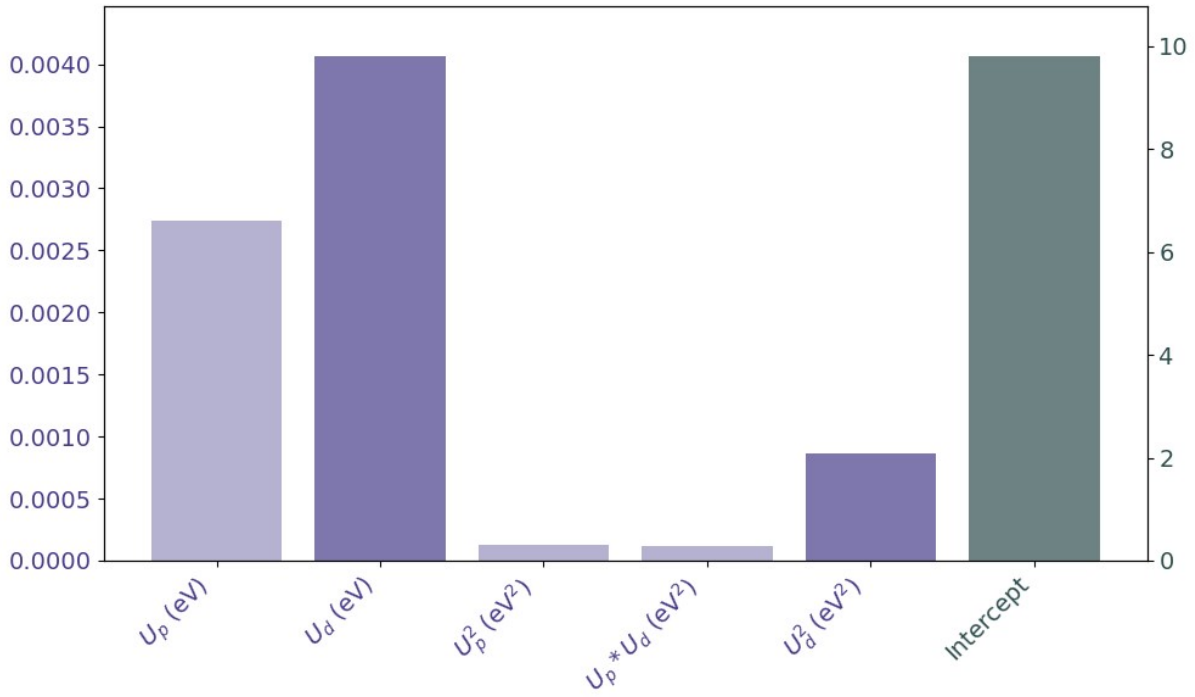

Figure S24. Feature importance of the PR model for predicting the rPBE lattice constant (c) of anatase TiO_2. Lighter shades indicate features with negative contributions.

Table S9. Influence of U_d and U_p on anatase TiO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)	% Deviation in a = b	% Deviation in c	% Deviation in E_g	% Deviation in c/a
0	0	3.8292	9.8019	2.486	1.16	3.05	-22.31	1.86
2	0	3.8558	9.8173	2.664	1.87	3.21	-16.75	1.32
2	2	3.8489	9.8104	2.711	1.69	3.14	-15.28	1.43
2	3	3.8454	9.8065	2.735	1.59	3.10	-14.53	1.48
2	4	3.8417	9.8024	2.761	1.50	3.06	-13.72	1.54
2	5	3.8380	9.7983	2.787	1.40	3.01	-12.91	1.59
2	6	3.8341	9.7940	2.815	1.29	2.97	-12.03	1.65
2	7	3.8302	9.7897	2.843	1.19	2.92	-11.16	1.71
2	8	3.8267	9.7797	2.871	1.10	2.82	-10.28	1.70
2	9	3.8220	9.7802	2.904	0.97	2.82	-9.25	1.83
2	10	3.8176	9.7764	2.936	0.86	2.78	-8.25	1.91
3	0	3.8718	9.8118	2.757	2.29	3.15	-13.84	0.84
3	2	3.8648	9.8029	2.806	2.11	3.06	-12.31	0.94
3	3	3.8614	9.7994	2.832	2.02	3.02	-11.50	0.99
3	4	3.8563	9.8091	2.864	1.88	3.13	-10.50	1.22
3	5	3.8526	9.8048	2.892	1.78	3.08	-9.63	1.27

3	6	3.8489	9.7994	2.920	1.69	3.02	-8.75	1.32
3	7	3.8440	9.7944	2.954	1.56	2.97	-7.69	1.39
3	8	3.8400	9.7895	2.985	1.45	2.92	-6.72	1.45
3	9	3.8359	9.7843	3.017	1.34	2.86	-5.72	1.50
3	10	3.8317	9.7784	3.051	1.23	2.80	-4.66	1.55
4	0	3.8826	9.8314	2.874	2.57	3.36	-10.19	0.77
4	2	3.8756	9.8268	2.926	2.39	3.31	-8.56	0.90
4	3	3.8721	9.8225	2.953	2.30	3.27	-7.72	0.95
4	4	3.8703	9.8075	2.975	2.25	3.11	-7.03	0.84
4	5	3.8648	9.8120	3.010	2.11	3.16	-5.94	1.03
4	6	3.8610	9.8074	3.041	2.01	3.11	-4.97	1.08
4	7	3.8571	9.8038	3.073	1.90	3.07	-3.97	1.15
4	8	3.8531	9.7978	3.106	1.80	3.01	-2.94	1.19
4	9	3.8490	9.7925	3.140	1.69	2.95	-1.88	1.24
4	10	3.8449	9.7858	3.176	1.58	2.88	-0.75	1.28
5	0	3.8945	9.8449	2.992	2.89	3.50	-6.50	0.59
5	2	3.8882	9.8364	3.045	2.72	3.41	-4.84	0.67
5	3	3.8847	9.8321	3.073	2.63	3.37	-3.97	0.72
5	4	3.8805	9.8286	3.105	2.52	3.33	-2.97	0.79
5	5	3.8774	9.8222	3.135	2.44	3.26	-2.03	0.81
5	6	3.8736	9.8186	3.167	2.34	3.22	-1.03	0.87
5	7	3.8698	9.8134	3.201	2.24	3.17	0.03	0.91
5	8	3.8664	9.8068	3.234	2.15	3.10	1.06	0.94
5	9	3.8622	9.8018	3.271	2.04	3.05	2.22	0.99
5	10	3.8569	9.7983	3.312	1.90	3.01	3.50	1.09
6	0	3.9069	9.8595	3.114	3.22	3.65	-2.69	0.42
6	2	3.9002	9.8504	3.171	3.04	3.56	-0.91	0.50
6	3	3.8968	9.8457	3.201	2.95	3.51	0.03	0.54
6	4	3.8933	9.8394	3.231	2.86	3.44	0.97	0.57
6	5	3.8897	9.8337	3.263	2.76	3.38	1.97	0.60
6	6	3.8858	9.8295	3.299	2.66	3.34	3.09	0.66
6	7	3.8824	9.8248	3.333	2.57	3.29	4.16	0.70
6	8	3.8785	9.8194	3.370	2.47	3.23	5.31	0.75
6	9	3.8743	9.8140	3.409	2.36	3.18	6.53	0.80
6	10	3.8699	9.8069	3.450	2.24	3.10	7.81	0.84
7	0	3.9184	9.8759	3.243	3.52	3.83	1.34	0.30
7	2	3.9117	9.8664	3.303	3.34	3.73	3.22	0.37
7	3	3.9083	9.8615	3.335	3.25	3.68	4.22	0.41
7	4	3.9048	9.8562	3.367	3.16	3.62	5.22	0.44
7	5	3.9014	9.8508	3.401	3.07	3.56	6.28	0.48
7	6	3.8975	9.8454	3.437	2.97	3.51	7.41	0.52
7	7	3.8937	9.8396	3.474	2.87	3.45	8.56	0.56
7	8	3.8898	9.8340	3.513	2.76	3.39	9.78	0.60
7	9	3.8857	9.8280	3.554	2.66	3.32	11.06	0.65
7	10	3.8816	9.8219	3.597	2.55	3.26	12.41	0.69
8	0	3.9295	9.8933	3.378	3.82	4.01	5.56	0.19

8	2	3.9232	9.8835	3.440	3.65	3.91	7.50	0.25
8	3	3.9197	9.8786	3.473	3.56	3.86	8.53	0.29
8	4	3.9162	9.8736	3.508	3.46	3.80	9.62	0.33
8	5	3.9125	9.8682	3.544	3.37	3.75	10.75	0.37
8	6	3.9087	9.8627	3.581	3.26	3.69	11.91	0.41
8	7	3.9049	9.8569	3.621	3.16	3.63	13.16	0.45
8	8	3.9010	9.8511	3.662	3.06	3.57	14.44	0.49
8	9	3.8970	9.8449	3.705	2.96	3.50	15.78	0.53
8	10	3.8929	9.8384	3.750	2.85	3.43	17.19	0.57
9	0	3.9407	9.9117	3.516	4.11	4.20	9.87	0.09
9	2	3.9338	9.9026	3.583	3.93	4.11	11.97	0.17
9	3	3.9304	9.8974	3.618	3.84	4.05	13.06	0.21
9	4	3.9264	9.8930	3.656	3.73	4.01	14.25	0.27
9	5	3.9234	9.8865	3.692	3.65	3.94	15.38	0.28
9	6	3.9197	9.8810	3.731	3.55	3.88	16.59	0.32
9	7	3.9157	9.8754	3.772	3.45	3.82	17.88	0.36
9	8	3.9119	9.8693	3.815	3.35	3.76	19.22	0.40
9	9	3.9079	9.8634	3.860	3.24	3.70	20.63	0.44
9	10	3.9037	9.8580	3.908	3.13	3.64	22.13	0.49
10	0	3.9510	9.9319	3.661	4.38	4.42	14.41	0.03
10	2	3.9444	9.9221	3.729	4.21	4.31	16.53	0.10
10	3	3.9405	9.9177	3.768	4.10	4.27	17.75	0.16
10	4	3.9370	9.9123	3.805	4.01	4.21	18.91	0.19
10	5	3.9335	9.9066	3.845	3.92	4.15	20.16	0.22
10	6	3.9298	9.9009	3.885	3.82	4.09	21.41	0.26
10	7	3.9264	9.8962	3.927	3.73	4.04	22.72	0.30
10	8	3.9225	9.8903	3.972	3.63	3.98	24.13	0.34
10	9	3.9185	9.8840	4.019	3.52	3.91	25.59	0.38
10	10	3.9145	9.8776	4.068	3.42	3.85	27.13	0.41

Table S10. Influence of U_d and U_p on anatase TiO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)
1	11	3.7984	9.7697	2.860
2	15	3.7972	9.7312	3.108
4	14	3.8269	9.7614	3.338

7	15	3.8594	9.7891	3.845
9	14	3.8859	9.8363	4.121
10	14	3.8965	9.8537	4.290
11	4	3.9473	9.9329	3.958
12	2	3.9642	9.9652	4.032
13	15	3.9221	9.9055	4.870
15	0	3.9985	10.0493	4.397

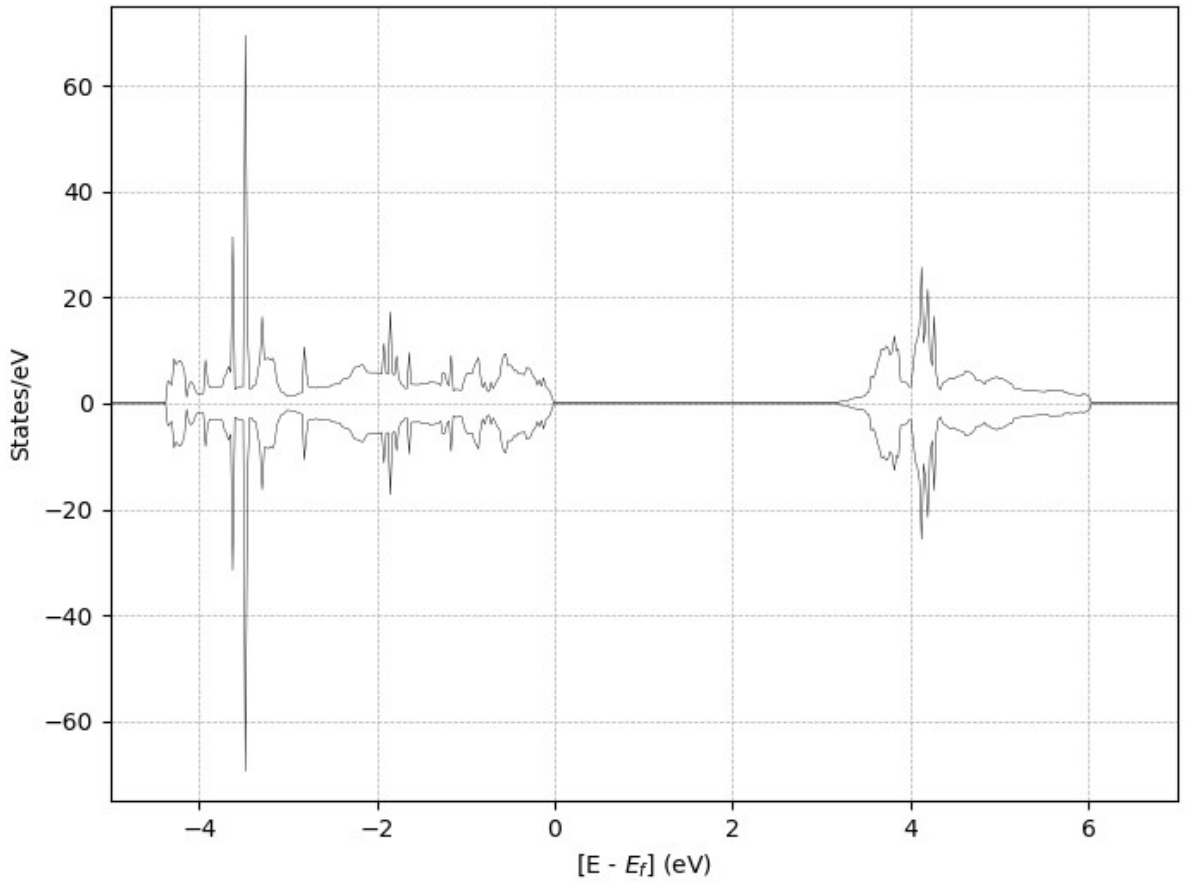

Figure S25. DOS for anatase TiO_2 with rPBE functional: U_p = 3 eV, U_d = 6 eV

PBE:

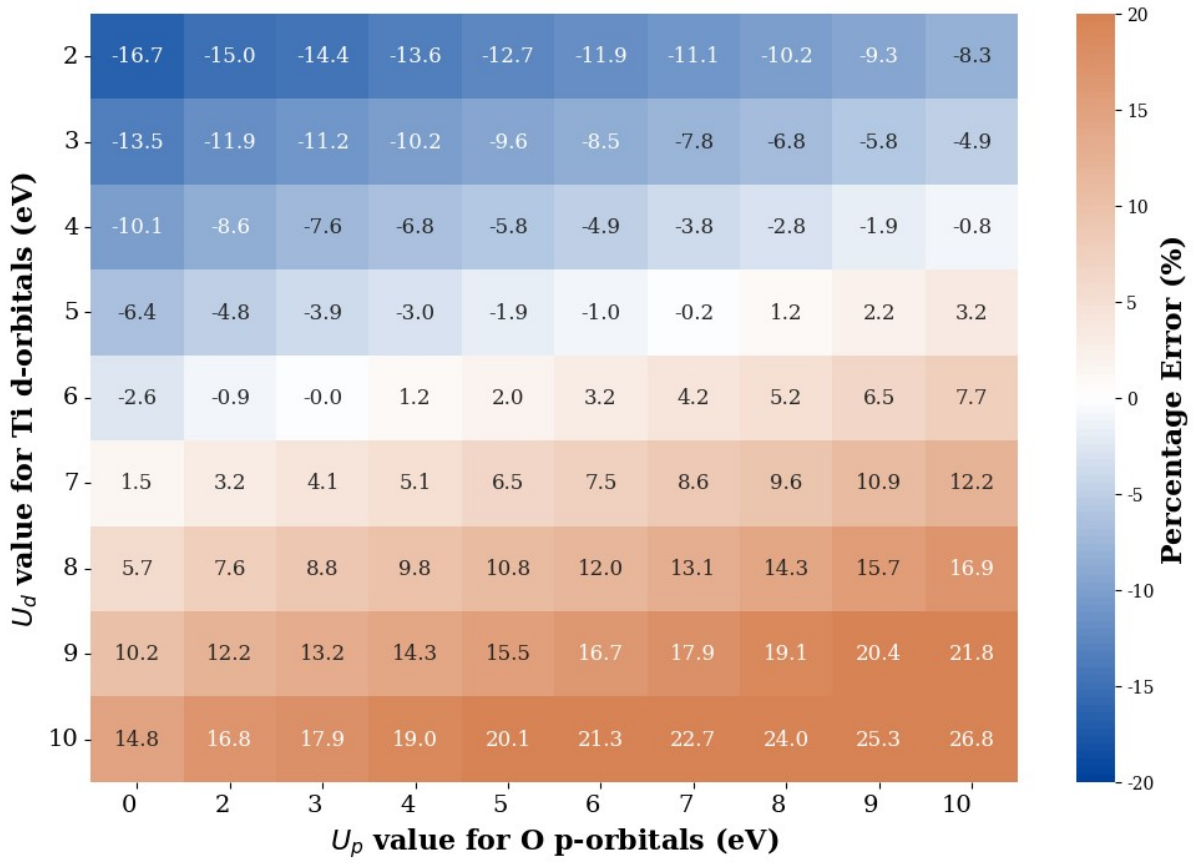

Figure S26. Heatmap of PBE predicted band gap for anatase TiO_2 as a function of the U_d and U_p parameters.

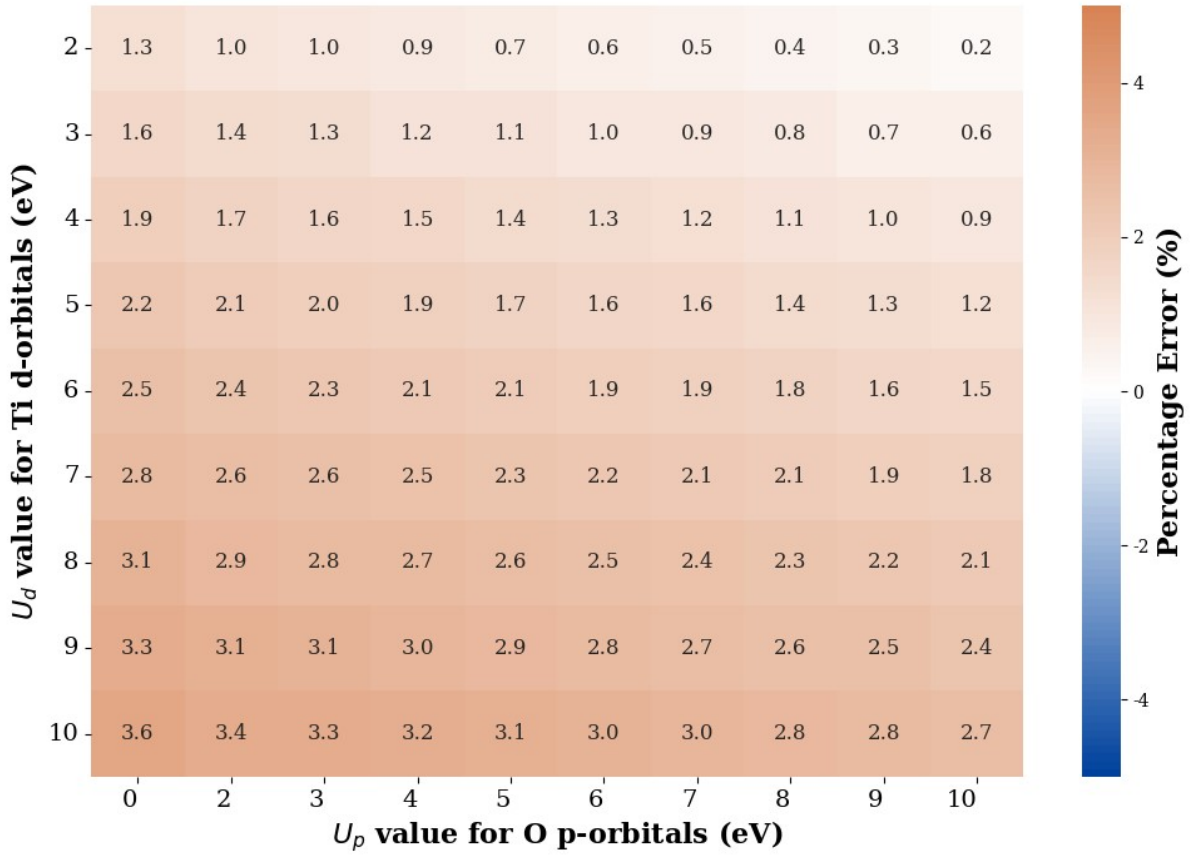

Figure S27. Heatmap of PBE predicted lattice constant (a = b) for anatase TiO_2 as a function of the U_d and U_p parameters.

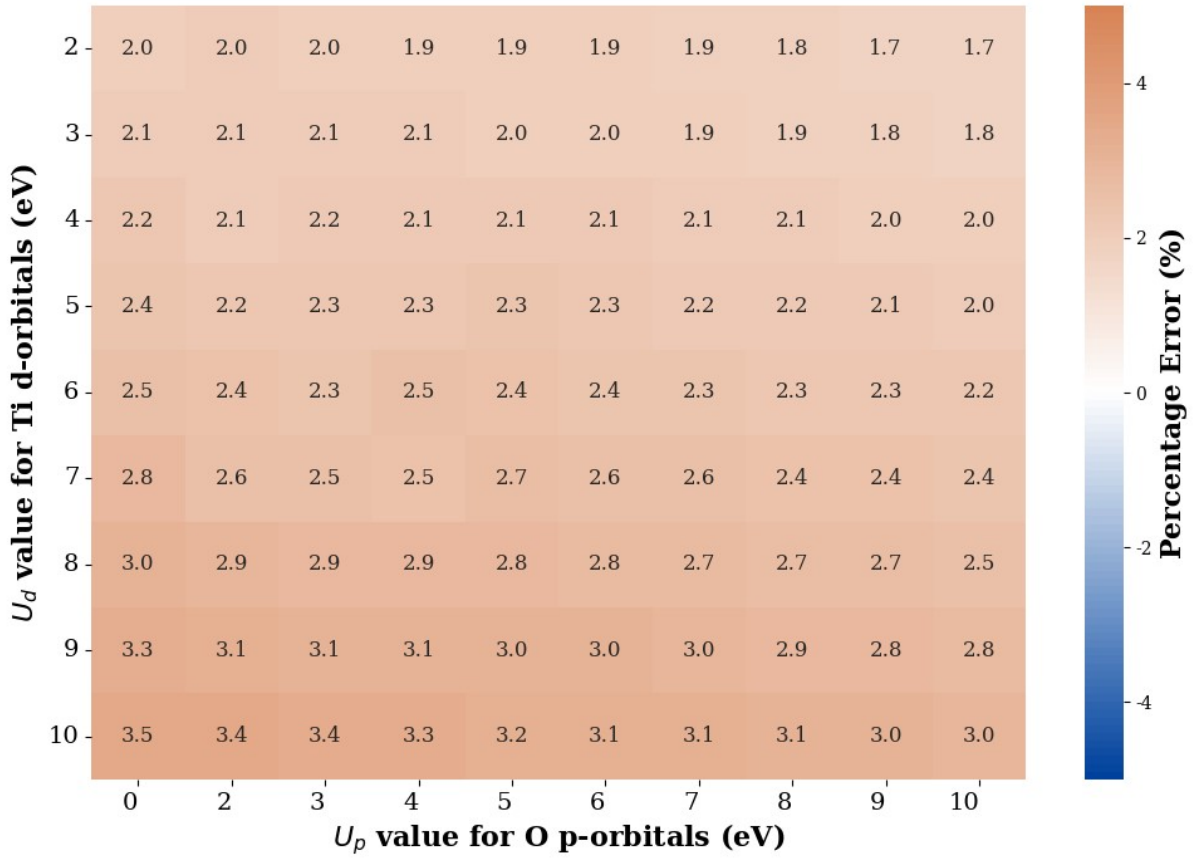

Figure S28. Heatmap of PBE predicted lattice constant (c) for anatase TiO_2 as a function of the U_d and U_p parameters.

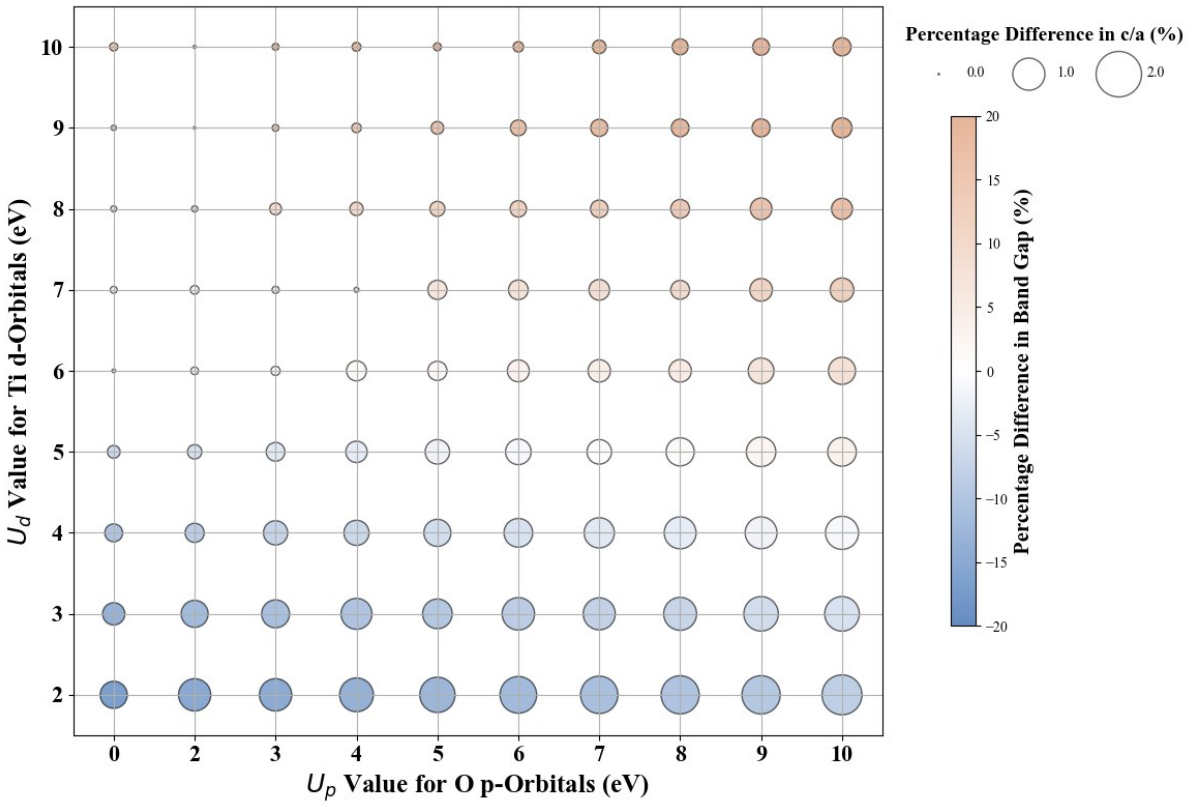

Figure S29. Effect of Hubbard U values on PBE band gap and lattice parameters of anatase TiO_2.

Table S11. Influence of U_d and U_p on anatase TiO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)	% Deviation in a = b	% Deviation in c	% Deviation in E_g	% Deviation in c/a
0	0	3.8044	9.7024	2.496	0.51	1.96	-22.00	1.49
2	0	3.8334	9.7019	2.666	1.26	1.96	-16.69	0.71
2	2	3.8246	9.7082	2.719	1.03	2.02	-15.03	1.01
2	3	3.8223	9.7031	2.738	0.97	1.97	-14.44	1.02
2	4	3.8180	9.7010	2.765	0.86	1.95	-13.59	1.11
2	5	3.8132	9.6983	2.793	0.74	1.92	-12.72	1.21
2	6	3.8097	9.6989	2.819	0.64	1.93	-11.91	1.31
2	7	3.8059	9.6939	2.845	0.55	1.88	-11.09	1.36
2	8	3.8015	9.6882	2.875	0.43	1.82	-10.16	1.41
2	9	3.7982	9.6807	2.901	0.34	1.74	-9.34	1.42
2	10	3.7933	9.6796	2.933	0.21	1.73	-8.34	1.55
3	0	3.8464	9.7122	2.768	1.59	2.06	-13.50	0.48
3	2	3.8391	9.7158	2.818	1.41	2.10	-11.94	0.71
3	3	3.8357	9.7117	2.842	1.32	2.06	-11.19	0.76
3	4	3.8306	9.7157	2.874	1.19	2.10	-10.19	0.93
3	5	3.8286	9.7031	2.894	1.14	1.97	-9.56	0.85
3	6	3.8232	9.7056	2.927	1.00	2.00	-8.53	1.02
3	7	3.8204	9.6961	2.952	0.92	1.90	-7.75	1.00
3	8	3.8165	9.6917	2.982	0.82	1.86	-6.81	1.05
3	9	3.8116	9.6890	3.015	0.69	1.83	-5.78	1.16
3	10	3.8085	9.6817	3.043	0.61	1.75	-4.91	1.16
4	0	3.8585	9.7266	2.878	1.90	2.21	-10.06	0.31
4	2	3.8523	9.7151	2.926	1.74	2.09	-8.56	0.36
4	3	3.8477	9.7241	2.957	1.63	2.18	-7.59	0.57
4	4	3.8446	9.7204	2.983	1.55	2.15	-6.78	0.61
4	5	3.8399	9.7180	3.014	1.43	2.12	-5.81	0.71
4	6	3.8363	9.7175	3.044	1.33	2.12	-4.88	0.80
4	7	3.8312	9.7129	3.077	1.20	2.07	-3.84	0.89
4	8	3.8275	9.7135	3.109	1.11	2.08	-2.84	0.99
4	9	3.8241	9.7044	3.139	1.02	1.98	-1.91	0.98
4	10	3.8199	9.7013	3.173	0.91	1.95	-0.84	1.06
5	0	3.8703	9.7414	2.995	2.20	2.36	-6.41	0.16
5	2	3.8643	9.7304	3.045	2.05	2.25	-4.84	0.20
5	3	3.8607	9.7349	3.075	1.96	2.29	-3.91	0.34
5	4	3.8569	9.7353	3.105	1.86	2.29	-2.97	0.44
5	5	3.8525	9.7373	3.138	1.75	2.32	-1.94	0.58

5	6	3.8485	9.7325	3.169	1.65	2.27	-0.97	0.63
5	7	3.8459	9.7209	3.195	1.58	2.15	-0.16	0.58
5	8	3.8398	9.7233	3.237	1.43	2.18	1.16	0.77
5	9	3.8359	9.7207	3.272	1.32	2.15	2.25	0.84
5	10	3.8326	9.7077	3.303	1.24	2.02	3.22	0.79
6	0	3.8823	9.7572	3.118	2.50	2.51	-2.56	0.01
6	2	3.8762	9.7463	3.170	2.35	2.41	-0.94	0.06
6	3	3.8728	9.7401	3.199	2.26	2.34	-0.03	0.08
6	4	3.8679	9.7576	3.237	2.14	2.52	1.16	0.39
6	5	3.8650	9.7473	3.264	2.07	2.42	2.00	0.36
6	6	3.8602	9.7455	3.301	1.94	2.40	3.16	0.46
6	7	3.8565	9.7385	3.333	1.85	2.33	4.16	0.49
6	8	3.8534	9.7310	3.365	1.77	2.25	5.16	0.49
6	9	3.8482	9.7328	3.408	1.64	2.27	6.50	0.64
6	10	3.8437	9.7280	3.446	1.53	2.22	7.69	0.71
7	0	3.8935	9.7886	3.249	2.78	2.83	1.53	0.05
7	2	3.8878	9.7626	3.301	2.64	2.57	3.16	-0.07
7	3	3.8845	9.7569	3.331	2.56	2.51	4.09	-0.05
7	4	3.8812	9.7509	3.362	2.47	2.45	5.06	-0.02
7	5	3.8747	9.7717	3.408	2.31	2.66	6.50	0.36
7	6	3.8714	9.7652	3.441	2.23	2.59	7.53	0.38
7	7	3.8682	9.7609	3.475	2.15	2.55	8.59	0.41
7	8	3.8652	9.7467	3.507	2.07	2.41	9.59	0.35
7	9	3.8599	9.7480	3.550	1.94	2.42	10.94	0.50
7	10	3.8563	9.7435	3.590	1.84	2.38	12.19	0.55
8	0	3.9044	9.8081	3.384	3.05	3.02	5.75	-0.04
8	2	3.8981	9.7993	3.444	2.90	2.93	7.62	0.04
8	3	3.8928	9.7958	3.482	2.77	2.90	8.81	0.14
8	4	3.8902	9.7930	3.513	2.70	2.87	9.78	0.17
8	5	3.8865	9.7880	3.547	2.61	2.82	10.84	0.22
8	6	3.8828	9.7830	3.583	2.52	2.77	11.97	0.26
8	7	3.8794	9.7781	3.619	2.43	2.72	13.09	0.30
8	8	3.8757	9.7730	3.658	2.34	2.67	14.31	0.34
8	9	3.8707	9.7712	3.702	2.21	2.65	15.69	0.46
8	10	3.8674	9.7604	3.742	2.13	2.55	16.94	0.43
9	0	3.9146	9.8345	3.528	3.31	3.28	10.25	-0.03
9	2	3.9076	9.8203	3.590	3.13	3.14	12.19	0.01
9	3	3.9043	9.8157	3.623	3.05	3.10	13.22	0.04
9	4	3.9008	9.8113	3.658	2.97	3.05	14.31	0.09
9	5	3.8966	9.8073	3.696	2.86	3.01	15.50	0.16
9	6	3.8930	9.8067	3.735	2.77	3.01	16.72	0.24
9	7	3.8892	9.8016	3.774	2.68	2.96	17.94	0.29
9	8	3.8859	9.7951	3.812	2.59	2.89	19.13	0.31
9	9	3.8826	9.7878	3.852	2.51	2.82	20.38	0.32
9	10	3.8780	9.7832	3.898	2.39	2.77	21.81	0.39
10	0	3.9250	9.8568	3.672	3.56	3.50	14.75	-0.07

10	2	3.9183	9.8474	3.738	3.40	3.41	16.81	0.01
10	3	3.9148	9.8422	3.772	3.31	3.36	17.88	0.05
10	4	3.9113	9.8365	3.808	3.23	3.30	19.00	0.08
10	5	3.9078	9.8262	3.844	3.14	3.20	20.13	0.06
10	6	3.9041	9.8212	3.883	3.05	3.15	21.34	0.11
10	7	3.9002	9.8187	3.925	2.95	3.13	22.66	0.18
10	8	3.8959	9.8144	3.969	2.84	3.08	24.03	0.25
10	9	3.8927	9.8092	4.011	2.76	3.03	25.34	0.28
10	10	3.8886	9.8032	4.058	2.66	2.97	26.81	0.32

Table S12. Influence of U_d and U_p on anatase TiO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b (Å)	c (Å)	E_g (eV)
1	11	3.7751	9.6747	2.854
2	15	3.7710	9.6548	3.096
4	14	3.8025	9.6718	3.319
7	15	3.8334	9.7126	3.821
9	14	3.8608	9.7508	4.095
10	14	3.8711	9.7735	4.265
11	4	3.9214	9.8581	3.961
12	2	3.9378	9.8935	4.041
13	15	3.8975	9.8310	4.837
15	0	3.9724	9.9767	4.427

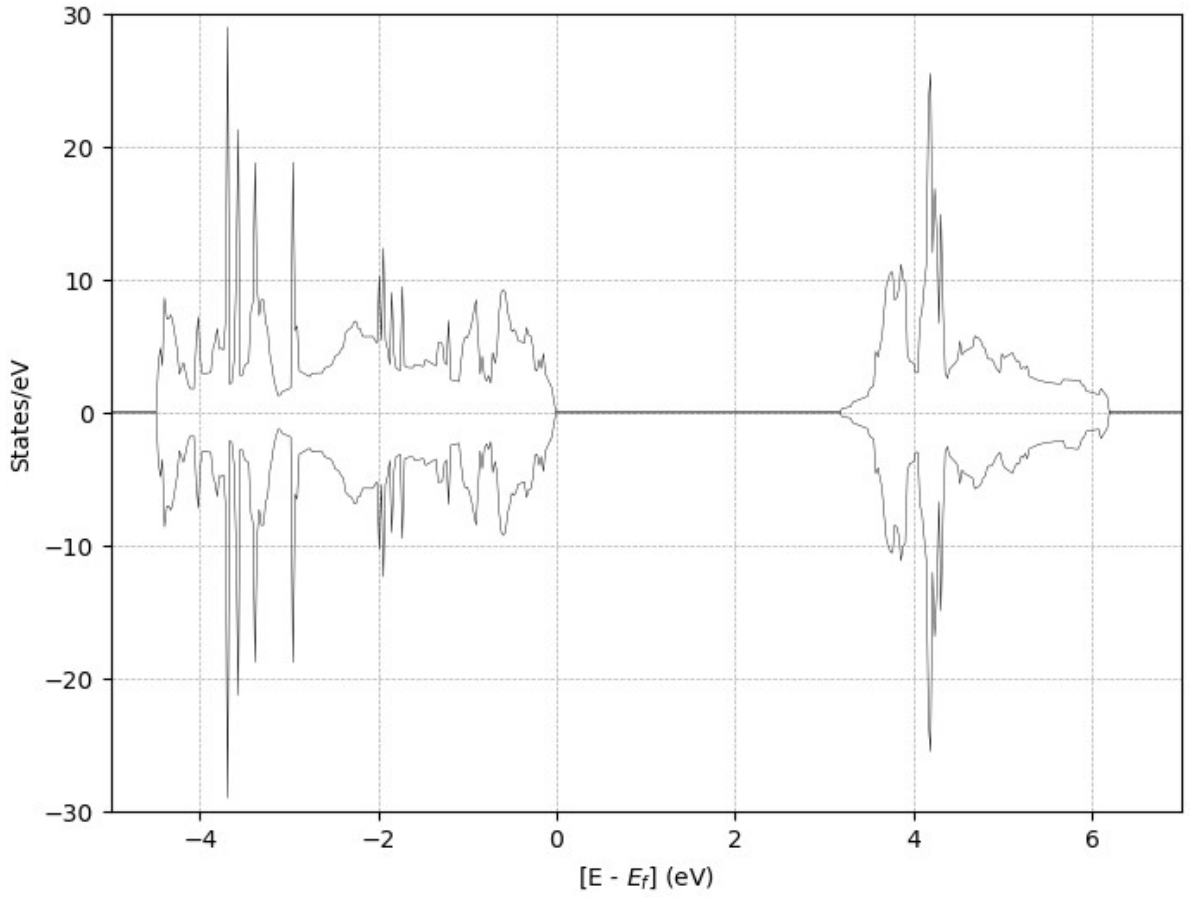

Figure S30. DOS for anatase TiO_2 with PBE functional: U_p = 3 eV, U_d = 6 eV

ZnO:

rPBE:

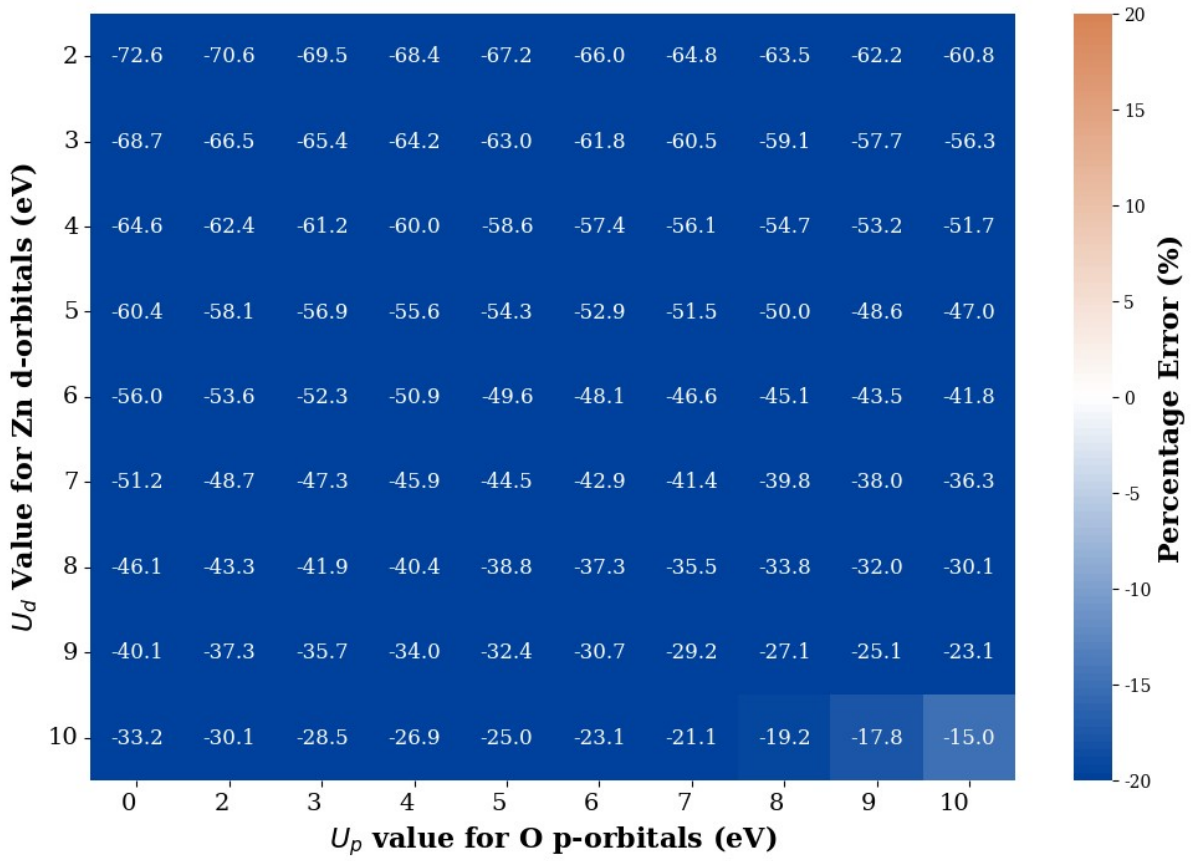

Figure S31. Heatmap of rPBE predicted band gap for cubic ZnO as a function of the U_d and U_p parameters.

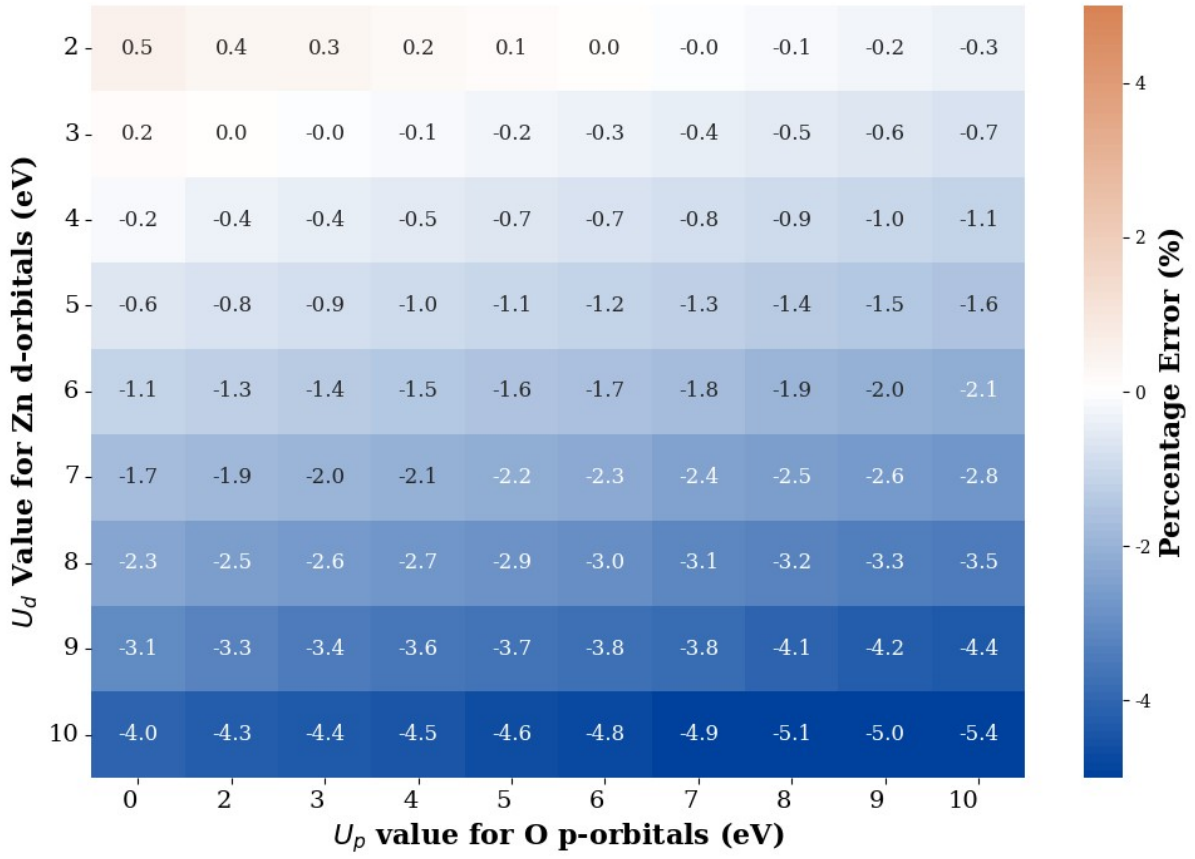

Figure S32. Heatmap of rPBE predicted lattice constant (a = b = c) for cubic ZnO as a function of the U_d and U_p parameters.

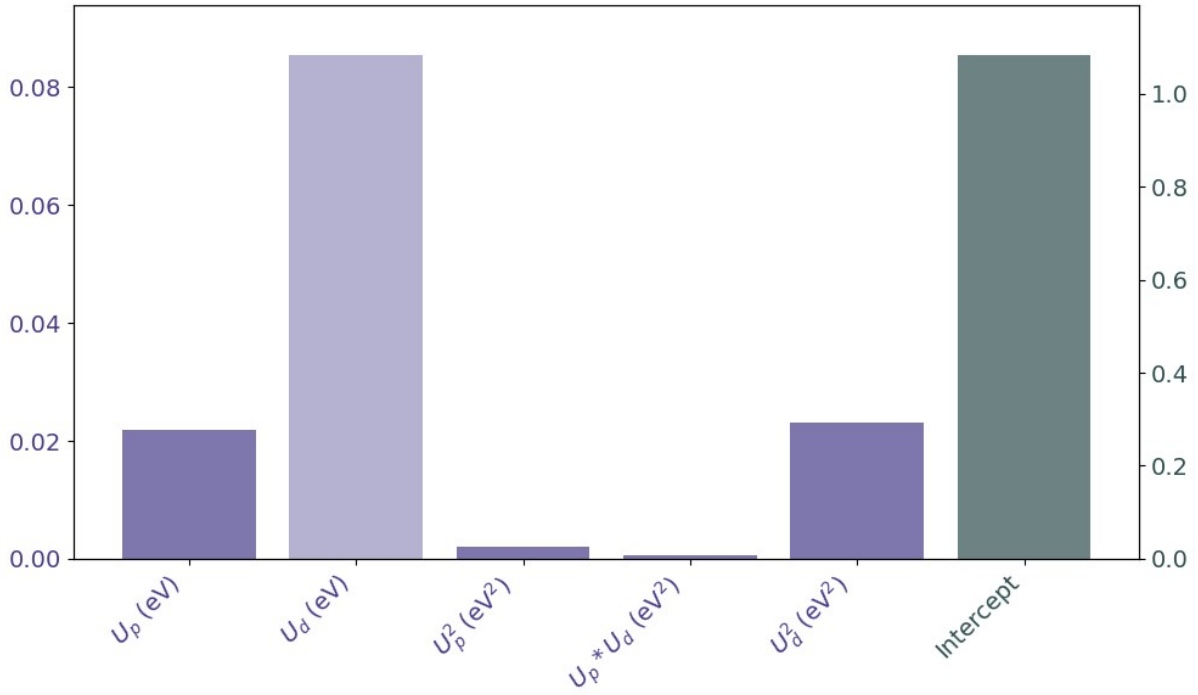

Figure S33. Feature importance of the PR model for predicting the rPBE band gap of c-ZnO. Lighter shades indicate features with negative contributions.

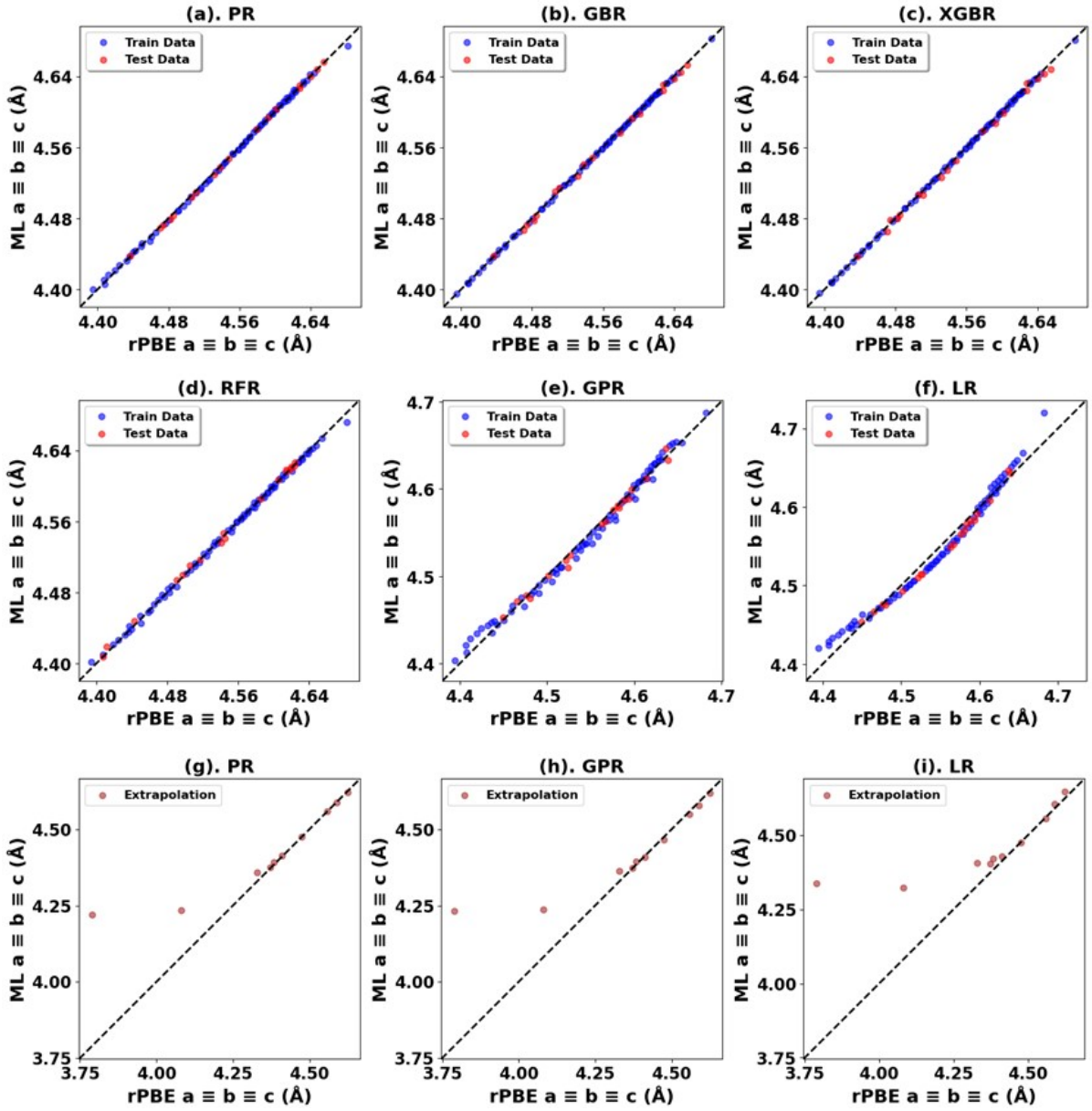

Figure S34. (a) - (f) Performance of models for rPBE lattice parameter (a = b = c) prediction of c-ZnO using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S13. Comparative performance of models for rPBE lattice constant (a = b = c) prediction in cubic ZnO.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Cubic ZnO	*PR	0.00	0.00	0.00	1.00	0.02	0.15	0.06	0.64
	GPR	0.00	0.00	0.00	1.00	0.02	0.15	0.07	0.62
	LR	0.00	0.01	0.01	0.97	0.04	0.19	0.10	0.37

	RFR	0.00	0.01	0.00	0.99	0.06	0.24	0.13	0.05
	GBR	0.00	0.00	0.00	1.00	0.06	0.24	0.13	0.05
	XGBR	0.00	0.01	0.00	0.99	0.06	0.24	0.13	0.05

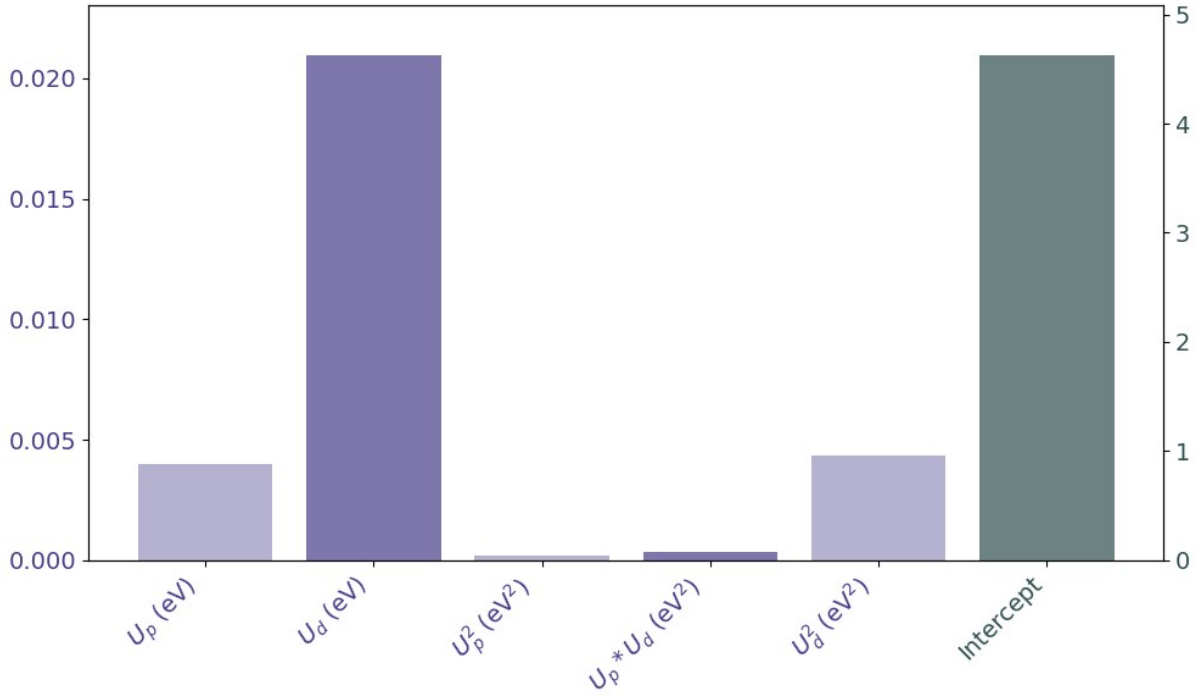

Figure S35. Feature importance of the PR model for predicting the rPBE lattice constant (a = b = c) of c-ZnO. Lighter shades indicate features with negative contributions.

Table S14. Influence of U_d and U_p on cubic ZnO DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	4.6823	0.658	1.13	-80.47
2	0	4.6549	0.923	0.54	-72.61
2	2	4.6479	0.992	0.39	-70.56
2	3	4.6441	1.029	0.30	-69.47
2	4	4.6402	1.066	0.22	-68.37
2	5	4.6361	1.105	0.13	-67.21
2	6	4.6320	1.145	0.04	-66.02
2	7	4.6277	1.187	-0.05	-64.78
2	8	4.6233	1.231	-0.15	-63.47
2	9	4.6190	1.275	-0.24	-62.17
2	10	4.6143	1.322	-0.34	-60.77
3	0	4.6390	1.056	0.20	-68.66
3	2	4.6316	1.128	0.04	-66.53
3	3	4.6278	1.166	-0.05	-65.40

3	4	4.6238	1.206	-0.13	-64.21
3	5	4.6196	1.246	-0.23	-63.03
3	6	4.6153	1.289	-0.32	-61.75
3	7	4.6110	1.332	-0.41	-60.47
3	8	4.6065	1.378	-0.51	-59.11
3	9	4.6019	1.424	-0.61	-57.74
3	10	4.5971	1.473	-0.71	-56.29
4	0	4.6211	1.192	-0.19	-64.63
4	2	4.6134	1.268	-0.36	-62.37
4	3	4.6095	1.307	-0.44	-61.22
4	4	4.6050	1.349	-0.54	-59.97
4	5	4.5995	1.394	-0.66	-58.64
4	6	4.5969	1.435	-0.71	-57.42
4	7	4.5924	1.481	-0.81	-56.05
4	8	4.5879	1.528	-0.91	-54.66
4	9	4.5831	1.577	-1.01	-53.20
4	10	4.5781	1.628	-1.12	-51.69
5	0	4.6013	1.333	-0.62	-60.45
5	2	4.5935	1.412	-0.79	-58.10
5	3	4.5894	1.454	-0.88	-56.85
5	4	4.5852	1.497	-0.97	-55.58
5	5	4.5809	1.541	-1.06	-54.27
5	6	4.5763	1.587	-1.16	-52.91
5	7	4.5716	1.635	-1.26	-51.48
5	8	4.5668	1.685	-1.37	-50.00
5	9	4.5634	1.733	-1.44	-48.58
5	10	4.5585	1.786	-1.54	-47.00
6	0	4.5790	1.482	-1.10	-56.02
6	2	4.5708	1.565	-1.28	-53.56
6	3	4.5666	1.609	-1.37	-52.26
6	4	4.5629	1.653	-1.45	-50.95
6	5	4.5585	1.699	-1.54	-49.58
6	6	4.5530	1.749	-1.66	-48.10
6	7	4.5482	1.799	-1.77	-46.62
6	8	4.5432	1.851	-1.87	-45.07
6	9	4.5381	1.905	-1.98	-43.47
6	10	4.5332	1.961	-2.09	-41.81
7	0	4.5520	1.645	-1.68	-51.19
7	2	4.5449	1.730	-1.84	-48.66
7	3	4.5407	1.776	-1.93	-47.30
7	4	4.5361	1.823	-2.03	-45.91
7	5	4.5314	1.872	-2.13	-44.45
7	6	4.5265	1.924	-2.23	-42.91
7	7	4.5214	1.976	-2.34	-41.36
7	8	4.5167	2.030	-2.45	-39.76
7	9	4.5108	2.089	-2.57	-38.01

7	10	4.5054	2.148	-2.69	-36.26
8	0	4.5246	1.818	-2.28	-46.05
8	2	4.5158	1.911	-2.47	-43.29
8	3	4.5111	1.959	-2.57	-41.87
8	4	4.5062	2.010	-2.67	-40.36
8	5	4.5017	2.061	-2.77	-38.84
8	6	4.4973	2.114	-2.87	-37.27
8	7	4.4902	2.174	-3.02	-35.49
8	8	4.4850	2.232	-3.13	-33.77
8	9	4.4803	2.290	-3.23	-32.05
8	10	4.4740	2.354	-3.37	-30.15
9	0	4.4909	2.017	-3.00	-40.15
9	2	4.4822	2.114	-3.19	-37.27
9	3	4.4763	2.168	-3.32	-35.67
9	4	4.4703	2.224	-3.45	-34.01
9	5	4.4654	2.279	-3.55	-32.37
9	6	4.4607	2.335	-3.66	-30.71
9	7	4.4586	2.386	-3.70	-29.20
9	8	4.4492	2.457	-3.90	-27.09
9	9	4.4425	2.524	-4.05	-25.10
9	10	4.4367	2.591	-4.17	-23.12
10	0	4.4503	2.250	-3.88	-33.23
10	2	4.4399	2.357	-4.11	-30.06
10	3	4.4362	2.409	-4.19	-28.52
10	4	4.4323	2.463	-4.27	-26.91
10	5	4.4244	2.529	-4.44	-24.96
10	6	4.4191	2.590	-4.55	-23.15
10	7	4.4118	2.659	-4.71	-21.10
10	8	4.4071	2.722	-4.81	-19.23
10	9	4.4077	2.771	-4.80	-17.77
10	10	4.3944	2.864	-5.09	-15.01

Table S15. Influence of U_d and U_p on cubic ZnO DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)
1	11	4.6242	1.220
2	15	4.5884	1.583
4	14	4.5585	1.849
7	15	4.4756	2.480
9	14	4.4114	2.885
10	14	4.3724	3.164
11	4	4.3840	2.757
12	2	4.3285	3.021
13	15	4.0808	5.194
15	0	3.7887	5.935

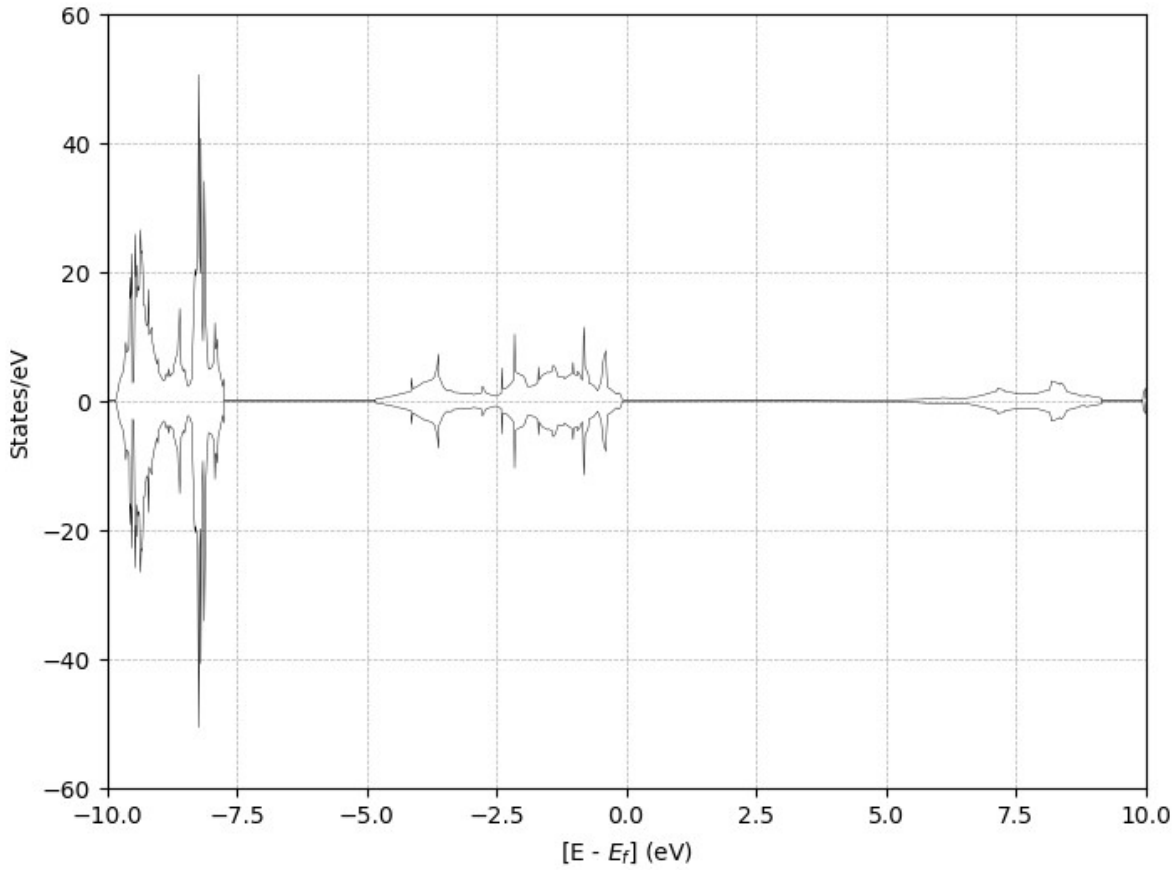

Figure S36. DOS for cubic ZnO with rPBE functional: U_p = 6 eV, U_d = 12 eV

PBE:

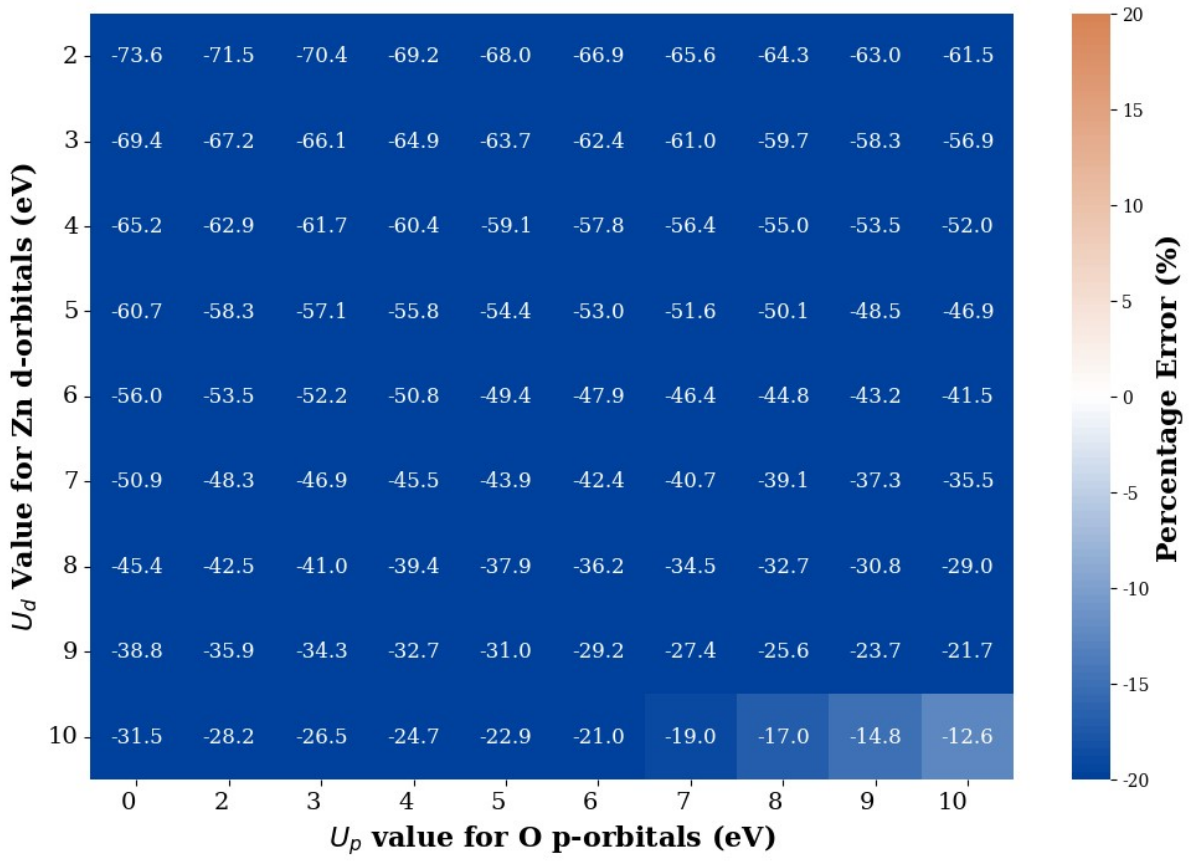

Figure S37. Heatmap of PBE predicted band gap for cubic ZnO as a function of the U_d and U_p parameters.

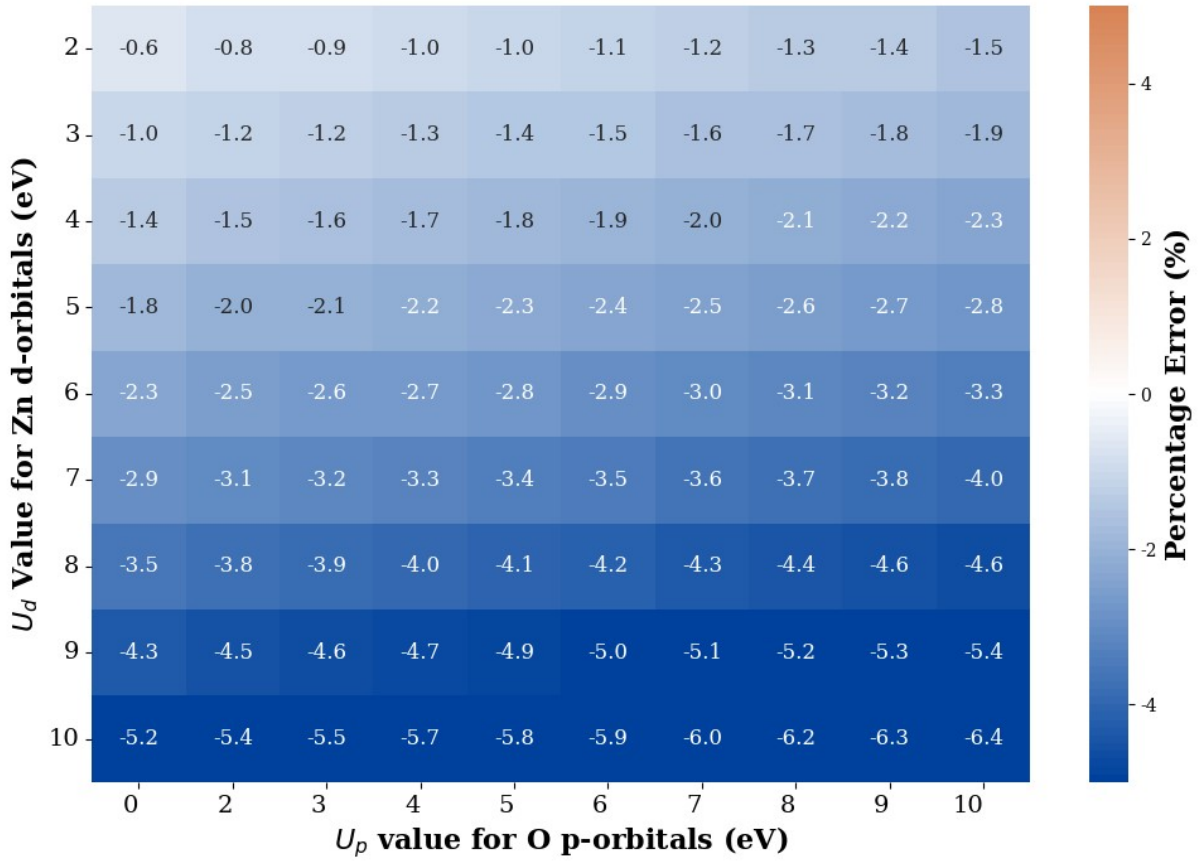

Figure S38. Heatmap of PBE predicted lattice constant (a = b = c) for cubic ZnO as a function of the U_d and U_p parameters.

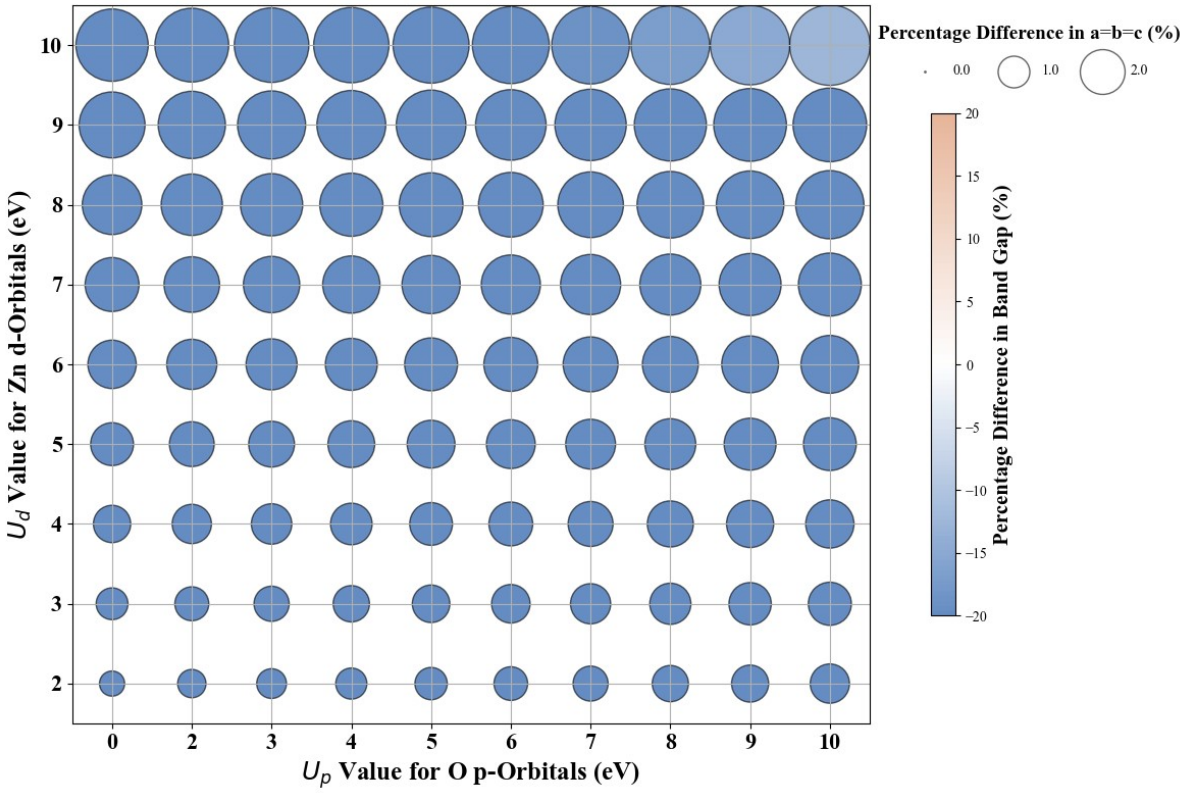

Figure S39. Effect of Hubbard U values on PBE band gap and lattice parameters of c-ZnO.

Table S16. Influence of U_d and U_p on cubic ZnO DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	4.6291	0.615	-0.02	-81.75
2	0	4.6007	0.891	-0.63	-73.56
2	2	4.5928	0.962	-0.80	-71.45
2	3	4.5890	0.999	-0.89	-70.36
2	4	4.5851	1.037	-0.97	-69.23
2	5	4.5816	1.077	-1.05	-68.04
2	6	4.5775	1.117	-1.13	-66.85
2	7	4.5732	1.160	-1.23	-65.58
2	8	4.5692	1.203	-1.31	-64.30
2	9	4.5664	1.246	-1.37	-63.03
2	10	4.5585	1.298	-1.54	-61.48
3	0	4.5831	1.032	-1.01	-69.38
3	2	4.5766	1.104	-1.15	-67.24
3	3	4.5728	1.143	-1.24	-66.08
3	4	4.5688	1.183	-1.32	-64.90
3	5	4.5647	1.224	-1.41	-63.68
3	6	4.5613	1.266	-1.48	-62.43
3	7	4.5552	1.313	-1.61	-61.04
3	8	4.5516	1.358	-1.69	-59.70
3	9	4.5470	1.405	-1.79	-58.31
3	10	4.5441	1.452	-1.86	-56.91
4	0	4.5655	1.174	-1.39	-65.16
4	2	4.5585	1.250	-1.54	-62.91
4	3	4.5541	1.291	-1.64	-61.69
4	4	4.5499	1.334	-1.73	-60.42
4	5	4.5454	1.377	-1.83	-59.14
4	6	4.5410	1.422	-1.92	-57.80
4	7	4.5365	1.469	-2.02	-56.41
4	8	4.5319	1.517	-2.12	-54.99
4	9	4.5272	1.567	-2.22	-53.50
4	10	4.5222	1.618	-2.33	-51.99
5	0	4.5449	1.324	-1.84	-60.71
5	2	4.5371	1.404	-2.01	-58.34
5	3	4.5330	1.447	-2.10	-57.06
5	4	4.5287	1.491	-2.19	-55.76
5	5	4.5243	1.536	-2.28	-54.42
5	6	4.5197	1.583	-2.38	-53.03
5	7	4.5150	1.632	-2.48	-51.57

5	8	4.5102	1.683	-2.59	-50.06
5	9	4.5052	1.735	-2.69	-48.52
5	10	4.5012	1.788	-2.78	-46.94
6	0	4.5217	1.482	-2.34	-56.02
6	2	4.5137	1.566	-2.51	-53.53
6	3	4.5095	1.611	-2.60	-52.20
6	4	4.5050	1.657	-2.70	-50.83
6	5	4.5004	1.705	-2.80	-49.41
6	6	4.4953	1.756	-2.91	-47.89
6	7	4.4905	1.807	-3.01	-46.38
6	8	4.4855	1.860	-3.12	-44.81
6	9	4.4805	1.915	-3.23	-43.18
6	10	4.4752	1.973	-3.34	-41.45
7	0	4.4954	1.653	-2.91	-50.95
7	2	4.4872	1.742	-3.08	-48.31
7	3	4.4830	1.788	-3.18	-46.94
7	4	4.4784	1.837	-3.27	-45.49
7	5	4.4733	1.889	-3.38	-43.95
7	6	4.4680	1.942	-3.50	-42.37
7	7	4.4627	1.997	-3.61	-40.74
7	8	4.4577	2.053	-3.72	-39.08
7	9	4.4520	2.112	-3.85	-37.33
7	10	4.4466	2.172	-3.96	-35.55
8	0	4.4657	1.841	-3.55	-45.37
8	2	4.4557	1.938	-3.76	-42.49
8	3	4.4508	1.989	-3.87	-40.98
8	4	4.4458	2.041	-3.98	-39.44
8	5	4.4417	2.093	-4.07	-37.89
8	6	4.4366	2.149	-4.18	-36.23
8	7	4.4306	2.208	-4.31	-34.48
8	8	4.4248	2.269	-4.43	-32.67
8	9	4.4190	2.332	-4.56	-30.80
8	10	4.4147	2.392	-4.65	-29.02
9	0	4.4288	2.061	-4.35	-38.84
9	2	4.4208	2.159	-4.52	-35.93
9	3	4.4157	2.213	-4.63	-34.33
9	4	4.4105	2.268	-4.74	-32.70
9	5	4.4054	2.325	-4.85	-31.01
9	6	4.4000	2.385	-4.97	-29.23
9	7	4.3945	2.446	-5.09	-27.42
9	8	4.3895	2.508	-5.19	-25.58
9	9	4.3852	2.570	-5.29	-23.74
9	10	4.3794	2.638	-5.41	-21.72
10	0	4.3883	2.310	-5.22	-31.45
10	2	4.3782	2.420	-5.44	-28.19
10	3	4.3731	2.478	-5.55	-26.47

10	4	4.3679	2.537	-5.66	-24.72
10	5	4.3624	2.598	-5.78	-22.91
10	6	4.3566	2.663	-5.90	-20.98
10	7	4.3506	2.729	-6.03	-19.02
10	8	4.3446	2.798	-6.17	-16.97
10	9	4.3382	2.870	-6.30	-14.84
10	10	4.3314	2.946	-6.45	-12.58

Table S17. Influence of U_d and U_p on cubic ZnO DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)
1	11	4.5692	1.190
2	15	4.5340	1.561
4	14	4.4808	1.888
7	15	4.4152	2.515
9	14	4.3499	2.951
10	14	4.3030	3.277
11	4	4.3156	2.866
12	2	4.2626	3.151
15	0	4.0938	4.756

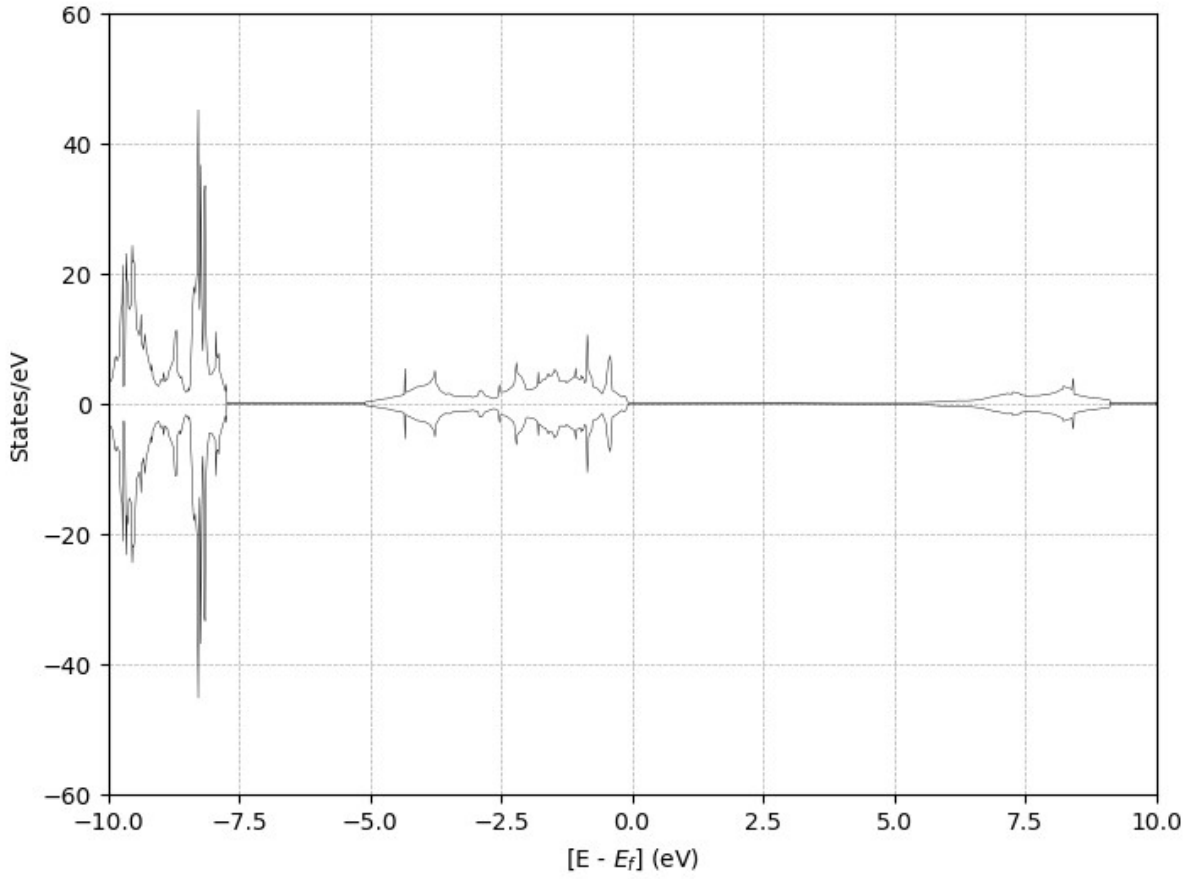

Figure S40. DOS for cubic ZnO with PBE functional: U_p = 5 eV, U_d = 12 eV

ZnO_2:

rPBE:

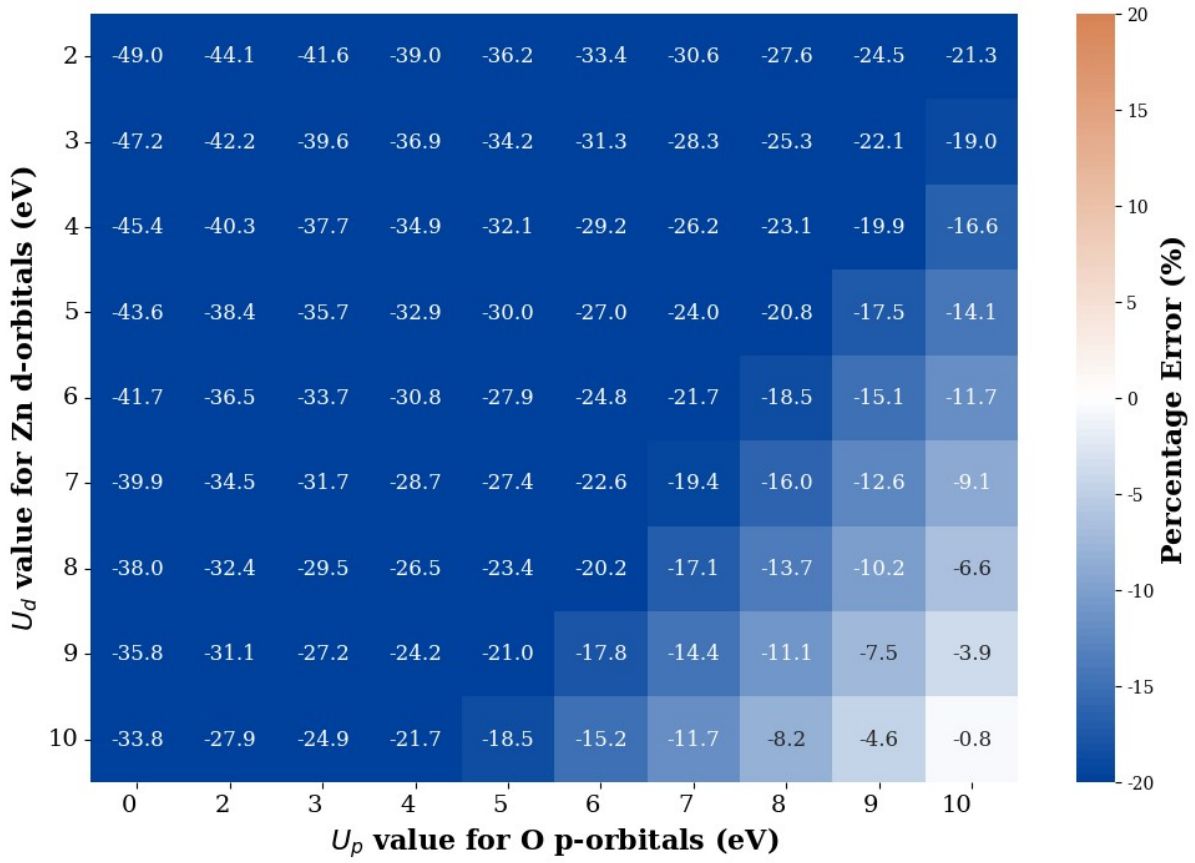

Figure S41. Heatmap of rPBE predicted band gap for cubic ZnO_2 as a function of the U_d and U_p parameters.

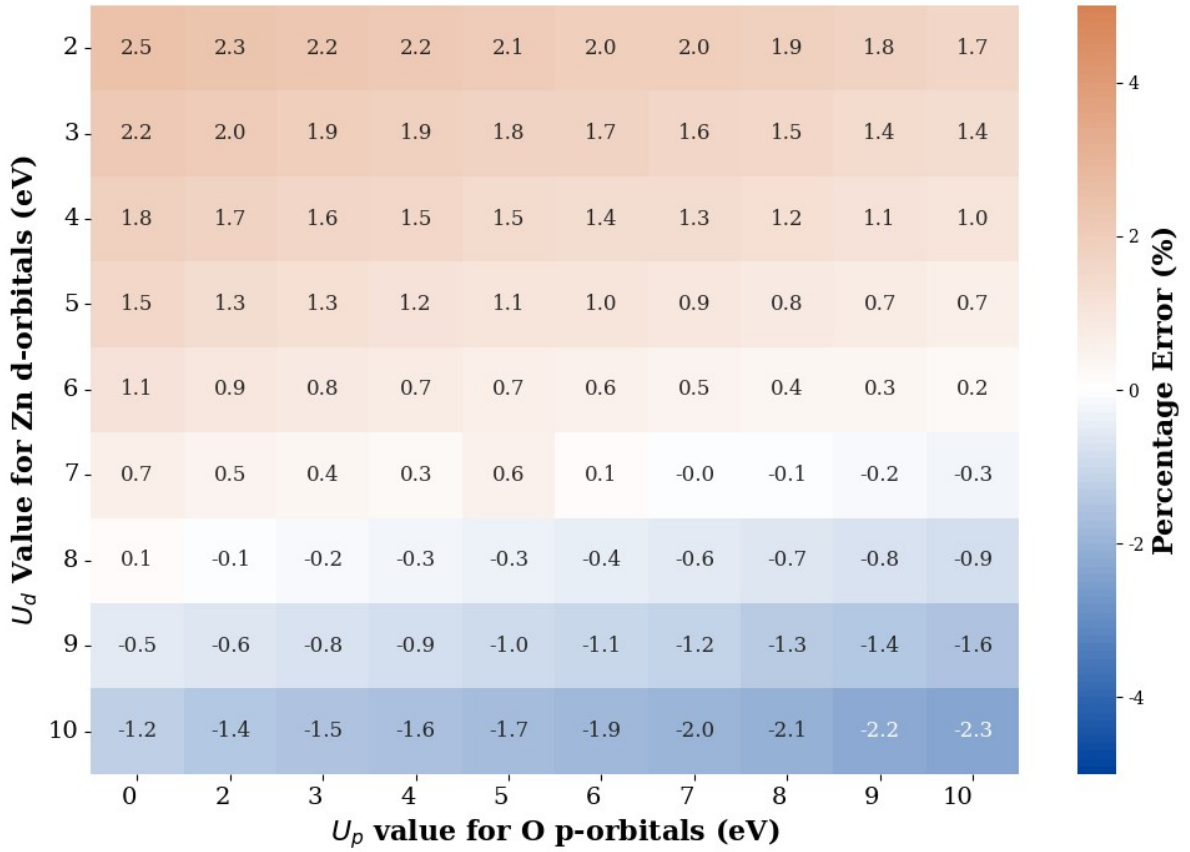

Figure S42. Heatmap of rPBE predicted lattice constant (a = b = c) for cubic ZnO_2 as a function of the U_d and U_p parameters.

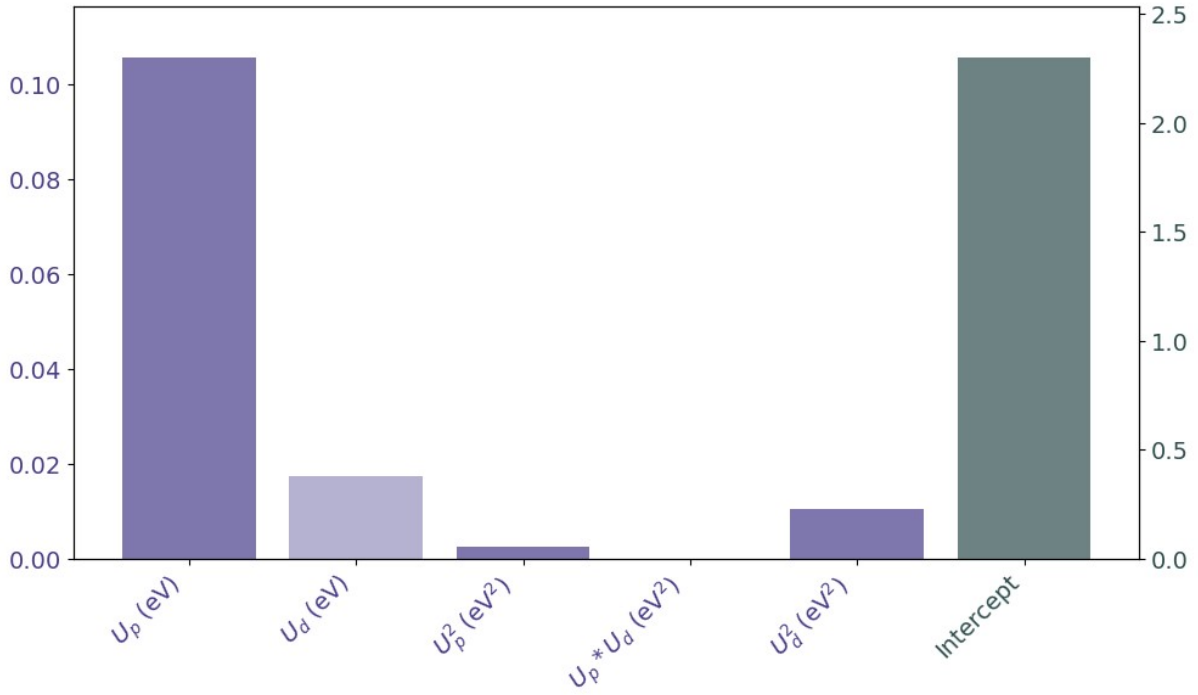

Figure S43. Feature importance of the PR model for predicting the rPBE band gap of c-ZnO_2. Lighter shades indicate features with negative contributions.

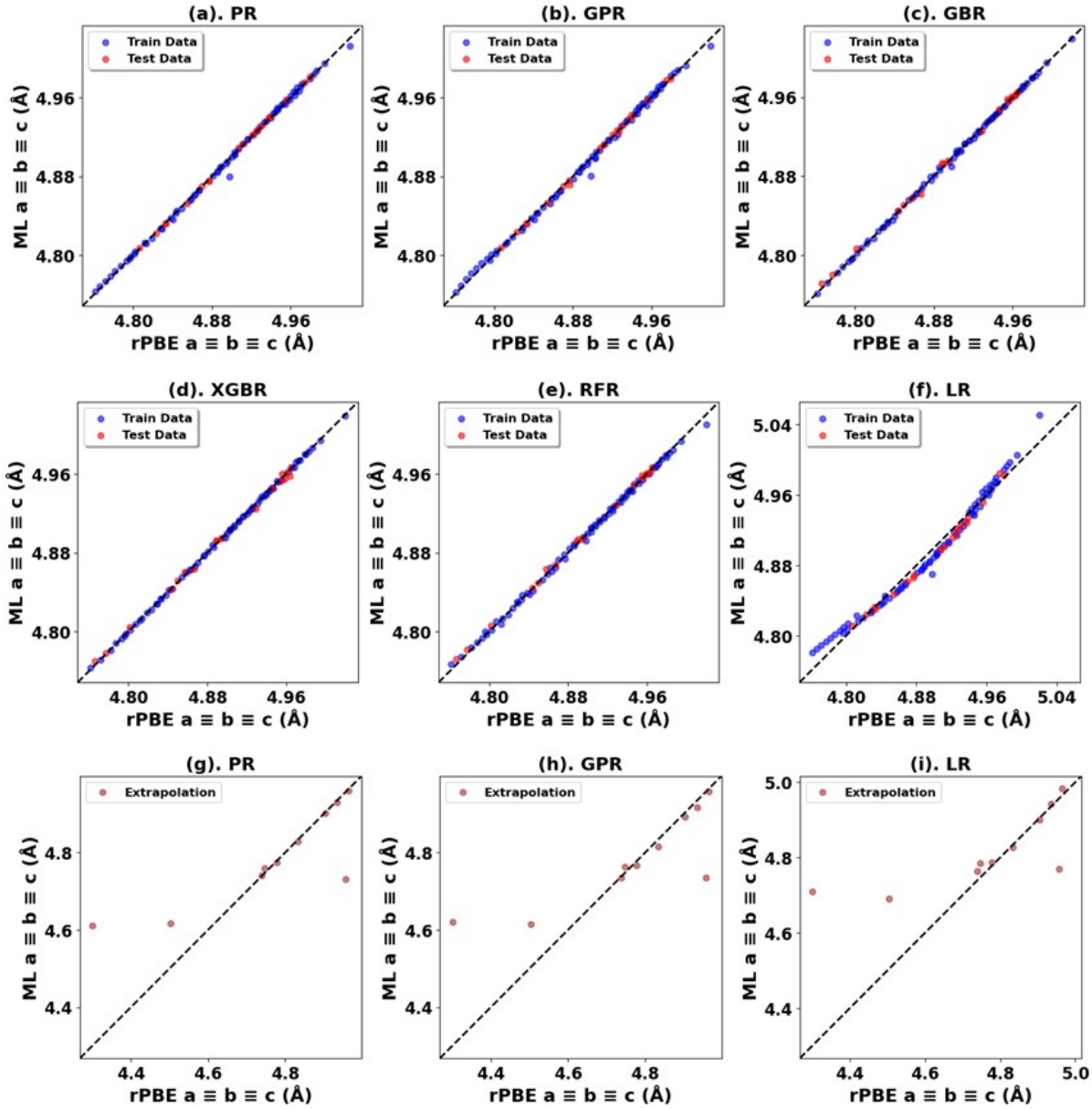

Figure S44. (a) - (f) Performance of models for rPBE lattice parameter (a = b = c) prediction of c-ZnO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S18. Comparative performance of models for rPBE lattice constant (a = b = c) prediction in cubic ZnO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Cubic ZnO_2	*PR	0.00	0.00	0.00	1.00	0.02	0.13	0.07	0.61
	GPR	0.00	0.00	0.00	1.00	0.02	0.13	0.07	0.60
	LR	0.00	0.01	0.01	0.97	0.02	0.16	0.09	0.42

	RFR	0.00	0.01	0.00	0.99	0.04	0.19	0.11	0.14
	GBR	0.00	0.00	0.00	0.99	0.04	0.19	0.11	0.14
	XGBR	0.00	0.01	0.00	0.99	0.04	0.19	0.11	0.14

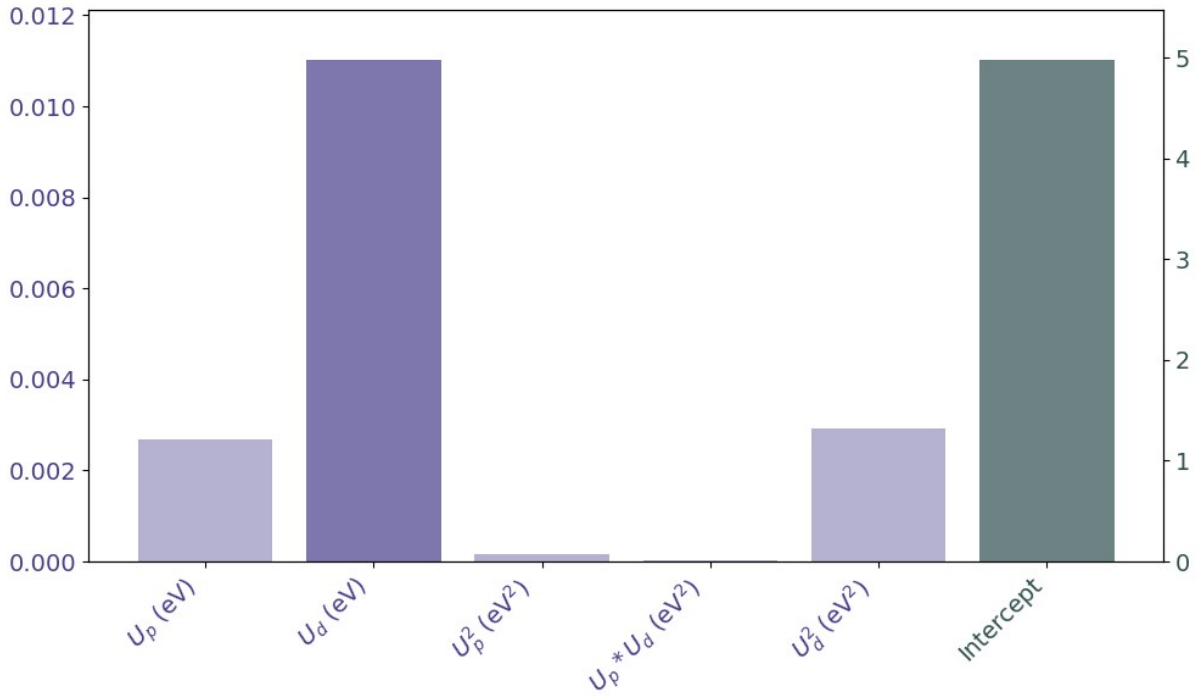

Figure S45. Feature importance of the PR model for predicting the rPBE lattice constant (a = b = c) of c-ZnO_2. Lighter shades indicate features with negative contributions.

Table S19. Influence of U_d and U_p on cubic ZnO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	5.0199	2.130	3.06	-52.67
2	0	4.9945	2.295	2.53	-49.00
2	2	4.9865	2.514	2.37	-44.13
2	3	4.9831	2.629	2.30	-41.58
2	4	4.9794	2.746	2.22	-38.98
2	5	4.9745	2.870	2.12	-36.22
2	6	4.9701	2.995	2.03	-33.44
2	7	4.9686	3.124	2.00	-30.58
2	8	4.9637	3.258	1.90	-27.60
2	9	4.9588	3.397	1.80	-24.51
2	10	4.9546	3.540	1.72	-21.33
3	0	4.9796	2.376	2.23	-47.20

3	2	4.9716	2.601	2.07	-42.20
3	3	4.9664	2.718	1.96	-39.60
3	4	4.9649	2.838	1.93	-36.93
3	5	4.9600	2.963	1.83	-34.16
3	6	4.9558	3.092	1.74	-31.29
3	7	4.9508	3.225	1.64	-28.33
3	8	4.9468	3.362	1.56	-25.29
3	9	4.9423	3.504	1.46	-22.13
3	10	4.9397	3.647	1.41	-18.96
4	0	4.9623	2.458	1.87	-45.38
4	2	4.9556	2.686	1.74	-40.31
4	3	4.9522	2.805	1.67	-37.67
4	4	4.9466	2.930	1.55	-34.89
4	5	4.9439	3.055	1.50	-32.11
4	6	4.9394	3.187	1.40	-29.18
4	7	4.9352	3.322	1.32	-26.18
4	8	4.9309	3.462	1.23	-23.07
4	9	4.9267	3.606	1.14	-19.87
4	10	4.9223	3.755	1.05	-16.56
5	0	4.9454	2.538	1.53	-43.60
5	2	4.9374	2.771	1.36	-38.42
5	3	4.9333	2.893	1.28	-35.71
5	4	4.9291	3.019	1.19	-32.91
5	5	4.9248	3.149	1.11	-30.02
5	6	4.9206	3.283	1.02	-27.04
5	7	4.9162	3.421	0.93	-23.98
5	8	4.9113	3.565	0.83	-20.78
5	9	4.9070	3.712	0.74	-17.51
5	10	4.9029	3.866	0.66	-14.09
6	0	4.9256	2.622	1.12	-41.73
6	2	4.9164	2.859	0.93	-36.47
6	3	4.9122	2.984	0.85	-33.69
6	4	4.9075	3.113	0.75	-30.82
6	5	4.9033	3.245	0.66	-27.89
6	6	4.8997	3.384	0.59	-24.80
6	7	4.8952	3.525	0.50	-21.67
6	8	4.8898	3.668	0.39	-18.49
6	9	4.8862	3.822	0.31	-15.07
6	10	4.8809	3.973	0.20	-11.71
7	0	4.9030	2.706	0.66	-39.87
7	2	4.8942	2.949	0.48	-34.47
7	3	4.8886	3.075	0.36	-31.67
7	4	4.8853	3.209	0.29	-28.69
7	5	4.8981	3.266	0.56	-27.42
7	6	4.8762	3.485	0.11	-22.56
7	7	4.8700	3.626	-0.02	-19.42

7	8	4.8670	3.778	-0.08	-16.04
7	9	4.8620	3.931	-0.19	-12.64
7	10	4.8573	4.089	-0.28	-9.13
8	0	4.8769	2.792	0.12	-37.96
8	2	4.8672	3.041	-0.08	-32.42
8	3	4.8634	3.173	-0.16	-29.49
8	4	4.8588	3.307	-0.25	-26.51
8	5	4.8542	3.446	-0.35	-23.42
8	6	4.8495	3.589	-0.44	-20.24
8	7	4.8432	3.732	-0.57	-17.07
8	8	4.8382	3.884	-0.67	-13.69
8	9	4.8331	4.039	-0.78	-10.24
8	10	4.8280	4.201	-0.88	-6.64
9	0	4.8444	2.889	-0.55	-35.80
9	2	4.8407	3.100	-0.62	-31.11
9	3	4.8328	3.274	-0.78	-27.24
9	4	4.8290	3.411	-0.86	-24.20
9	5	4.8233	3.553	-0.98	-21.04
9	6	4.8190	3.699	-1.07	-17.80
9	7	4.8133	3.850	-1.18	-14.44
9	8	4.8067	4.001	-1.32	-11.09
9	9	4.8014	4.161	-1.43	-7.53
9	10	4.7958	4.325	-1.54	-3.89
10	0	4.8116	2.981	-1.22	-33.76
10	2	4.8022	3.244	-1.41	-27.91
10	3	4.7973	3.381	-1.51	-24.87
10	4	4.7929	3.523	-1.60	-21.71
10	5	4.7873	3.668	-1.72	-18.49
10	6	4.7818	3.817	-1.83	-15.18
10	7	4.7770	3.972	-1.93	-11.73
10	8	4.7716	4.131	-2.04	-8.20
10	9	4.7661	4.295	-2.15	-4.56
10	10	4.7614	4.464	-2.25	-0.80

Table S20. Influence of U_d and U_p on cubic ZnO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)
1	11	4.9650	3.573
2	15	4.9351	4.323
4	14	4.9042	4.401
7	15	4.8337	4.959
9	14	4.7779	5.043
10	14	4.7387	5.193
11	4	4.7475	3.646
12	2	4.9573	3.283
13	15	4.5036	6.062
15	0	4.3008	5.189

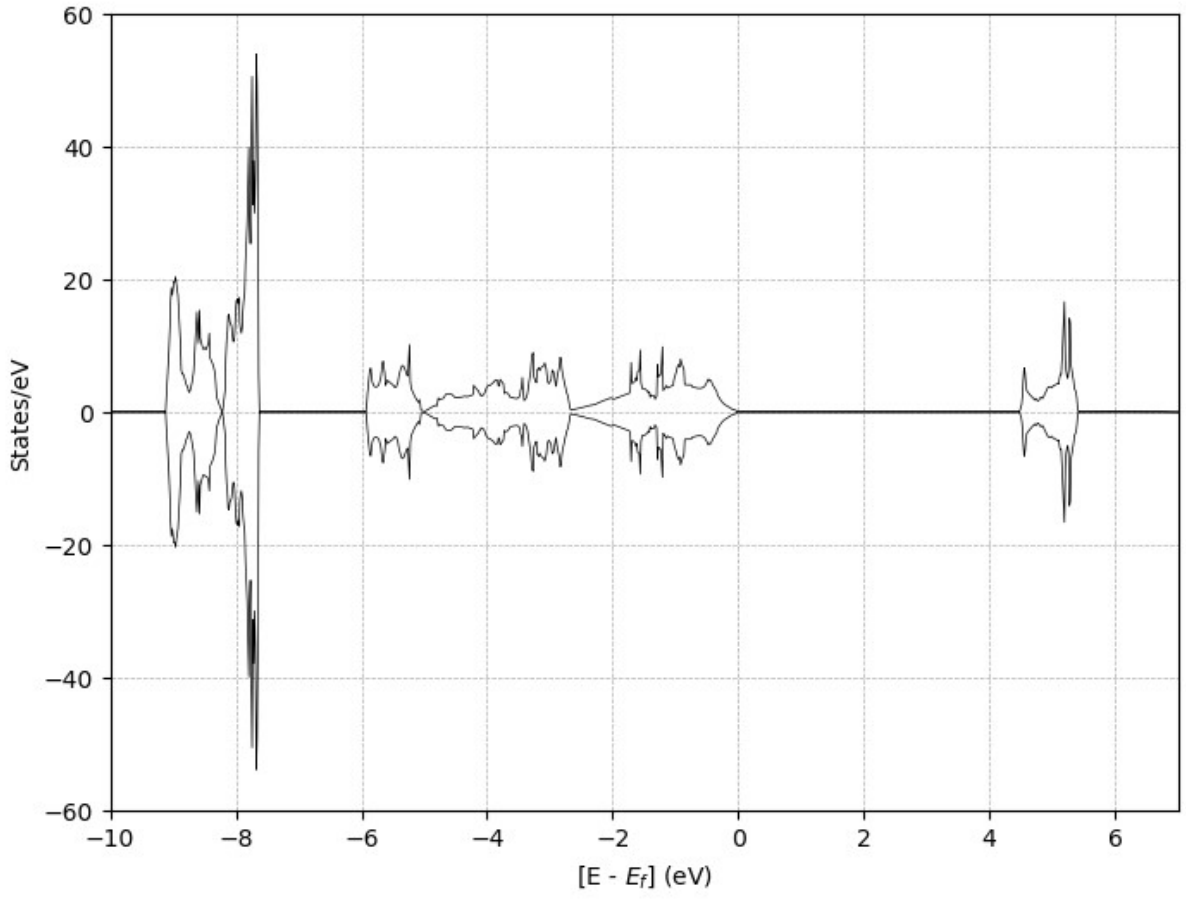

Figure S46. DOS for cubic ZnO_2 with rPBE functional: U_p = 10 eV, U_d = 10 eV

PBE:

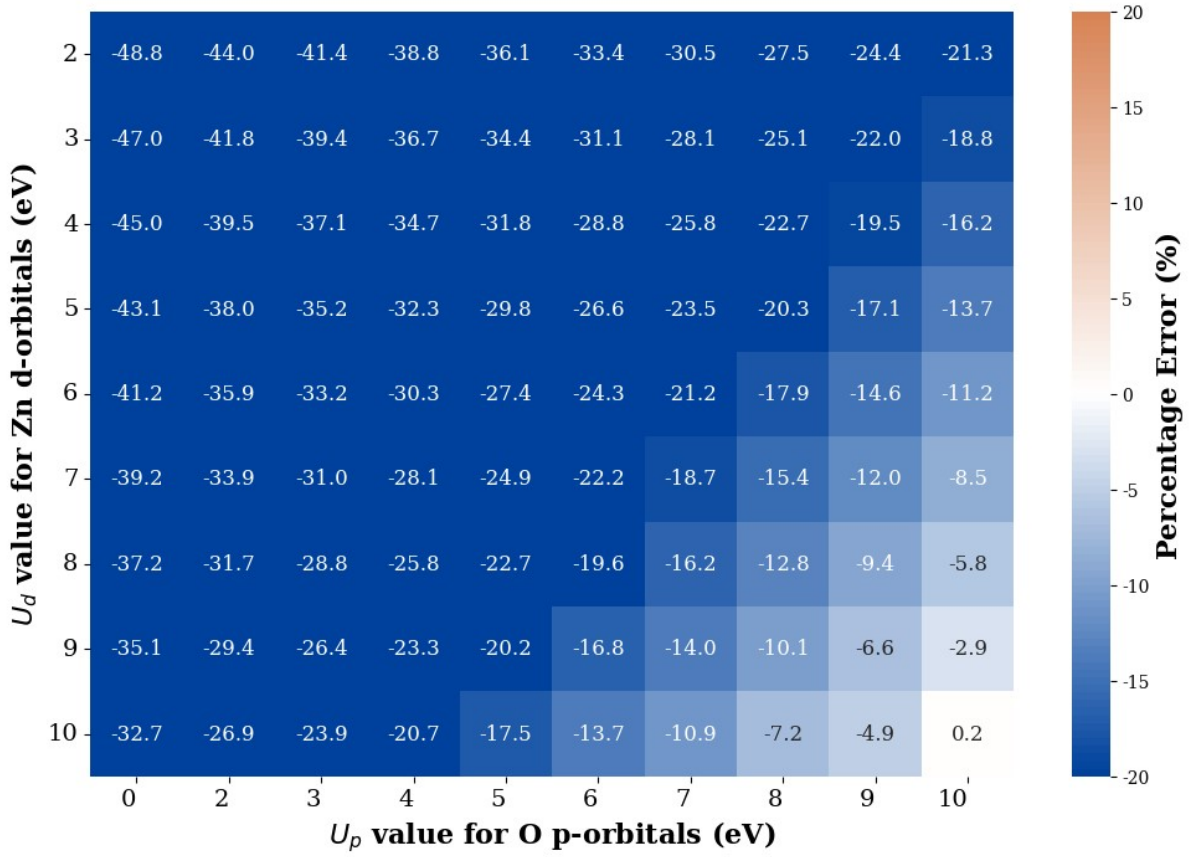

Figure S47. Heatmap of PBE predicted band gap for cubic ZnO_2 as a function of the U_d and U_p parameters.

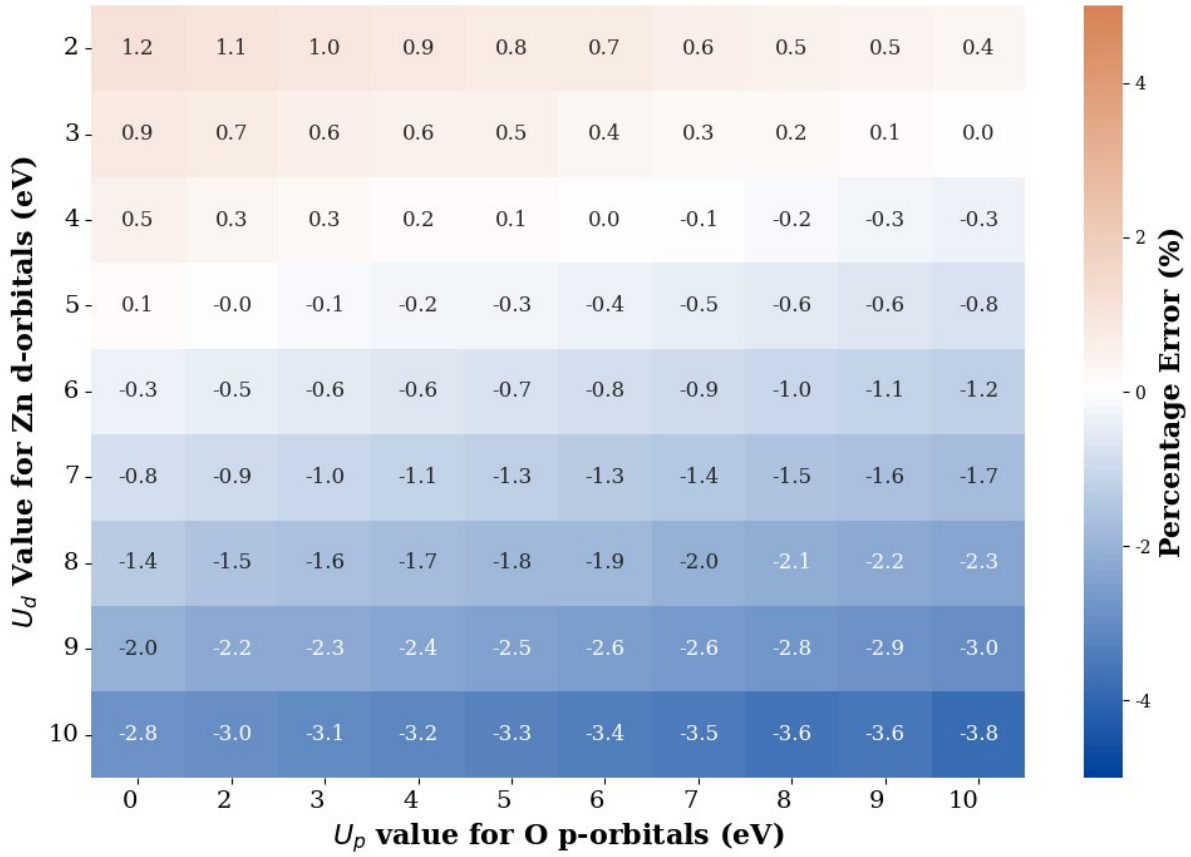

Figure S48. Heatmap of PBE predicted lattice constant (a = b = c) for cubic ZnO_2 as a function of the U_d and U_p parameters.

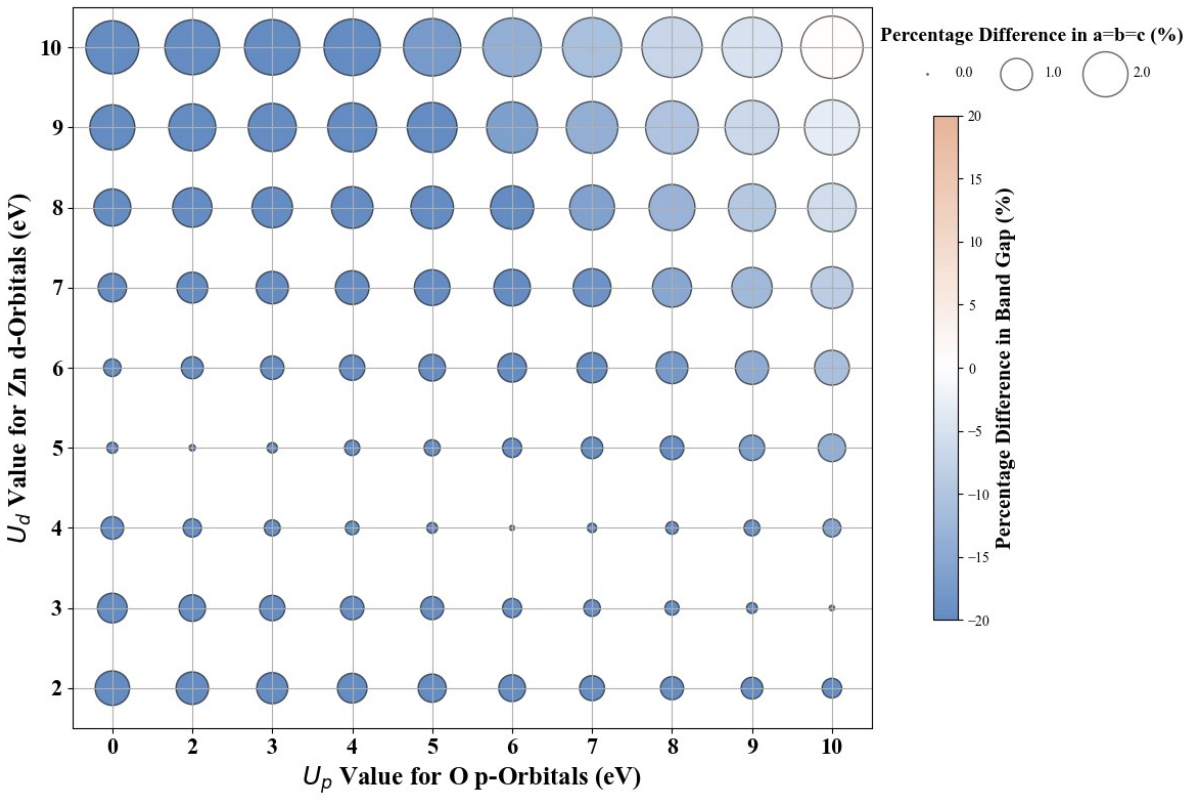

Figure S49. Effect of Hubbard U values on PBE band gap and lattice parameters of c-ZnO_2.

Table S21. Influence of U_d and U_p on cubic ZnO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	4.9573	2.128	1.77	-52.71
2	0	4.9573	2.302	1.18	-48.84
2	2	4.9222	2.521	1.05	-43.98
2	3	4.9180	2.635	0.97	-41.44
2	4	4.9137	2.753	0.88	-38.82
2	5	4.9095	2.874	0.79	-36.13
2	6	4.9058	2.999	0.71	-33.36
2	7	4.9013	3.129	0.62	-30.47
2	8	4.8970	3.262	0.53	-27.51
2	9	4.8939	3.400	0.47	-24.44
2	10	4.8898	3.542	0.39	-21.29
3	0	4.9573	2.387	0.88	-46.96
3	2	4.9053	2.621	0.70	-41.76
3	3	4.9022	2.728	0.64	-39.38
3	4	4.8979	2.849	0.55	-36.69
3	5	4.8969	2.953	0.53	-34.38
3	6	4.8889	3.102	0.37	-31.07
3	7	4.8845	3.235	0.28	-28.11
3	8	4.8810	3.370	0.20	-25.11
3	9	4.8767	3.511	0.12	-21.98
3	10	4.8724	3.655	0.03	-18.78
4	0	4.9573	2.473	0.51	-45.04
4	2	4.8874	2.721	0.34	-39.53
4	3	4.8835	2.829	0.26	-37.13
4	4	4.8802	2.940	0.19	-34.67
4	5	4.8766	3.071	0.12	-31.76
4	6	4.8722	3.203	0.03	-28.82
4	7	4.8668	3.339	-0.09	-25.80
4	8	4.8632	3.477	-0.16	-22.73
4	9	4.8587	3.621	-0.25	-19.53
4	10	4.8552	3.769	-0.32	-16.24
5	0	4.9573	2.559	0.12	-43.13
5	2	4.8690	2.792	-0.04	-37.96
5	3	4.8658	2.914	-0.11	-35.24
5	4	4.8596	3.045	-0.23	-32.33
5	5	4.8584	3.160	-0.26	-29.78
5	6	4.8529	3.304	-0.37	-26.58
5	7	4.8482	3.443	-0.47	-23.49
5	8	4.8436	3.585	-0.56	-20.33

5	9	4.8397	3.732	-0.64	-17.07
5	10	4.8341	3.883	-0.76	-13.71
6	0	4.9573	2.644	-0.31	-41.24
6	2	4.8473	2.884	-0.49	-35.91
6	3	4.8442	3.008	-0.55	-33.16
6	4	4.8398	3.137	-0.64	-30.29
6	5	4.8364	3.267	-0.71	-27.40
6	6	4.8308	3.407	-0.83	-24.29
6	7	4.8266	3.548	-0.91	-21.16
6	8	4.8218	3.694	-1.01	-17.91
6	9	4.8171	3.843	-1.11	-14.60
6	10	4.8122	3.997	-1.21	-11.18
7	0	4.9573	2.734	-0.81	-39.24
7	2	4.8248	2.976	-0.95	-33.87
7	3	4.8202	3.104	-1.04	-31.02
7	4	4.8156	3.236	-1.14	-28.09
7	5	4.8091	3.380	-1.27	-24.89
7	6	4.8060	3.501	-1.33	-22.20
7	7	4.8017	3.657	-1.42	-18.73
7	8	4.7970	3.806	-1.52	-15.42
7	9	4.7919	3.959	-1.62	-12.02
7	10	4.7869	4.116	-1.73	-8.53
8	0	4.9573	2.825	-1.37	-37.22
8	2	4.7958	3.075	-1.54	-31.67
8	3	4.7912	3.206	-1.64	-28.76
8	4	4.7867	3.340	-1.73	-25.78
8	5	4.7826	3.479	-1.81	-22.69
8	6	4.7803	3.618	-1.86	-19.60
8	7	4.7733	3.770	-2.01	-16.22
8	8	4.7684	3.922	-2.11	-12.84
8	9	4.7629	4.078	-2.22	-9.38
8	10	4.7581	4.239	-2.32	-5.80
9	0	4.9573	2.922	-2.02	-35.07
9	2	4.7638	3.178	-2.20	-29.38
9	3	4.7590	3.312	-2.30	-26.40
9	4	4.7545	3.450	-2.39	-23.33
9	5	4.7506	3.592	-2.47	-20.18
9	6	4.7451	3.746	-2.58	-16.76
9	7	4.7419	3.872	-2.65	-13.96
9	8	4.7357	4.045	-2.78	-10.11
9	9	4.7306	4.205	-2.88	-6.56
9	10	4.7252	4.370	-2.99	-2.89
10	0	4.9573	3.028	-2.80	-32.71
10	2	4.7254	3.290	-2.99	-26.89
10	3	4.7222	3.426	-3.05	-23.87
10	4	4.7164	3.568	-3.17	-20.71

10	5	4.7118	3.714	-3.27	-17.47
10	6	4.7055	3.885	-3.40	-13.67
10	7	4.7015	4.011	-3.48	-10.87
10	8	4.6952	4.178	-3.61	-7.16
10	9	4.6965	4.279	-3.58	-4.91
10	10	4.6837	4.511	-3.84	0.24

Table S22. Influence of U_d and U_p on cubic ZnO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)
1	11	4.9195	3.520
2	15	4.8679	4.316
4	14	4.8381	4.410
7	15	4.7639	4.981
9	14	4.7048	5.081
10	14	4.6627	5.240
11	4	4.6677	3.703
12	2	4.6163	3.568
15	0	4.1032	5.670

Figure S50. DOS for cubic ZnO_2 with PBE functional: U_p = 10 eV, U_d = 10 eV

ZrO_2:

rPBE:

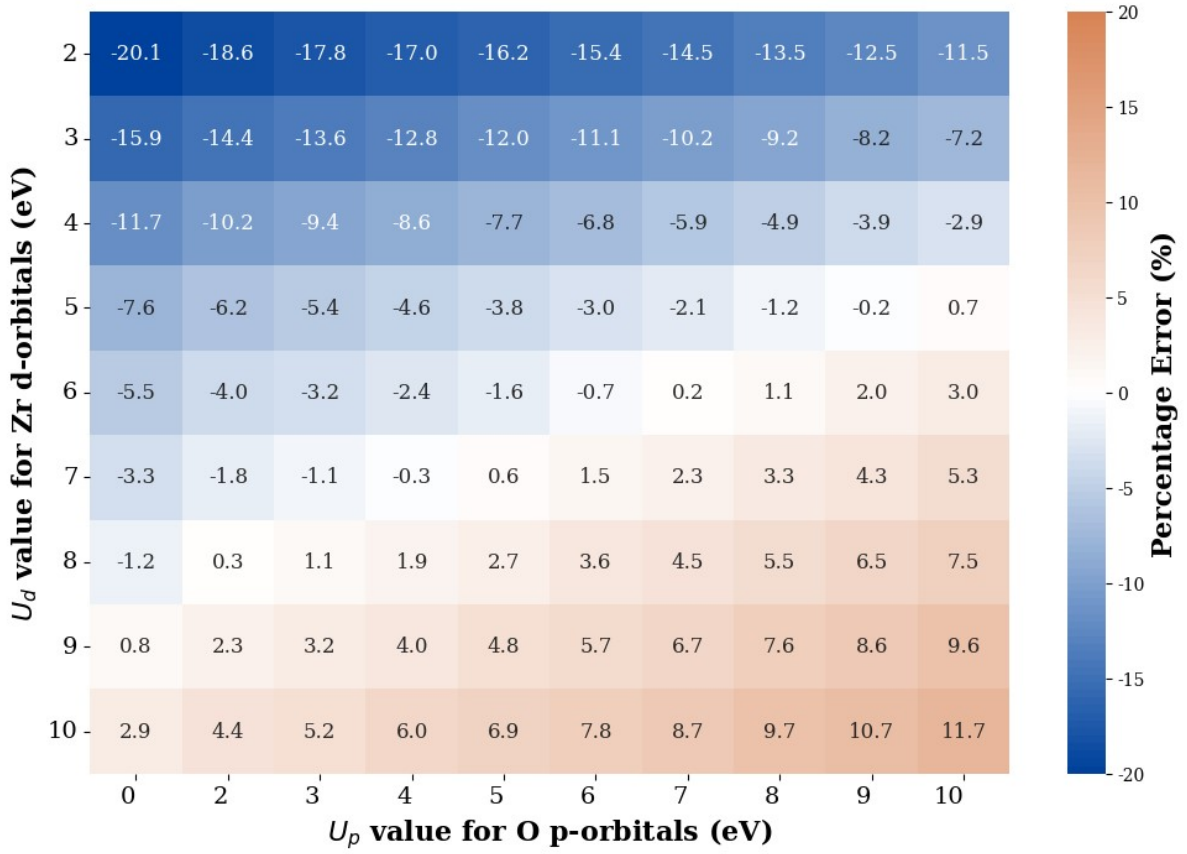

Figure S51. Heatmap of rPBE predicted band gap for cubic ZrO_2 as a function of the U_d and U_p parameters.

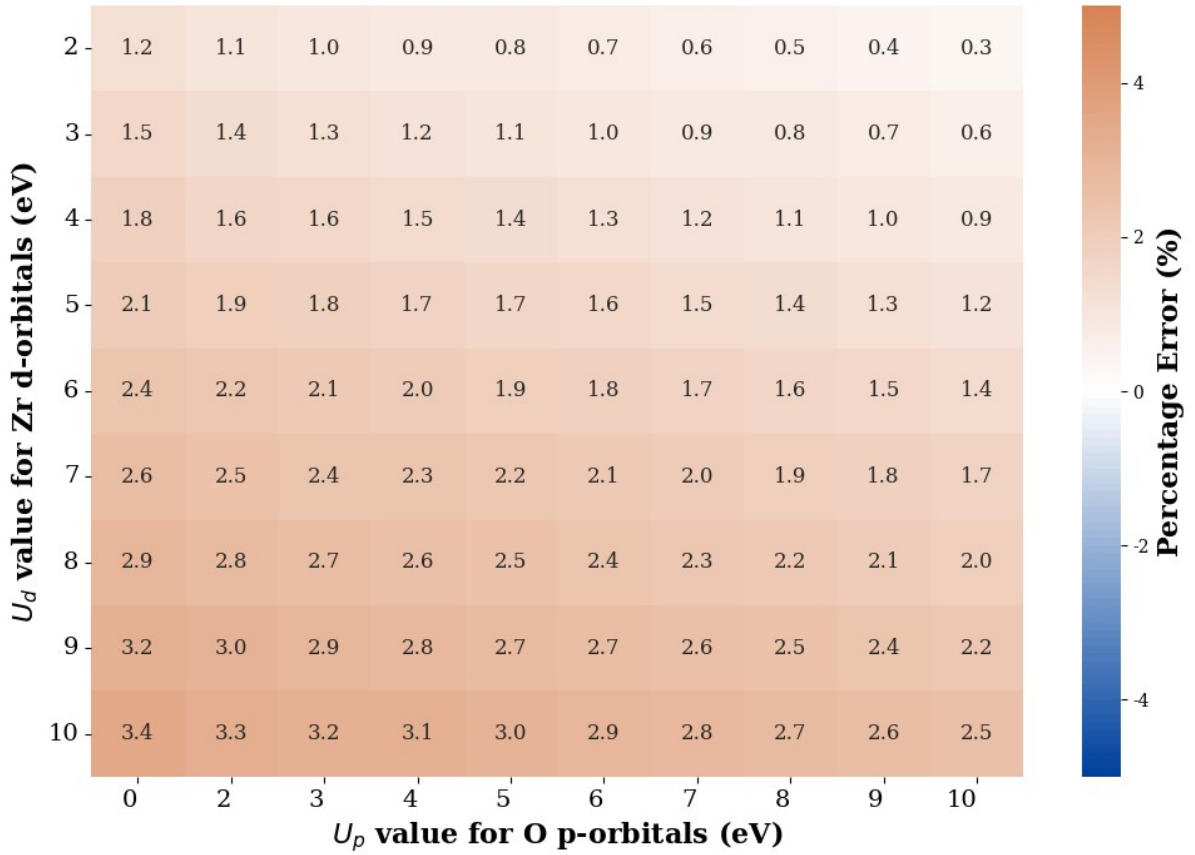

Figure S52. Heatmap of rPBE predicted lattice constant (a = b = c) for cubic ZrO_2 as a function of the U_d and U_p parameters.

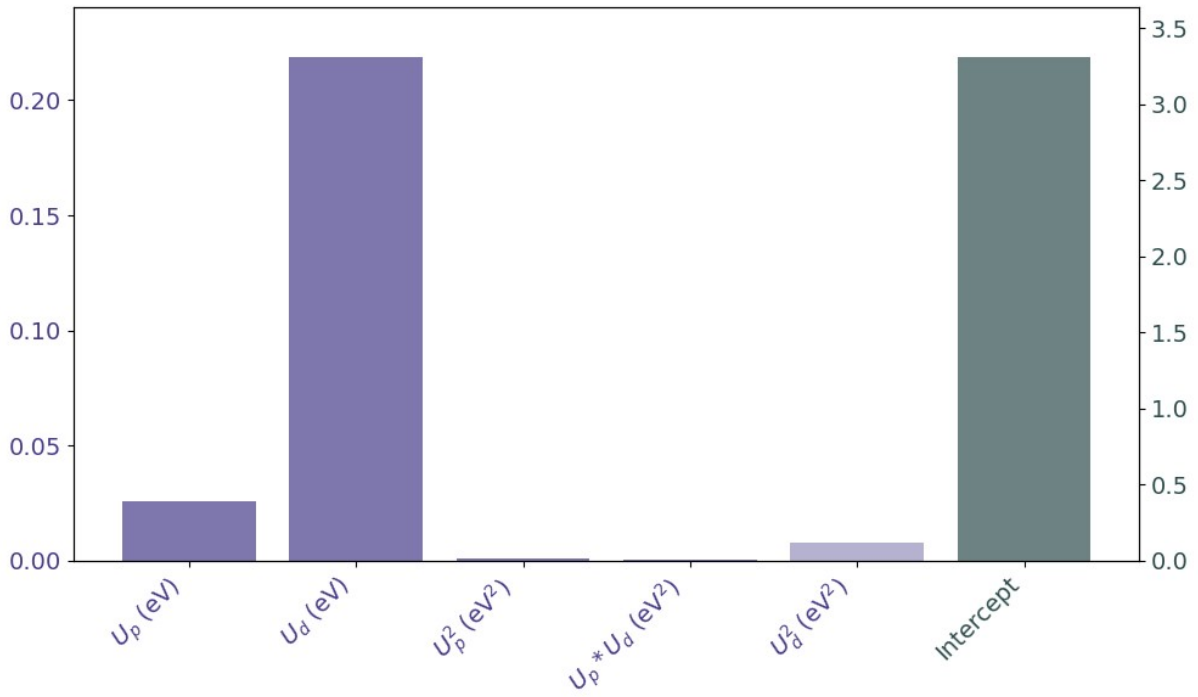

Figure S53. Feature importance of the PR model for predicting the rPBE band gap of c-ZrO_2. Lighter shades indicate features with negative contributions.

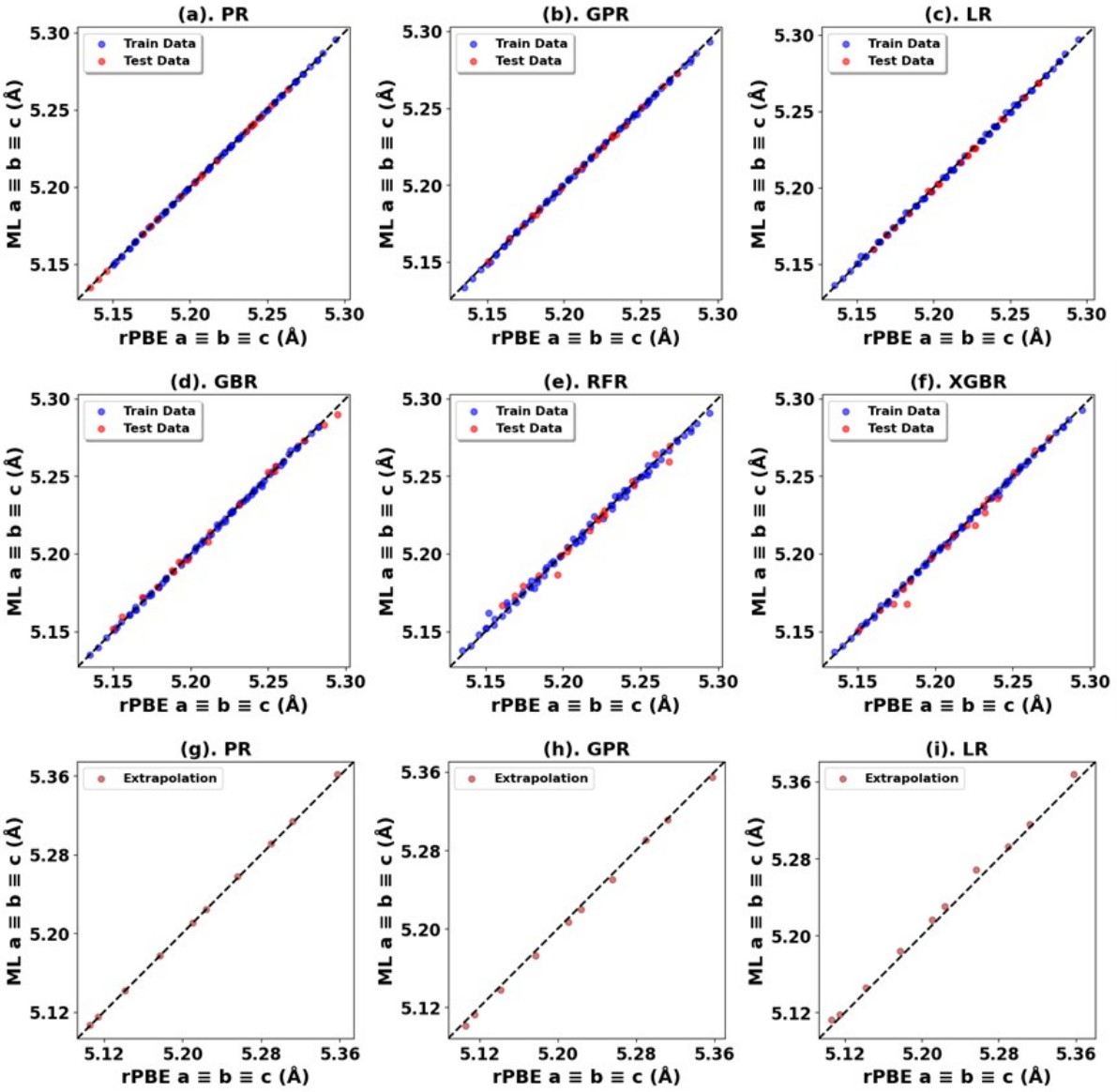

Figure S54. (a) - (f) Performance of models for rPBE lattice parameter (a = b = c) prediction of c-ZrO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_d from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_d values beyond these initial ranges.

Table S23. Comparative performance of models for rPBE lattice constant (a = b = c) prediction in cubic ZrO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Cubic ZrO_2	*PR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	GPR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	LR	0.00	0.00	0.00	1.00	0.00	0.01	0.01	0.99
	GBR	0.00	0.00	0.00	0.99	0.00	0.03	0.03	0.87

	XGBR	0.00	0.01	0.00	0.98	0.00	0.03	0.03	0.86
	RFR	0.00	0.01	0.00	0.98	0.00	0.03	0.03	0.85

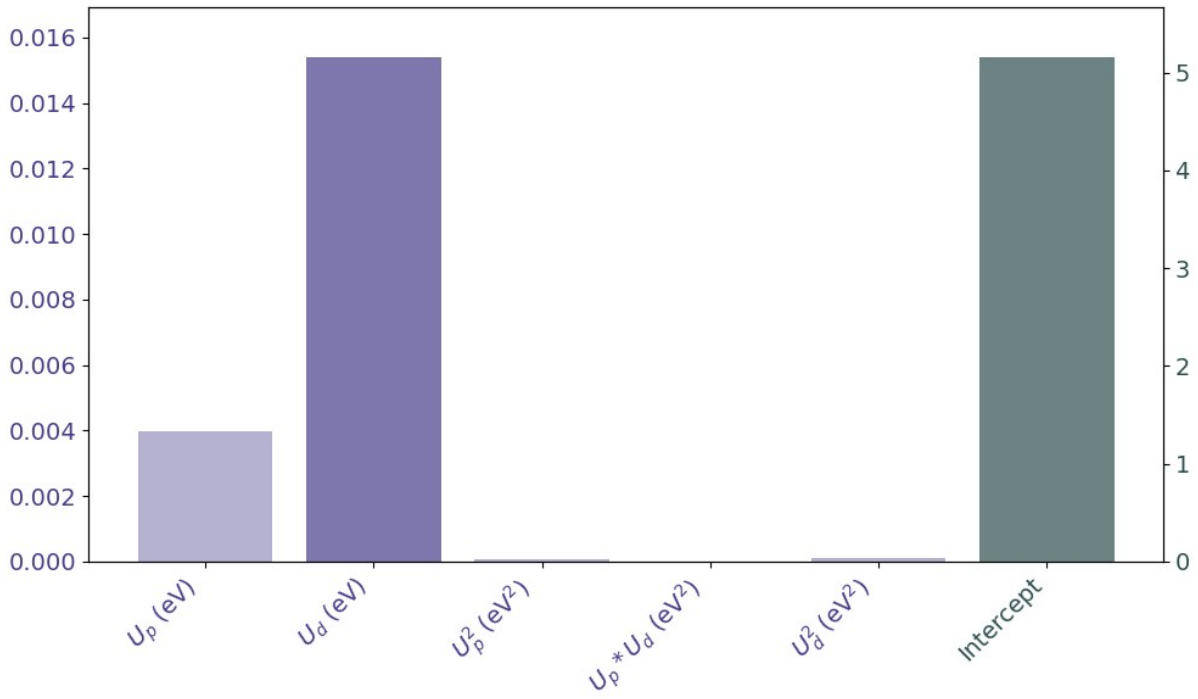

Figure S55. Feature importance of the PR model for predicting the rPBE lattice constant (a = b = c) of c-ZrO_2. Lighter shades indicate features with negative contributions.

Table S24. Influence of U_d and U_p on cubic ZrO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	5.1523	3.295	0.65	-28.37
2	0	5.1817	3.675	1.23	-20.11
2	2	5.1733	3.743	1.06	-18.63
2	3	5.1689	3.779	0.98	-17.85
2	4	5.1644	3.816	0.89	-17.04
2	5	5.1607	3.853	0.82	-16.24
2	6	5.1558	3.893	0.72	-15.37
2	7	5.1508	3.935	0.62	-14.46
2	8	5.1457	3.979	0.52	-13.50
2	9	5.1405	4.024	0.42	-12.52
2	10	5.1351	4.071	0.32	-11.50
3	0	5.1965	3.867	1.52	-15.93
3	2	5.1881	3.937	1.35	-14.41

3	3	5.1837	3.973	1.27	-13.63
3	4	5.1792	4.011	1.18	-12.80
3	5	5.1745	4.050	1.09	-11.96
3	6	5.1698	4.091	0.99	-11.07
3	7	5.1649	4.133	0.90	-10.15
3	8	5.1608	4.175	0.82	-9.24
3	9	5.1555	4.221	0.71	-8.24
3	10	5.1501	4.268	0.61	-7.22
4	0	5.2113	4.060	1.80	-11.74
4	2	5.2028	4.131	1.64	-10.20
4	3	5.1983	4.168	1.55	-9.39
4	4	5.1938	4.206	1.46	-8.57
4	5	5.1891	4.246	1.37	-7.70
4	6	5.1844	4.287	1.28	-6.80
4	7	5.1794	4.330	1.18	-5.87
4	8	5.1744	4.374	1.08	-4.91
4	9	5.1692	4.420	0.98	-3.91
4	10	5.1639	4.468	0.88	-2.87
5	0	5.2258	4.249	2.09	-7.63
5	2	5.2172	4.315	1.92	-6.20
5	3	5.2128	4.350	1.83	-5.43
5	4	5.2082	4.387	1.75	-4.63
5	5	5.2036	4.424	1.65	-3.83
5	6	5.1987	4.463	1.56	-2.98
5	7	5.1939	4.503	1.47	-2.11
5	8	5.1888	4.545	1.36	-1.20
5	9	5.1835	4.589	1.26	-0.24
5	10	5.1782	4.634	1.16	0.74
6	0	5.2402	4.349	2.37	-5.46
6	2	5.2316	4.416	2.20	-4.00
6	3	5.2271	4.451	2.11	-3.24
6	4	5.2225	4.488	2.02	-2.43
6	5	5.2178	4.526	1.93	-1.61
6	6	5.2130	4.566	1.84	-0.74
6	7	5.2080	4.607	1.74	0.15
6	8	5.2030	4.649	1.64	1.07
6	9	5.1977	4.693	1.54	2.02
6	10	5.1924	4.739	1.44	3.02
7	0	5.2544	4.447	2.65	-3.33
7	2	5.2457	4.515	2.48	-1.85
7	3	5.2413	4.551	2.39	-1.07
7	4	5.2367	4.588	2.30	-0.26
7	5	5.2319	4.627	2.21	0.59
7	6	5.2271	4.667	2.11	1.46
7	7	5.2221	4.708	2.02	2.35
7	8	5.2171	4.751	1.92	3.28

7	9	5.2118	4.796	1.81	4.26
7	10	5.2064	4.842	1.71	5.26
8	0	5.2684	4.544	2.92	-1.22
8	2	5.2597	4.613	2.75	0.28
8	3	5.2552	4.649	2.66	1.07
8	4	5.2506	4.687	2.57	1.89
8	5	5.2459	4.726	2.48	2.74
8	6	5.2410	4.766	2.39	3.61
8	7	5.2360	4.808	2.29	4.52
8	8	5.2309	4.851	2.19	5.46
8	9	5.2256	4.897	2.08	6.46
8	10	5.2202	4.943	1.98	7.46
9	0	5.2822	4.638	3.19	0.83
9	2	5.2735	4.708	3.02	2.35
9	3	5.2690	4.745	2.93	3.15
9	4	5.2644	4.783	2.84	3.98
9	5	5.2596	4.823	2.75	4.85
9	6	5.2547	4.863	2.65	5.72
9	7	5.2498	4.906	2.56	6.65
9	8	5.2446	4.950	2.45	7.61
9	9	5.2393	4.995	2.35	8.59
9	10	5.2338	5.043	2.25	9.63
10	0	5.2946	4.733	3.43	2.89
10	2	5.2860	4.804	3.26	4.43
10	3	5.2826	4.839	3.20	5.20
10	4	5.2779	4.878	3.11	6.04
10	5	5.2731	4.917	3.01	6.89
10	6	5.2682	4.959	2.92	7.80
10	7	5.2632	5.002	2.82	8.74
10	8	5.2580	5.046	2.72	9.70
10	9	5.2527	5.092	2.61	10.70
10	10	5.2472	5.140	2.51	11.74

Table S25. Influence of U_d and U_p on cubic ZrO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)
1	11	5.1146	3.922
2	15	5.1060	4.336
4	14	5.1415	4.680
7	15	5.1771	5.103
9	14	5.2104	5.252
10	14	5.2238	5.352
11	4	5.2901	4.972
12	2	5.3120	4.985
13	15	5.2560	5.698
15	0	5.3577	4.824

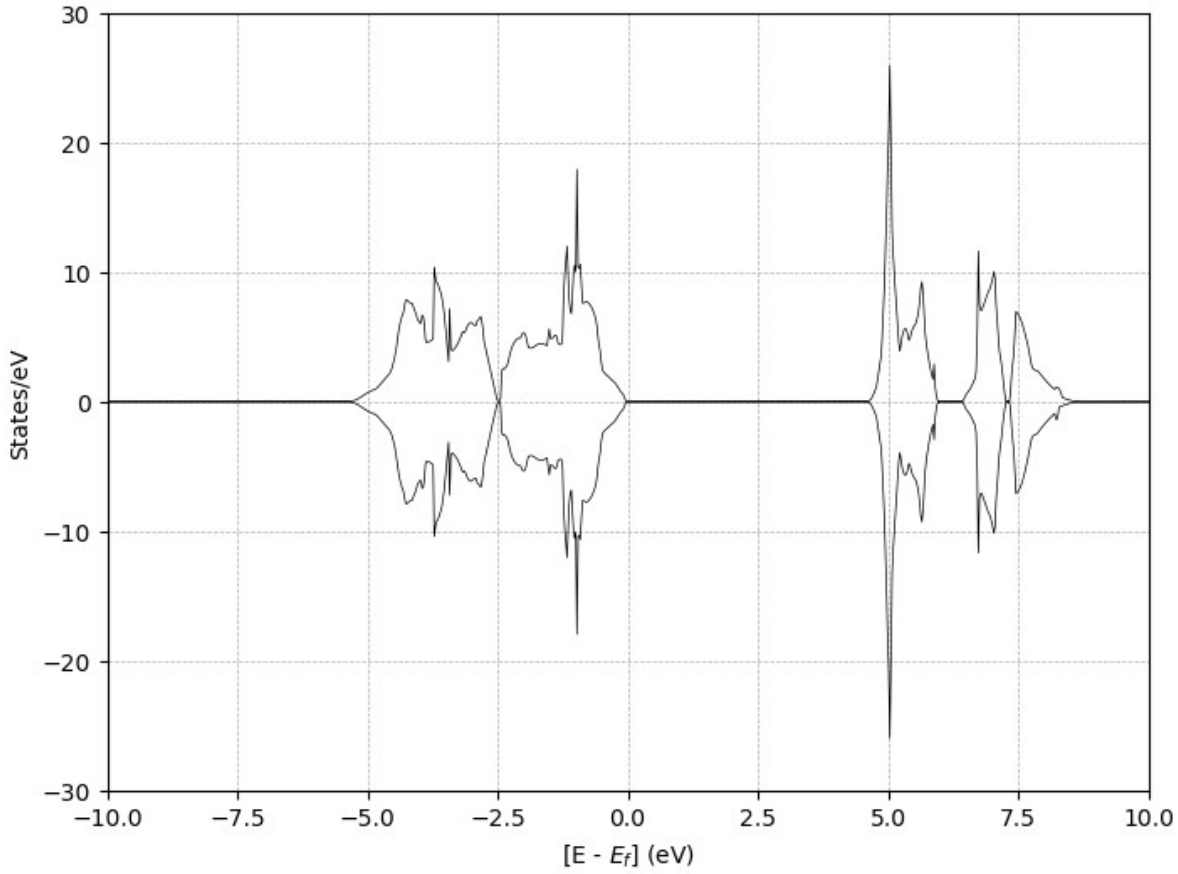

Figure S56. DOS for cubic ZrO_2 with rPBE functional: U_p = 9 eV, U_d = 5 eV

PBE:

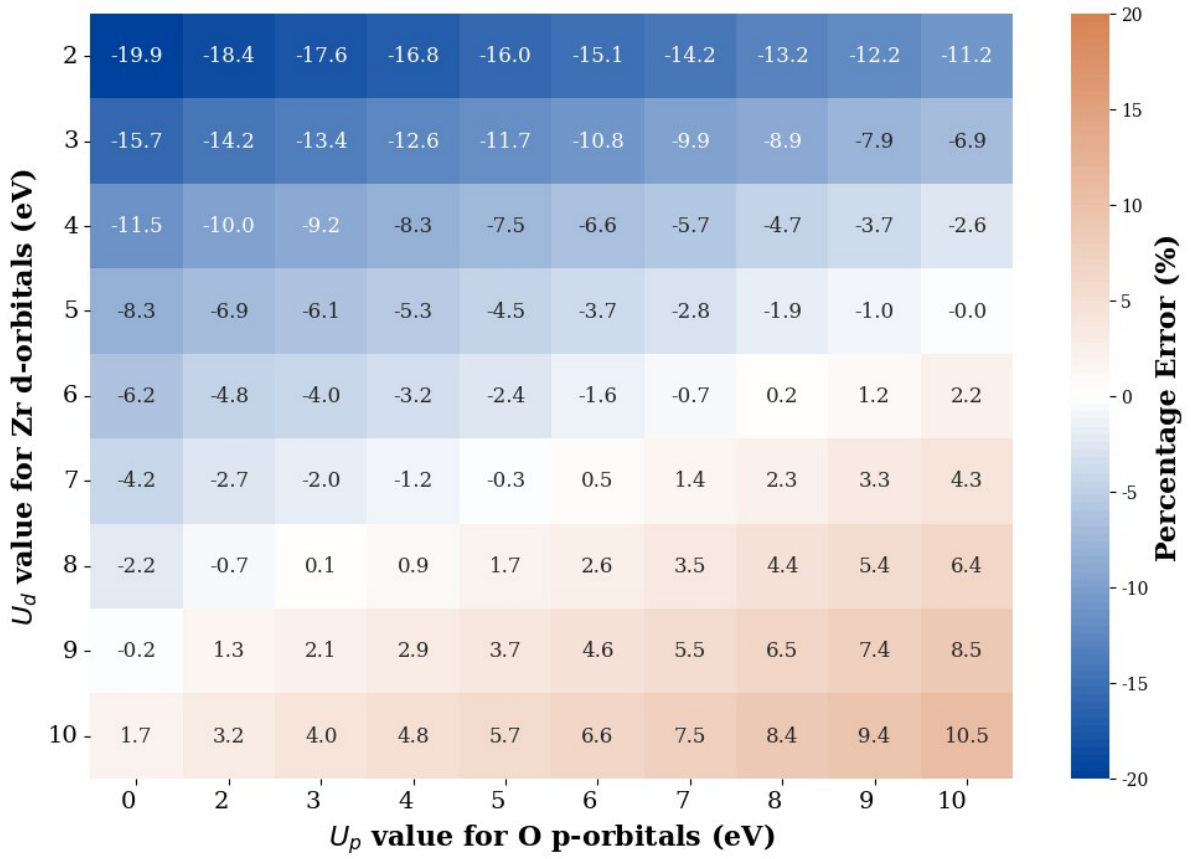

Figure S57. Heatmap of PBE predicted band gap for cubic ZrO_2 as a function of the U_d and U_p parameters.

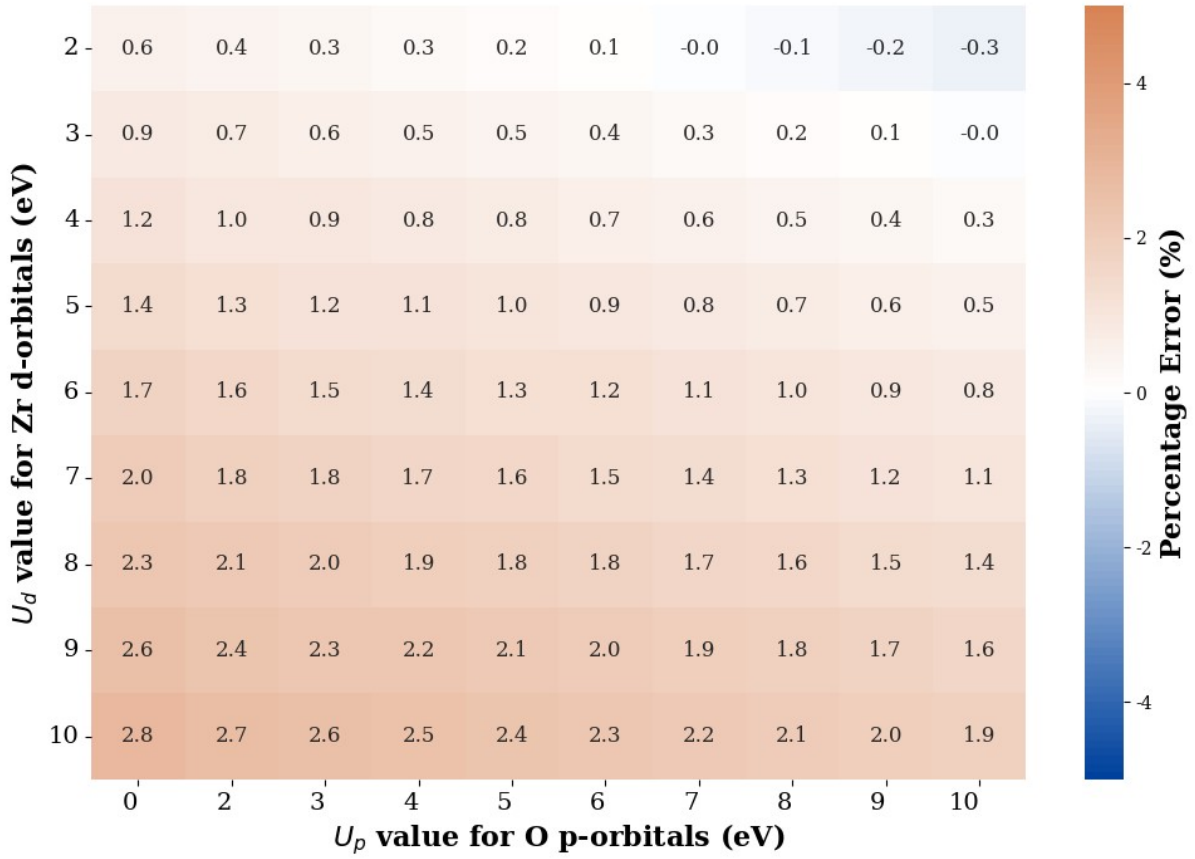

Figure S58. Heatmap of PBE predicted lattice constant (a = b = c) for cubic ZrO_2 as a function of the U_d and U_p parameters.

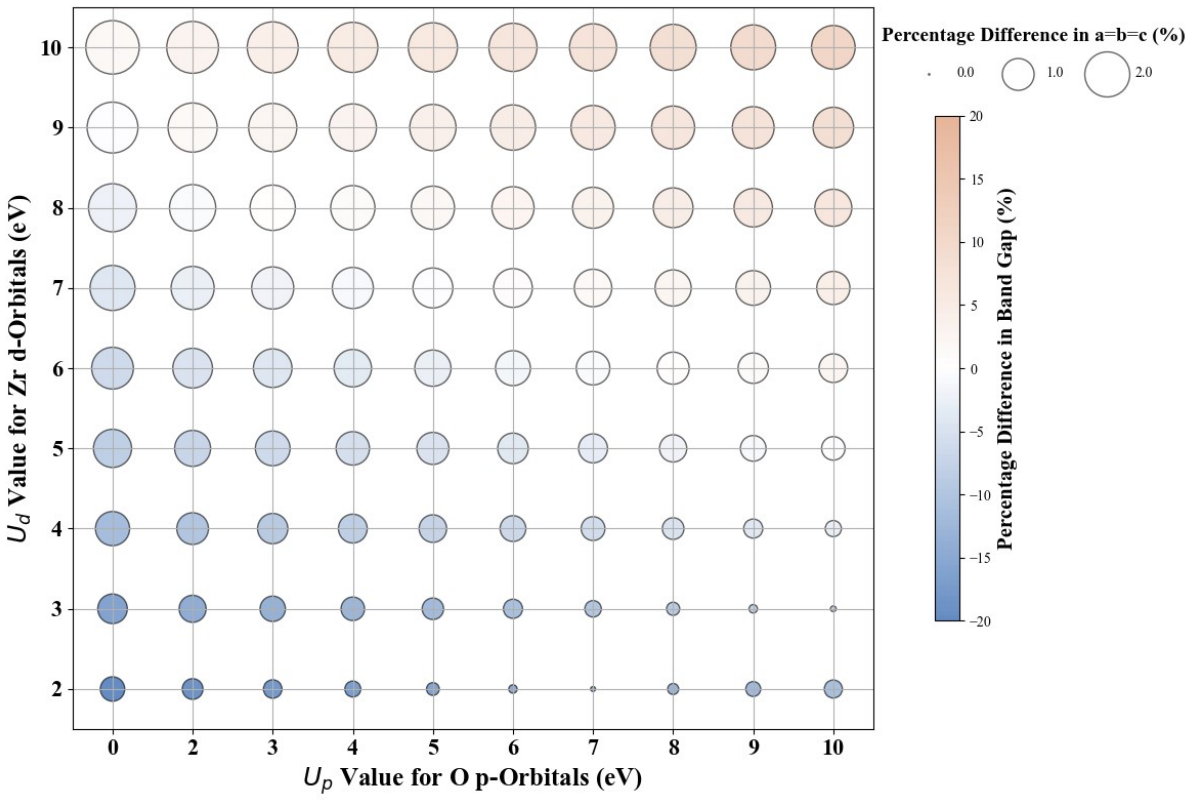

Figure S59. Effect of Hubbard U values on PBE band gap and lattice parameters of c-ZrO_2.

Table S26. Influence of U_d and U_p on cubic ZrO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_d (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	5.1184	3.307	-0.01	-28.11
2	0	5.1491	3.683	0.59	-19.93
2	2	5.1407	3.753	0.43	-18.41
2	3	5.1363	3.789	0.34	-17.63
2	4	5.1318	3.827	0.25	-16.80
2	5	5.1272	3.866	0.16	-15.96
2	6	5.1225	3.907	0.07	-15.07
2	7	5.1177	3.949	-0.02	-14.15
2	8	5.1127	3.993	-0.12	-13.20
2	9	5.1076	4.039	-0.22	-12.20
2	10	5.1024	4.086	-0.32	-11.17
3	0	5.1633	3.877	0.87	-15.72
3	2	5.1559	3.945	0.72	-14.24
3	3	5.1515	3.982	0.64	-13.43
3	4	5.1470	4.020	0.55	-12.61
3	5	5.1423	4.060	0.46	-11.74
3	6	5.1375	4.101	0.36	-10.85
3	7	5.1327	4.144	0.27	-9.91
3	8	5.1276	4.189	0.17	-8.93
3	9	5.1225	4.235	0.07	-7.93
3	10	5.1172	4.283	-0.03	-6.89
4	0	5.1781	4.069	1.16	-11.54
4	2	5.1698	4.140	0.99	-10.00
4	3	5.1654	4.178	0.91	-9.17
4	4	5.1610	4.216	0.82	-8.35
4	5	5.1574	4.254	0.75	-7.52
4	6	5.1525	4.296	0.66	-6.61
4	7	5.1476	4.340	0.56	-5.65
4	8	5.1426	4.385	0.46	-4.67
4	9	5.1374	4.432	0.36	-3.65
4	10	5.1320	4.480	0.26	-2.61
5	0	5.1927	4.218	1.44	-8.30
5	2	5.1843	4.284	1.28	-6.87
5	3	5.1800	4.319	1.19	-6.11
5	4	5.1755	4.355	1.11	-5.33
5	5	5.1709	4.392	1.02	-4.52
5	6	5.1662	4.431	0.92	-3.67
5	7	5.1614	4.471	0.83	-2.80
5	8	5.1564	4.513	0.73	-1.89

5	9	5.1522	4.554	0.65	-1.00
5	10	5.1468	4.599	0.54	-0.02
6	0	5.2072	4.313	1.73	-6.24
6	2	5.1988	4.380	1.56	-4.78
6	3	5.1944	4.415	1.47	-4.02
6	4	5.1899	4.452	1.39	-3.22
6	5	5.1853	4.489	1.30	-2.41
6	6	5.1806	4.528	1.21	-1.57
6	7	5.1758	4.569	1.11	-0.67
6	8	5.1709	4.611	1.02	0.24
6	9	5.1656	4.655	0.91	1.20
6	10	5.1604	4.700	0.81	2.17
7	0	5.2215	4.407	2.00	-4.20
7	2	5.2130	4.475	1.84	-2.72
7	3	5.2086	4.510	1.75	-1.96
7	4	5.2041	4.547	1.66	-1.15
7	5	5.1995	4.585	1.57	-0.33
7	6	5.1947	4.625	1.48	0.54
7	7	5.1899	4.666	1.39	1.43
7	8	5.1850	4.708	1.29	2.35
7	9	5.1797	4.752	1.19	3.30
7	10	5.1745	4.798	1.09	4.30
8	0	5.2356	4.499	2.28	-2.20
8	2	5.2272	4.567	2.11	-0.72
8	3	5.2227	4.603	2.03	0.07
8	4	5.2182	4.641	1.94	0.89
8	5	5.2135	4.679	1.85	1.72
8	6	5.2087	4.719	1.76	2.59
8	7	5.2038	4.760	1.66	3.48
8	8	5.1988	4.803	1.56	4.41
8	9	5.1937	4.848	1.46	5.39
8	10	5.1883	4.894	1.36	6.39
9	0	5.2495	4.589	2.55	-0.24
9	2	5.2410	4.658	2.39	1.26
9	3	5.2365	4.695	2.30	2.07
9	4	5.2320	4.732	2.21	2.87
9	5	5.2273	4.771	2.12	3.72
9	6	5.2225	4.812	2.02	4.61
9	7	5.2176	4.853	1.93	5.50
9	8	5.2126	4.897	1.83	6.46
9	9	5.2074	4.942	1.73	7.43
9	10	5.2021	4.989	1.62	8.46
10	0	5.2632	4.677	2.82	1.67
10	2	5.2547	4.747	2.65	3.20
10	3	5.2502	4.784	2.57	4.00
10	4	5.2457	4.822	2.48	4.83

10	5	5.2410	4.861	2.38	5.67
10	6	5.2362	4.902	2.29	6.57
10	7	5.2312	4.944	2.19	7.48
10	8	5.2262	4.988	2.10	8.43
10	9	5.2210	5.034	1.99	9.43
10	10	5.2156	5.081	1.89	10.46

Table S27. Influence of U_d and U_p on cubic ZrO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_d (eV)	**U_p (eV)**	**a = b = c (Å)**	**E_g (eV)**
1	11	5.0822	3.938
2	15	5.0742	4.353
4	14	5.1094	4.696
7	15	5.1464	5.054
9	14	5.1795	5.194
10	14	5.1927	5.289
11	4	5.2591	4.910
12	2	5.2803	4.921
13	15	5.2254	5.618
15	0	5.3264	4.797

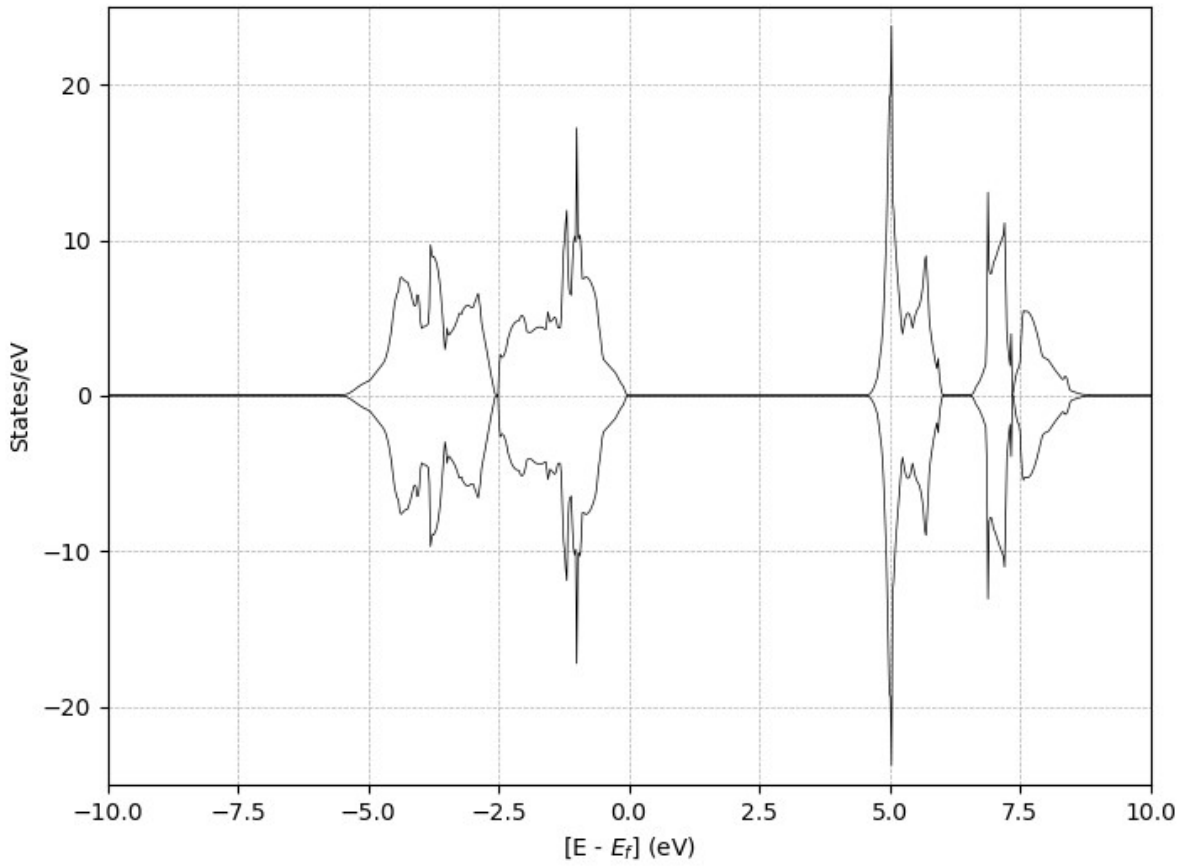

Figure S60. DOS for cubic ZrO_2 with PBE functional: U_p = 9 eV, U_d = 5 eV

CeO_2:

rPBE:

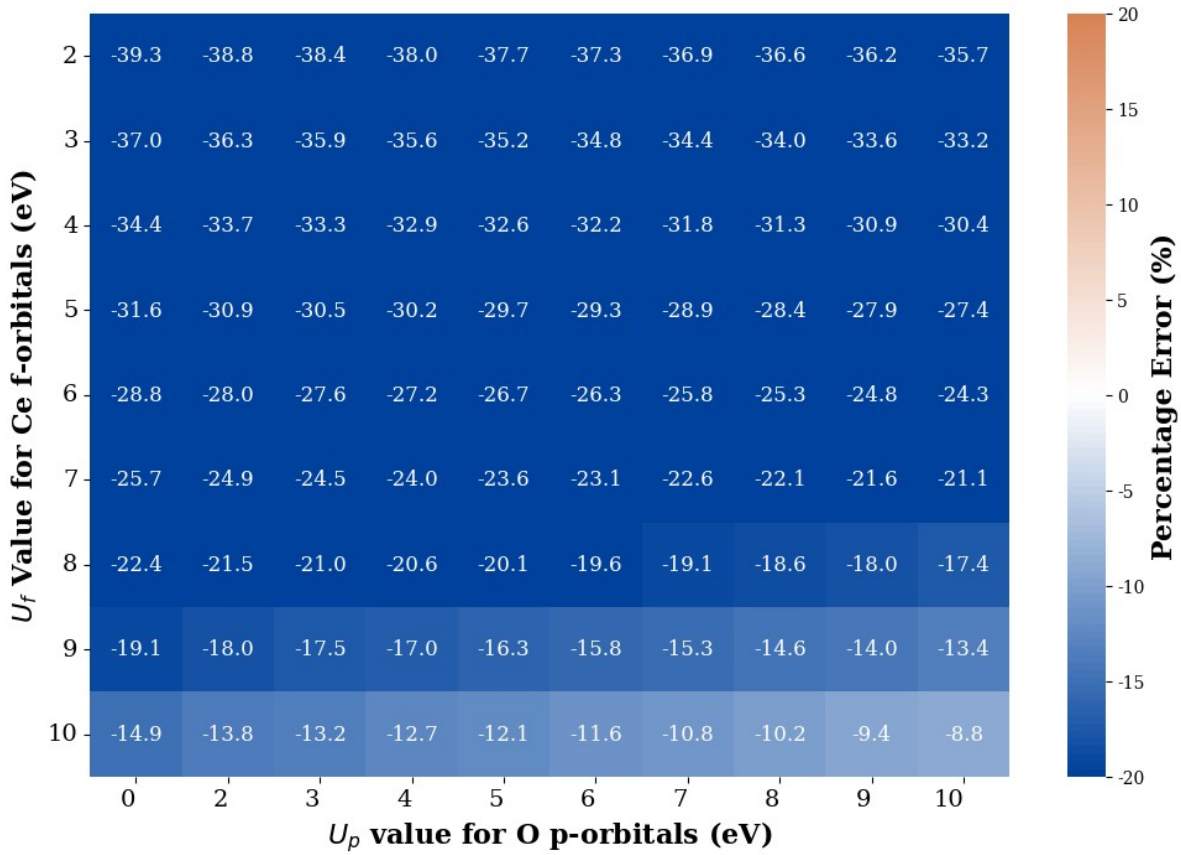

Figure S61. Heatmap of rPBE predicted band gap for cubic CeO_2 as a function of the U_f and U_p parameters.

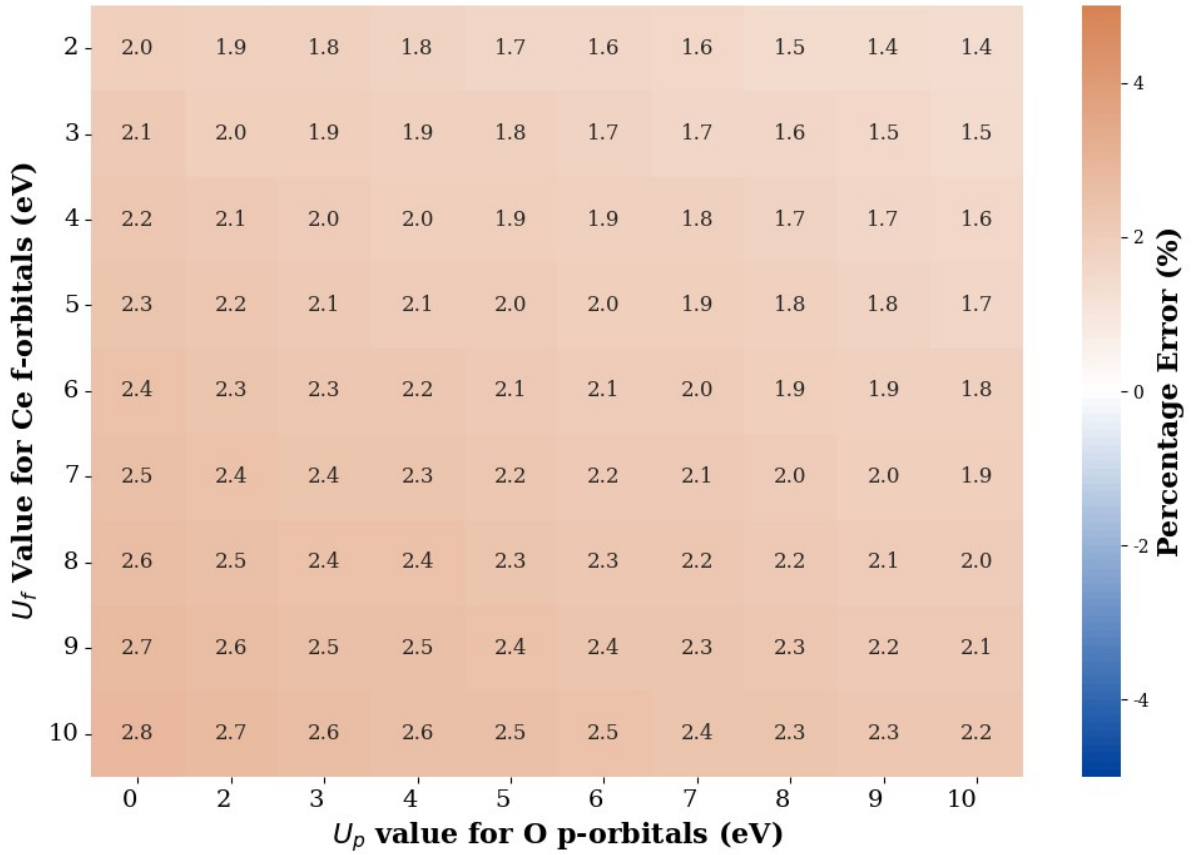

Figure S62. Heatmap of rPBE predicted lattice constant (a = b = c) for cubic CeO_2 as a function of the U_f and U_p parameters.

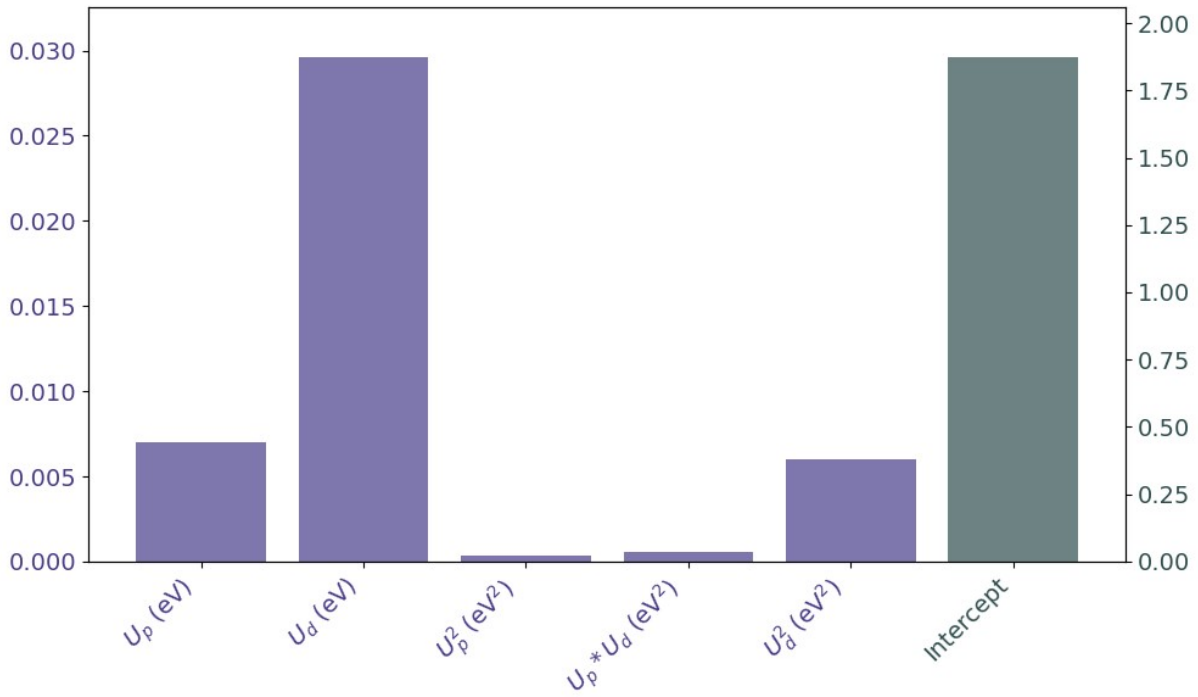

Figure S63. Feature importance of the PR model for predicting the rPBE band gap of c-CeO_2.

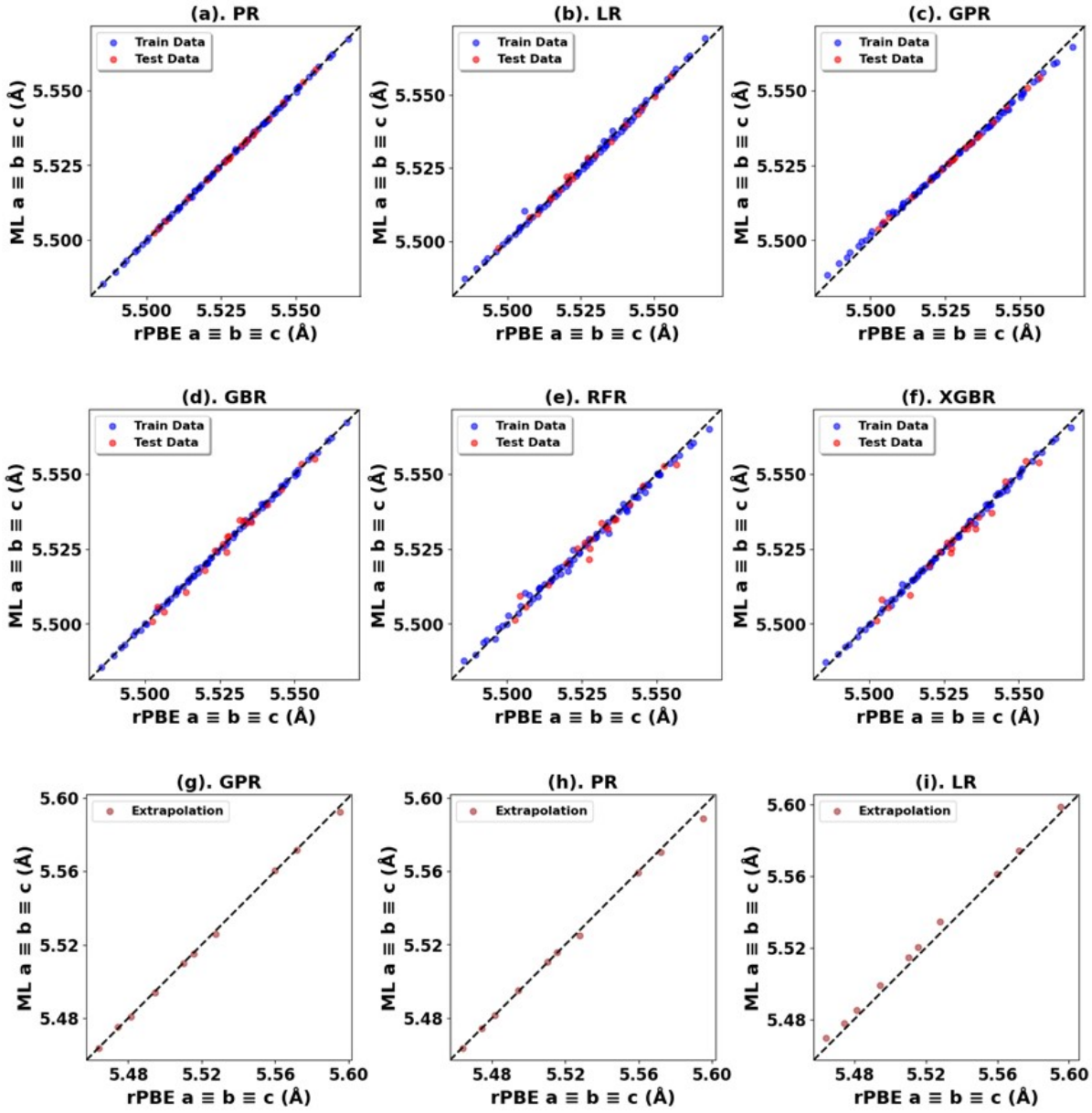

Figure S64. (a) - (f) Performance of models for rPBE lattice parameter (a = b = c) prediction of c-CeO_2 using the initial range of U_p from 0.00 eV to 10.00 eV and U_f from 2.00 eV to 10.00 eV. (g) - (i) Performance of top three models in extrapolation using U_p and U_f values beyond these initial ranges.

Table S28. Comparative performance of models for rPBE lattice constant (a = b = c) prediction in cubic CeO_2.

Oxide	Model	Initial Range				Extrapolation			
		MSE (Å²)	RMSE (Å)	MAE (Å)	R^2	MSE (Å²)	RMSE (Å)	MAE (Å)	R^2
Cubic CeO_2	GPR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	*PR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00
	LR	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.99

	GBR	0.00	0.00	0.00	0.98	0.00	0.02	0.02	0.84
	XGBR	0.00	0.00	0.00	0.97	0.00	0.02	0.02	0.82
	RFR	0.00	0.00	0.00	0.97	0.00	0.02	0.02	0.82

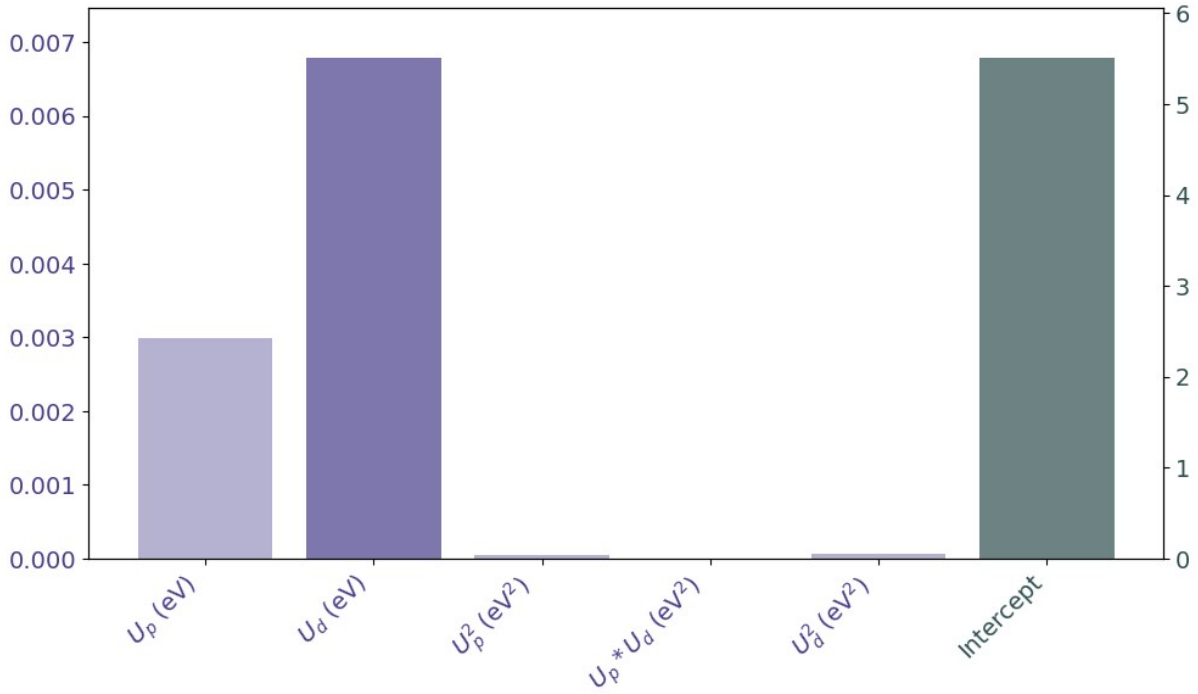

Figure S65. Feature importance of the PR model for predicting the rPBE lattice constant (a = b = c) of c-CeO_2. Lighter shades indicate features with negative contributions.

Table S29. Influence of U_f and U_p on cubic CeO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_f (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	5.5059	1.816	1.75	-43.25
2	0	5.5203	1.942	2.02	-39.31
2	2	5.5151	1.960	1.92	-38.75
2	3	5.5110	1.972	1.85	-38.38
2	4	5.5075	1.983	1.78	-38.03
2	5	5.5042	1.994	1.72	-37.69
2	6	5.5005	2.006	1.65	-37.31
2	7	5.4969	2.018	1.59	-36.94
2	8	5.4932	2.030	1.52	-36.56
2	9	5.4895	2.043	1.45	-36.16
2	10	5.4854	2.057	1.38	-35.72
3	0	5.5273	2.017	2.15	-36.97
3	2	5.5210	2.039	2.03	-36.28

3	3	5.5178	2.050	1.97	-35.94
3	4	5.5144	2.062	1.91	-35.56
3	5	5.5110	2.073	1.85	-35.22
3	6	5.5073	2.085	1.78	-34.84
3	7	5.5038	2.098	1.71	-34.44
3	8	5.4999	2.111	1.64	-34.03
3	9	5.4960	2.125	1.57	-33.59
3	10	5.4921	2.139	1.50	-33.16
4	0	5.5339	2.100	2.27	-34.38
4	2	5.5276	2.122	2.15	-33.69
4	3	5.5240	2.135	2.09	-33.28
4	4	5.5207	2.147	2.03	-32.91
4	5	5.5173	2.158	1.96	-32.56
4	6	5.5137	2.171	1.90	-32.16
4	7	5.5103	2.184	1.84	-31.75
4	8	5.5063	2.198	1.76	-31.31
4	9	5.5025	2.212	1.69	-30.88
4	10	5.4985	2.227	1.62	-30.41
5	0	5.5401	2.188	2.39	-31.63
5	2	5.5338	2.211	2.27	-30.91
5	3	5.5299	2.224	2.20	-30.50
5	4	5.5270	2.235	2.14	-30.16
5	5	5.5235	2.249	2.08	-29.72
5	6	5.5199	2.262	2.01	-29.31
5	7	5.5162	2.276	1.94	-28.88
5	8	5.5126	2.290	1.88	-28.44
5	9	5.5086	2.306	1.80	-27.94
5	10	5.5045	2.322	1.73	-27.44
6	0	5.5461	2.280	2.50	-28.75
6	2	5.5398	2.304	2.38	-28.00
6	3	5.5365	2.317	2.32	-27.59
6	4	5.5330	2.331	2.25	-27.16
6	5	5.5295	2.345	2.19	-26.72
6	6	5.5259	2.358	2.12	-26.31
6	7	5.5222	2.373	2.06	-25.84
6	8	5.5184	2.389	1.99	-25.34
6	9	5.5145	2.405	1.91	-24.84
6	10	5.5105	2.422	1.84	-24.31
7	0	5.5511	2.378	2.59	-25.69
7	2	5.5457	2.403	2.49	-24.91
7	3	5.5423	2.417	2.43	-24.47
7	4	5.5389	2.431	2.36	-24.03
7	5	5.5353	2.446	2.30	-23.56
7	6	5.5317	2.461	2.23	-23.09
7	7	5.5281	2.477	2.16	-22.59
7	8	5.5242	2.493	2.09	-22.09

7	9	5.5204	2.510	2.02	-21.56
7	10	5.5162	2.526	1.94	-21.06
8	0	5.5566	2.483	2.69	-22.41
8	2	5.5503	2.512	2.57	-21.50
8	3	5.5468	2.527	2.51	-21.03
8	4	5.5445	2.540	2.47	-20.63
8	5	5.5410	2.556	2.40	-20.13
8	6	5.5374	2.572	2.34	-19.63
8	7	5.5337	2.589	2.27	-19.09
8	8	5.5299	2.606	2.20	-18.56
8	9	5.5260	2.624	2.13	-18.00
8	10	5.5220	2.643	2.05	-17.41
9	0	5.5623	2.589	2.80	-19.09
9	2	5.5558	2.623	2.68	-18.03
9	3	5.5524	2.640	2.61	-17.50
9	4	5.5502	2.655	2.57	-17.03
9	5	5.5455	2.677	2.49	-16.34
9	6	5.5430	2.693	2.44	-15.84
9	7	5.5393	2.710	2.37	-15.31
9	8	5.5356	2.732	2.30	-14.63
9	9	5.5317	2.751	2.23	-14.03
9	10	5.5274	2.771	2.15	-13.41
10	0	5.5675	2.724	2.89	-14.88
10	2	5.5613	2.758	2.78	-13.81
10	3	5.5576	2.777	2.71	-13.22
10	4	5.5545	2.794	2.65	-12.69
10	5	5.5510	2.813	2.59	-12.09
10	6	5.5474	2.829	2.52	-11.59
10	7	5.5437	2.854	2.45	-10.81
10	8	5.5407	2.873	2.40	-10.22
10	9	5.5359	2.898	2.31	-9.44
10	10	5.5330	2.917	2.25	-8.84

Table S30. Influence of U_f and U_p on cubic CeO_2 DFT+U (rPBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_f (eV)	**U_p (eV)**	**a = b = c (Å)**	**E_g (eV)**

1	11	5.4744	1.996
2	15	5.4640	2.126
4	14	5.4815	2.288
7	15	5.4944	2.626
9	14	5.5102	2.858
10	14	5.5156	3.009
11	4	5.5598	2.959
12	2	5.5719	3.114
13	15	5.5278	3.617
15	0	5.5952	3.775

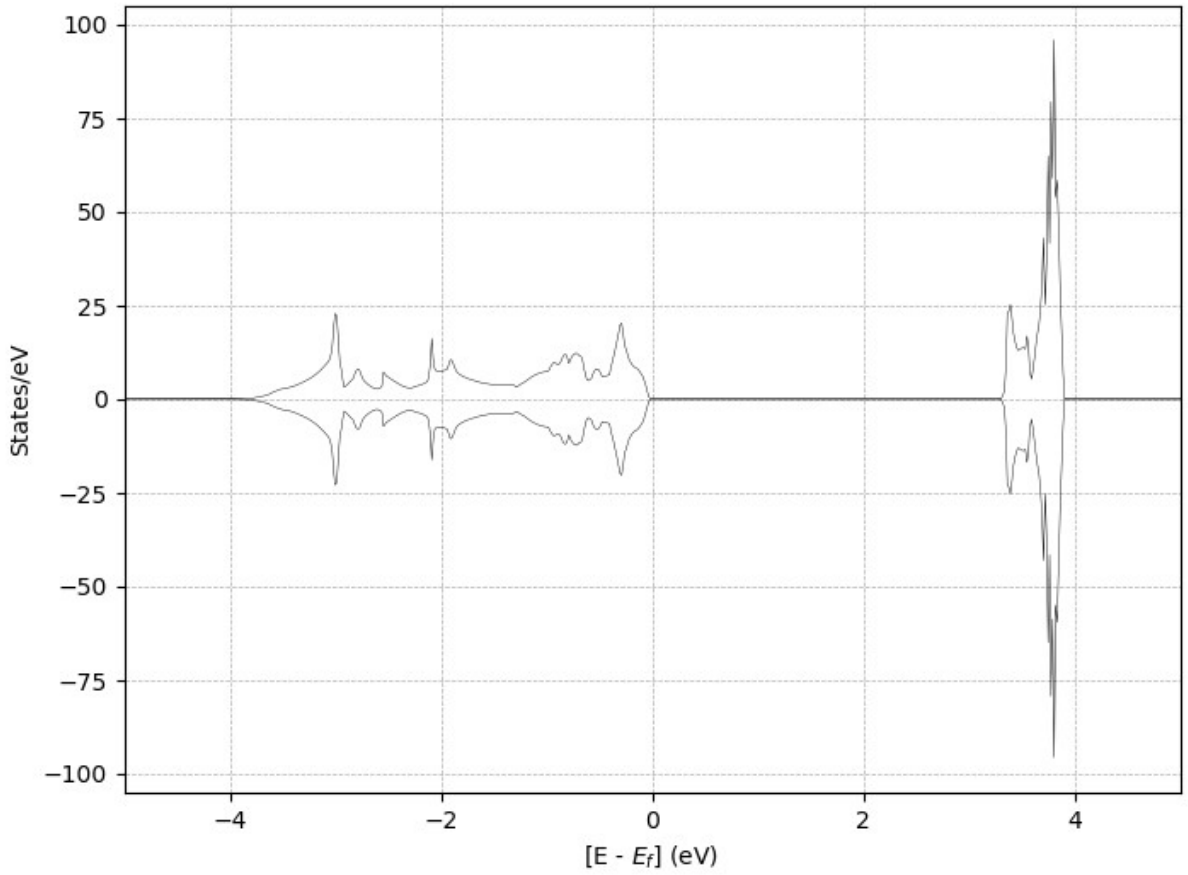

Figure S66. DOS for cubic CeO_2 with rPBE functional: U_p = 7 eV, U_f = 12 eV

PBE:

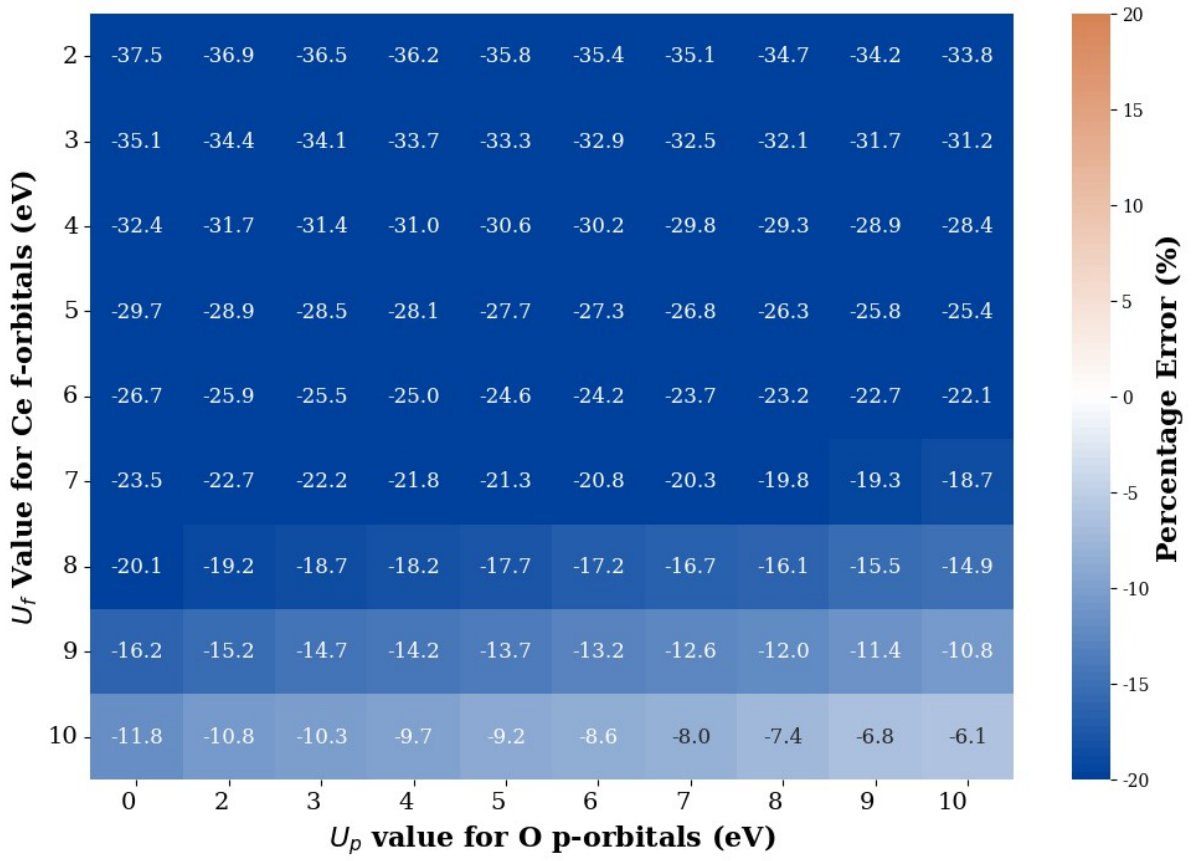

Figure S67. Heatmap of PBE predicted band gap for cubic CeO_2 as a function of the U_f and U_p parameters.

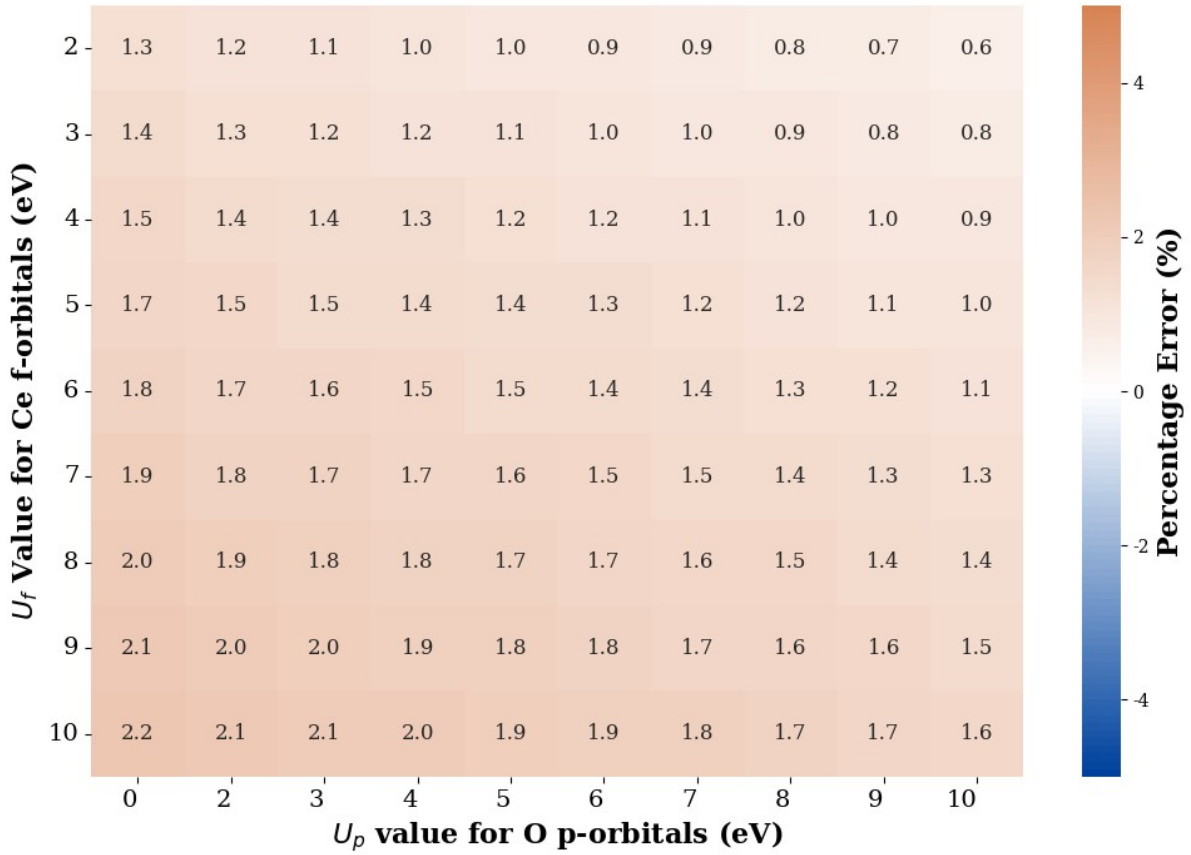

Figure S68. Heatmap of PBE predicted lattice constant (a = b = c) for cubic CeO_2 as a function of the U_f and U_p parameters.

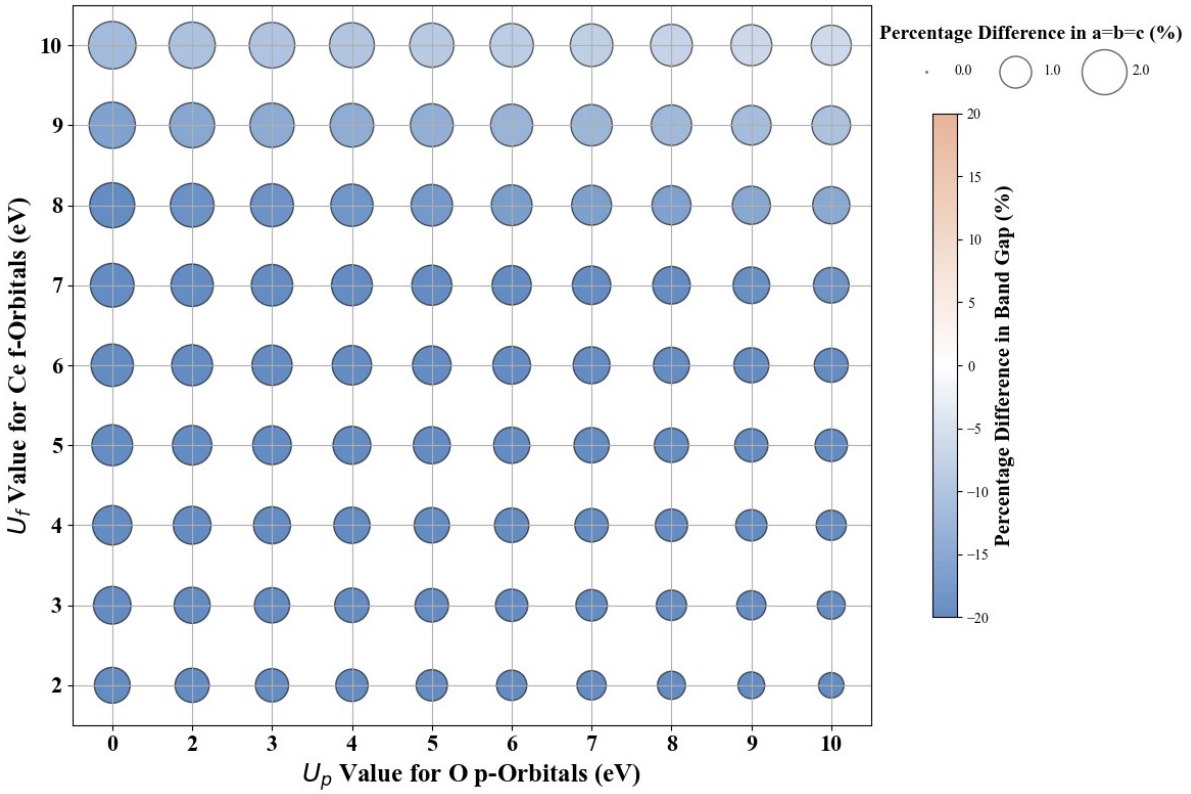

Figure S69. Effect of Hubbard U values on PBE band gap and lattice parameters of c-CeO_2.

Table S31. Influence of U_f and U_p on cubic CeO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g)

U_f (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)	% Deviation in a = b = c	% Deviation in E_g
0	0	5.4640	1.871	0.98	-41.53
2	0	5.4800	1.999	1.27	-37.53
2	2	5.4739	2.020	1.16	-36.88
2	3	5.4705	2.031	1.10	-36.53
2	4	5.4675	2.042	1.04	-36.19
2	5	5.4640	2.054	0.98	-35.81
2	6	5.4605	2.066	0.91	-35.44
2	7	5.4570	2.078	0.85	-35.06
2	8	5.4534	2.091	0.78	-34.66
2	9	5.4497	2.104	0.72	-34.25
2	10	5.4458	2.118	0.64	-33.81
3	0	5.4872	2.078	1.41	-35.06
3	2	5.4812	2.099	1.30	-34.41
3	3	5.4779	2.110	1.24	-34.06
3	4	5.4748	2.122	1.18	-33.69
3	5	5.4713	2.135	1.11	-33.28
3	6	5.4675	2.147	1.04	-32.91
3	7	5.4643	2.160	0.99	-32.50
3	8	5.4607	2.173	0.92	-32.09
3	9	5.4569	2.187	0.85	-31.66
3	10	5.4531	2.202	0.78	-31.19
4	0	5.4942	2.162	1.54	-32.44
4	2	5.4880	2.185	1.42	-31.72
4	3	5.4849	2.196	1.37	-31.38
4	4	5.4817	2.208	1.31	-31.00
4	5	5.4782	2.221	1.24	-30.59
4	6	5.4748	2.234	1.18	-30.19
4	7	5.4712	2.248	1.11	-29.75
4	8	5.4675	2.262	1.04	-29.31
4	9	5.4639	2.276	0.98	-28.88
4	10	5.4600	2.292	0.91	-28.38
5	0	5.5010	2.251	1.66	-29.66
5	2	5.4948	2.275	1.55	-28.91
5	3	5.4917	2.288	1.49	-28.50
5	4	5.4884	2.301	1.43	-28.09
5	5	5.4849	2.314	1.37	-27.69
5	6	5.4815	2.328	1.30	-27.25
5	7	5.4780	2.342	1.24	-26.81

5	8	5.4743	2.357	1.17	-26.34
5	9	5.4705	2.373	1.10	-25.84
5	10	5.4675	2.387	1.04	-25.41
6	0	5.5076	2.346	1.78	-26.69
6	2	5.5014	2.372	1.67	-25.88
6	3	5.4981	2.385	1.61	-25.47
6	4	5.4949	2.399	1.55	-25.03
6	5	5.4914	2.413	1.49	-24.59
6	6	5.4880	2.427	1.42	-24.16
6	7	5.4844	2.443	1.36	-23.66
6	8	5.4808	2.459	1.29	-23.16
6	9	5.4770	2.475	1.22	-22.66
6	10	5.4732	2.492	1.15	-22.13
7	0	5.5140	2.448	1.90	-23.50
7	2	5.5078	2.475	1.79	-22.66
7	3	5.5038	2.490	1.71	-22.19
7	4	5.5011	2.504	1.67	-21.75
7	5	5.4977	2.519	1.60	-21.28
7	6	5.4942	2.534	1.54	-20.81
7	7	5.4906	2.551	1.47	-20.28
7	8	5.4870	2.566	1.41	-19.81
7	9	5.4832	2.584	1.33	-19.25
7	10	5.4793	2.602	1.26	-18.69
8	0	5.5203	2.557	2.02	-20.09
8	2	5.5139	2.587	1.90	-19.16
8	3	5.5105	2.602	1.84	-18.69
8	4	5.5073	2.618	1.78	-18.19
8	5	5.5039	2.634	1.72	-17.69
8	6	5.5004	2.650	1.65	-17.19
8	7	5.4968	2.667	1.59	-16.66
8	8	5.4931	2.685	1.52	-16.09
8	9	5.4894	2.703	1.45	-15.53
8	10	5.4855	2.722	1.38	-14.94
9	0	5.5263	2.682	2.13	-16.19
9	2	5.5200	2.713	2.01	-15.22
9	3	5.5167	2.729	1.95	-14.72
9	4	5.5134	2.745	1.89	-14.22
9	5	5.5100	2.762	1.83	-13.69
9	6	5.5064	2.779	1.76	-13.16
9	7	5.5028	2.797	1.70	-12.59
9	8	5.4991	2.816	1.63	-12.00
9	9	5.4953	2.835	1.56	-11.41
9	10	5.4914	2.856	1.49	-10.75
10	0	5.5323	2.823	2.24	-11.78
10	2	5.5260	2.855	2.13	-10.78
10	3	5.5227	2.872	2.06	-10.25

10	4	5.5194	2.889	2.00	-9.72
10	5	5.5159	2.906	1.94	-9.19
10	6	5.5124	2.925	1.87	-8.59
10	7	5.5088	2.944	1.81	-8.00
10	8	5.5051	2.964	1.74	-7.38
10	9	5.5013	2.984	1.67	-6.75
10	10	5.4974	3.006	1.60	-6.06

Table S32. Influence of U_f and U_p on cubic CeO_2 DFT+U (PBE) predicted lattice parameters (a = b, c) and bandgap (E_g) [Extrapolation]

U_f (eV)	U_p (eV)	a = b = c (Å)	E_g (eV)
1	11	5.43445252	2.056
2	15	5.42535441	2.192
4	14	5.44371077	2.357
7	15	5.45838377	2.702
9	14	5.47476963	2.944
10	14	5.48063984	3.099
11	4	5.52537163	3.053
12	2	5.53703115	3.206
13	15	5.49396998	3.716
15	0	5.5612335	3.87

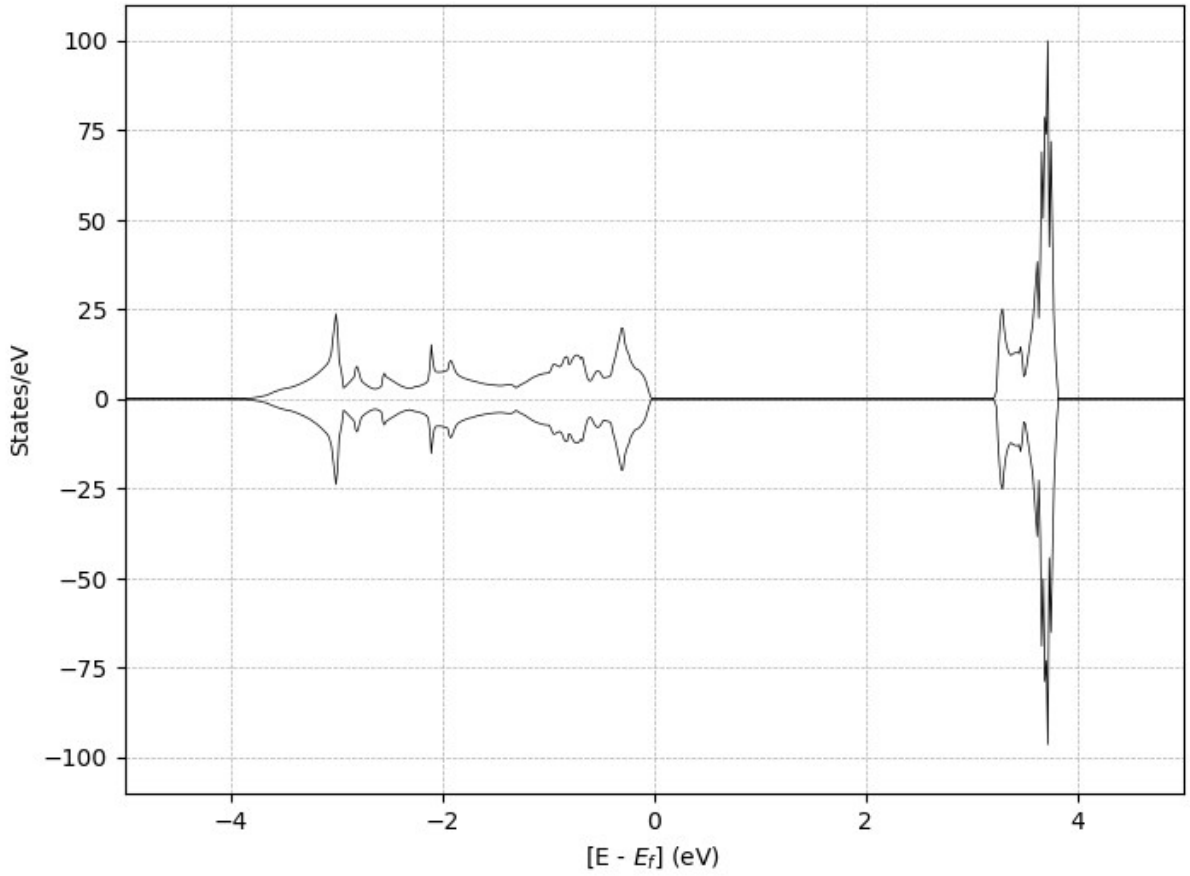

Figure S70. DOS for cubic CeO_2 with rPBE functional: U_p = 2 eV, U_f = 12 eV

Further Analysis:

Table S33. Descriptions of constituent elements and metal oxide features considered in model training across metal oxides. *Possible redundant feature.

Feature	Description
POSCAR Crystal System	Crystal system of the metal oxide structure from POSCAR data
Oxide	Metal oxide formula
Ud_Value/eV	U_d value applied to the d-orbitals of the metal (X)
Uf_Value/eV	U_f value applied to the f-orbitals of the metal (X)
Up_Value/eV	U_p value applied to the p-orbitals of oxygen
Number of X atoms	Number of metal (X) atoms in the metal oxide unit cell
Number of O atoms	Number of oxygen (O) atoms in the metal oxide unit cell
POSCAR α (°)	Alpha angle of the metal oxide structure in degrees
POSCAR β (°)	Beta angle of the metal oxide structure in degrees
POSCAR γ (°)	Gamma angle of the metal oxide structure in degrees
*POSCAR Volume (Å³)	Volume of the metal oxide structure in cubic angstroms (Å³)
POSCAR a (Å)	Lattice constant a of the metal oxide structure in angstroms (Å)
POSCAR b (Å)	Lattice constant b of the metal oxide structure in angstroms (Å)
POSCAR c (Å)	Lattice constant c of the metal oxide structure in angstroms (Å)
POSCAR Space Group	Space group of the metal oxide structure
POSCAR Hall Number	Hall number of the metal oxide structure
POSCAR International Number	International number of the metal oxide structure
*POSCAR Symbol	Symbol of the metal oxide structure
POSCAR Point Group	Point group of the metal oxide structure
Space_group_number_of_X	Space group number of the metal (X)
Space_group_of_X	Space group of the metal (X)
Structure_of_X	Structure type of metal (X)
Lattice_constant_a_of_X_pm	Lattice constant a of the metal (X) structure in picometers (pm)
Lattice_constant_b_of_X_pm	Lattice constant b of the metal (X) structure in picometers (pm)
Lattice_constant_c_of_X_pm	Lattice constant c of the metal (X) structure in picometers (pm)
Atomic_radius/pm_of_X	Atomic radius of the metal (X) in picometers (pm)
Van_der_Waals_radius/pm_of_X	Van der Waals radius of the metal (X) in picometers (pm)

Atomic_No_of_X	Atomic number of the metal (X)
Atomic_Mass/amu_of_X	Atomic mass of the metal (X) in atomic mass units (amu)
Period_of_X	Period of the metal (X) in the periodic table
First_ionization_energy/KJ/mol_of_X	First ionization energy of the metal (X) in kJ/mol
Density/Kg/m³_of_X	Density of the metal (X) in kg/m³
Electron_Affinity/eV_of_X	Electron affinity of the metal (X) in electron volts (eV)
Work_Function/eV_of_X	Work function of the metal (X) in electron volts (eV)
Pauling_Electronegativity/units_of_X	Pauling electronegativity of the metal (X)
d-shell_of_X	Number of electrons in the d-shell of the metal (X)
Lattice_angle_alpha_of_X_degree	Alpha angle of the metal (X) structure in degrees
Lattice_angle_beta_of_X_degree	Beta angle of the metal (X) structure in degrees
Lattice_angle_gamma_of_X_degree	Gamma angle of the metal (X) structure in degrees
Pauling_Electronegativity_Difference/units_of_O_and_X	Pauling electronegativity difference between oxygen (O) and metal (X)
Mean Metal Valence Electrons	Mean number of valence electrons for metal (X)
Mean Metal Bond Length (Å)	Mean bond length between metal (X) and its neighbors in angstroms (Å)
Min Metal Bond Length (Å)	Minimum bond length between metal (X) and its neighbors in angstroms (Å)
Max Metal Bond Length (Å)	Maximum bond length between metal (X) and its neighbors in angstroms (Å)
Std Metal Bond Length (Å)	Standard deviation of bond lengths for metal (X) and its neighbors in Å
Sum Metal Bond Length (Å)	Sum of bond lengths for metal (X) and its neighbors in angstroms (Å)
Mean Metal Coordination Number	Mean coordination number of metal (X)
Min Metal Coordination Number	Minimum coordination number of metal (X)
Max Metal Coordination Number	Maximum coordination number of metal (X)
Std Metal Coordination Number	Standard deviation of coordination numbers for metal (X)
Sum Metal Coordination Number	Sum of coordination numbers for metal (X)
Mean Metal Oxidation State	Mean oxidation state of metal (X)
Mean Oxygen Valence Electrons	Mean number of valence electrons for oxygen atoms
Mean Oxygen Bond Length (Å)	Mean bond length between oxygen and its neighbors in angstroms (Å)
Min Oxygen Bond Length (Å)	Minimum bond length between oxygen and its neighbors in angstroms (Å)
Max Oxygen Bond Length (Å)	Maximum bond length between oxygen and its neighbors in angstroms (Å)

Std Oxygen Bond Length (Å)	Standard deviation of bond lengths for oxygen and its neighbors in Å
Sum Oxygen Bond Length (Å)	Sum of bond lengths for oxygen and its neighbors in angstroms (Å)
Mean Oxygen Coordination Number	Mean coordination number of oxygen atoms
Min Oxygen Coordination Number	Minimum coordination number of oxygen atoms
Max Oxygen Coordination Number	Maximum coordination number of oxygen atoms
Std Oxygen Coordination Number	Standard deviation of coordination numbers for oxygen atoms
Sum Oxygen Coordination Number	Sum of coordination numbers for oxygen atoms
Mean Oxygen Oxidation State	Mean oxidation state of oxygen atoms

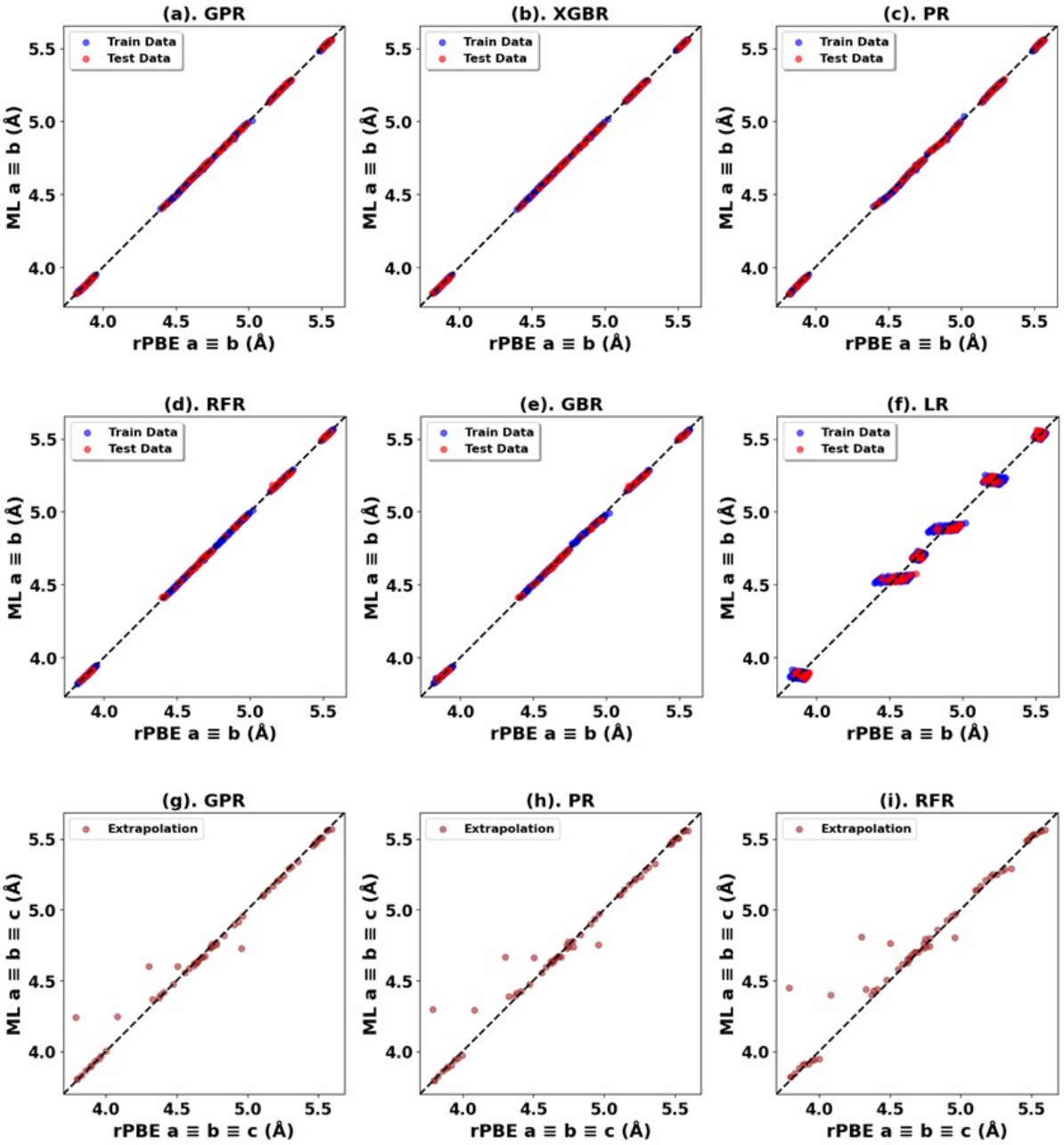

Figure S71. (a) - (f) Performance of ML models for rPBE lattice parameter (a = b) prediction across all six (6) primary metal oxides. (g) - (i) Performance of models in extrapolation using U_p and $U_{d/f}$ values beyond the initial range.

Table S34. Comparative performance of ML models for rPBE lattice parameter (a = b) prediction across all six primary metal oxides.

Oxides	Model	Initial Range				Extrapolation			
		MSE (Å²)	**RMSE (Å)**	**MAE (Å)**	**R^2**	**MSE (Å²)**	**RMSE (Å)**	**MAE (Å)**	**R^2**
All six (6) primary metal oxides in this study	*GPR	0.00	0.00	0.00	1.00	0.01	0.08	0.03	0.98
	PR	0.00	0.01	0.00	1.00	0.01	0.09	0.03	0.97
	RFR	0.00	0.01	0.00	1.00	0.02	0.12	0.05	0.95
	XGBR	0.00	0.00	0.00	1.00	0.02	0.12	0.05	0.95
	GBR	0.00	0.01	0.01	1.00	0.02	0.13	0.06	0.94
	LR	0.00	0.04	0.04	0.99	0.03	0.16	0.09	0.92

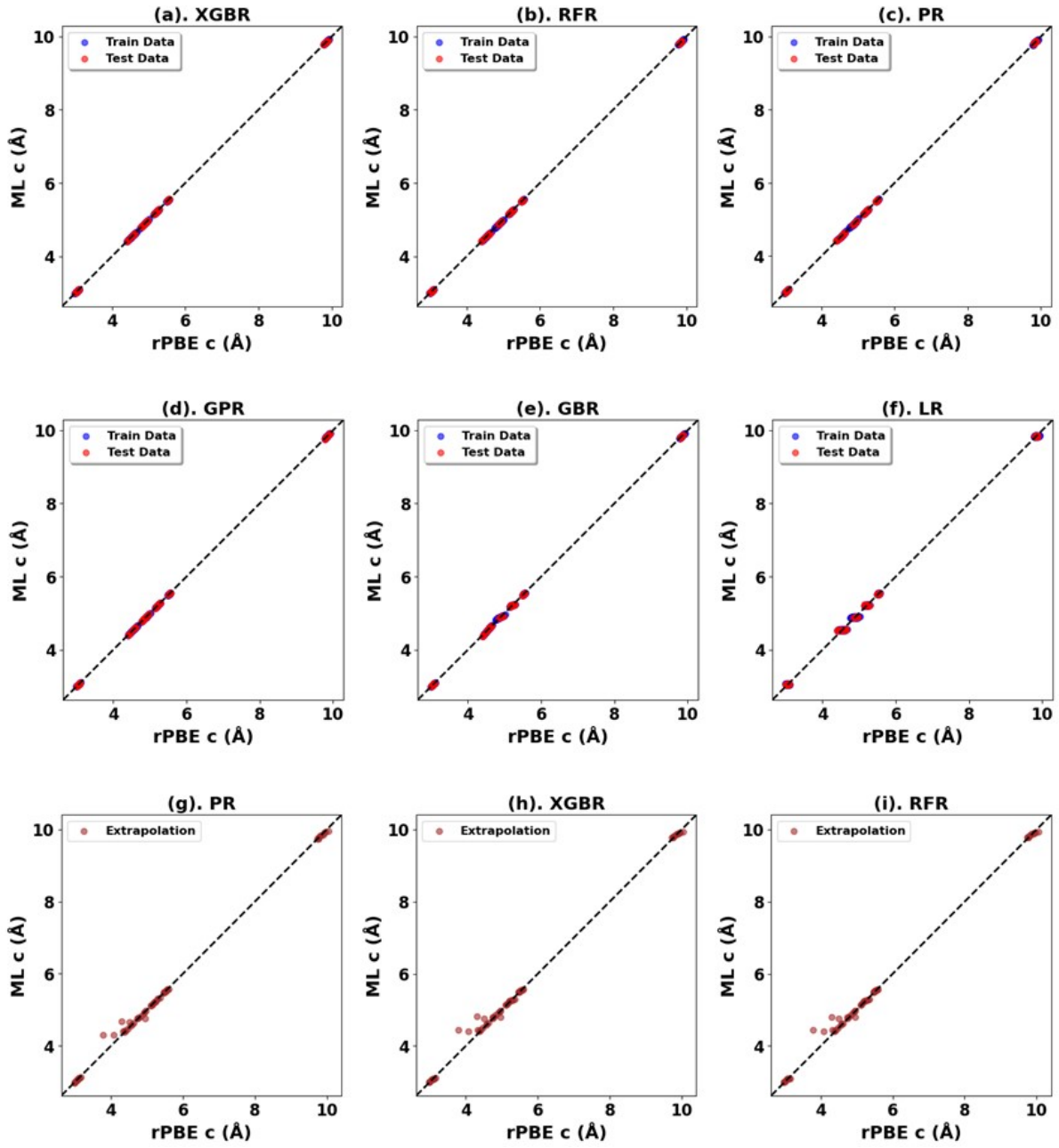

Figure S72. (a) - (f) Performance of ML models for rPBE lattice parameter (c) prediction across all six (6) primary metal oxides. (g) - (i) Performance of models in extrapolation using U_p and $U_{d/f}$ values beyond the initial range.

Table S35. Comparative performance of ML models for rPBE lattice parameter (c) prediction across all six primary metal oxides.

Oxides	Model	Initial Range				Extrapolation			
		MSE (Å²)	**RMSE (Å)**	**MAE (Å)**	**R^2**	**MSE (Å²)**	**RMSE (Å)**	**MAE (Å)**	**R^2**
All six (6) primary metal oxides in this study	PR	0.00	0.01	0.00	1.00	0.01	0.10	0.04	1.00
	*XGBR	0.00	0.00	0.00	1.00	0.02	0.13	0.06	1.00
	RFR	0.00	0.01	0.00	1.00	0.02	0.13	0.06	1.00
	GBR	0.00	0.02	0.01	1.00	0.02	0.14	0.06	1.00
	LR	0.00	0.05	0.04	1.00	0.03	0.17	0.10	0.99
	GPR	0.00	0.01	0.00	1.00	0.04	0.20	0.14	0.99

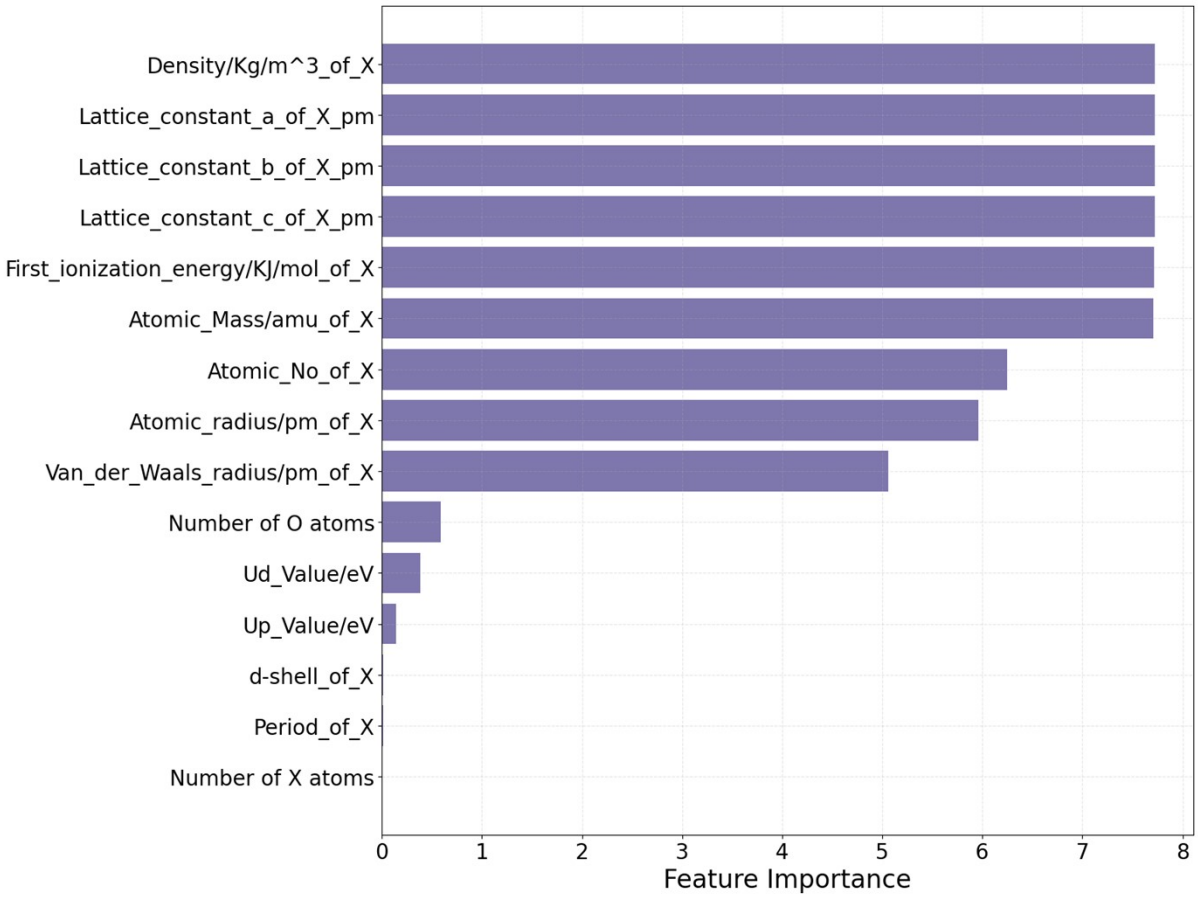

Figure S73. Feature importance analysis from the GPR Model for predicting the rPBE band gap across six primary metal oxides.

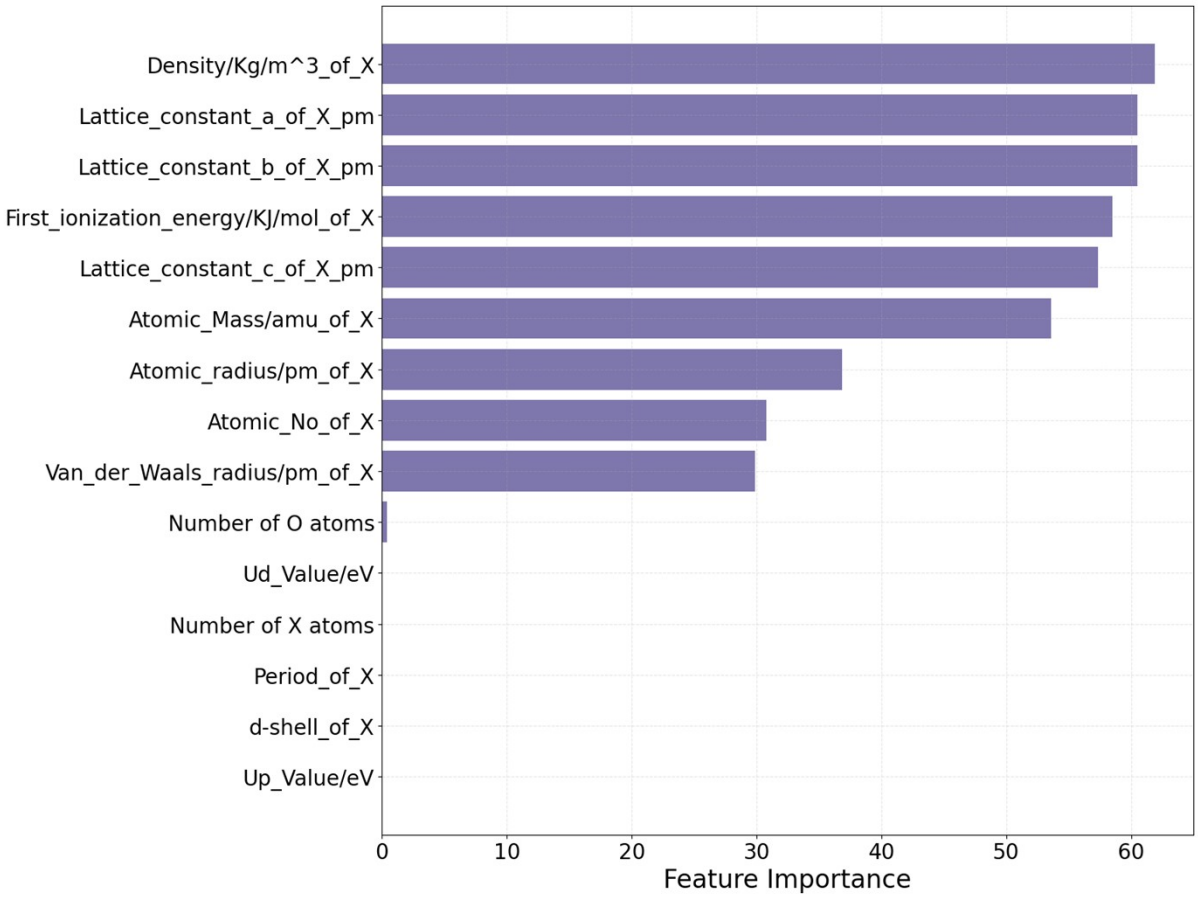

Figure S74. Feature importance analysis from the GPR Model for predicting the rPBE lattice constant (a = b) across six primary metal oxides.

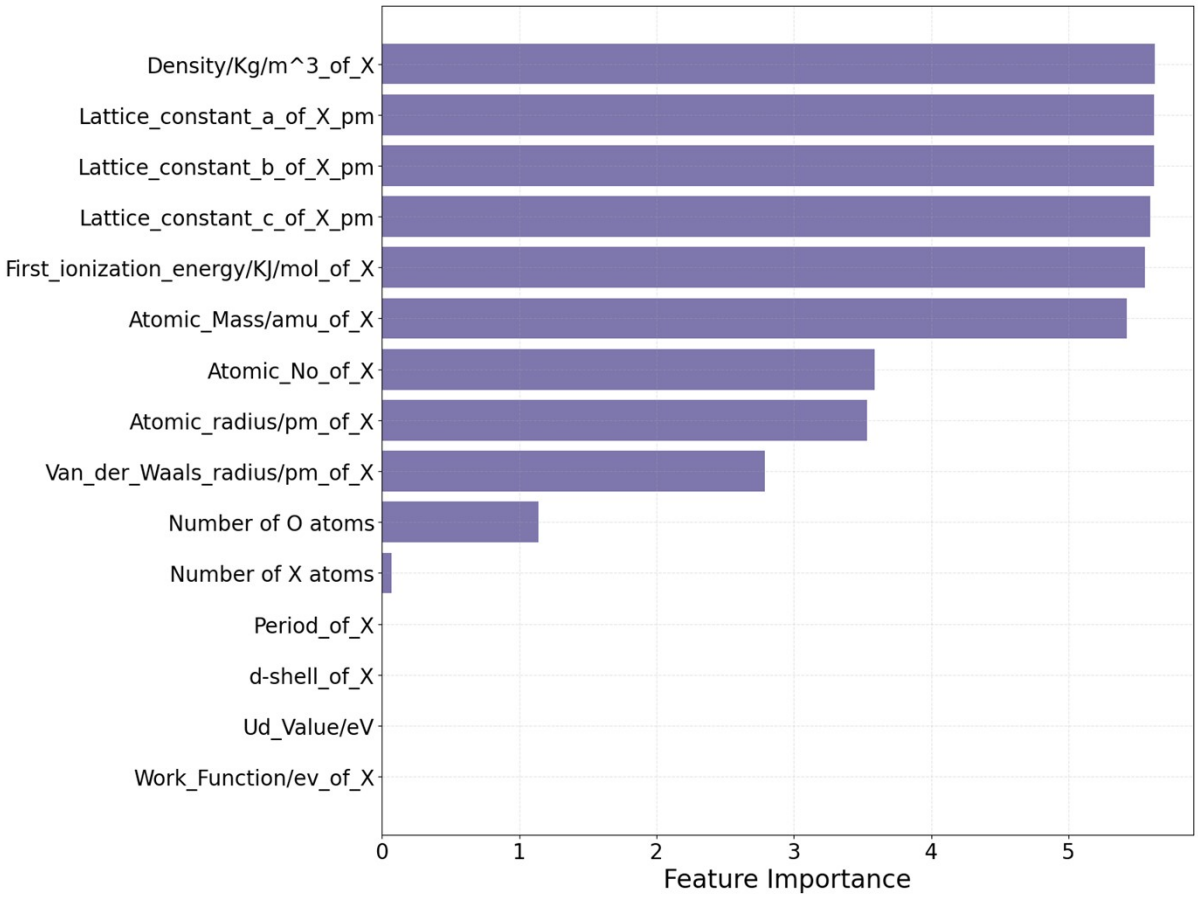

Figure S75. Feature importance analysis from the GPR Model for predicting the rPBE lattice constant (c) across six primary metal oxides.

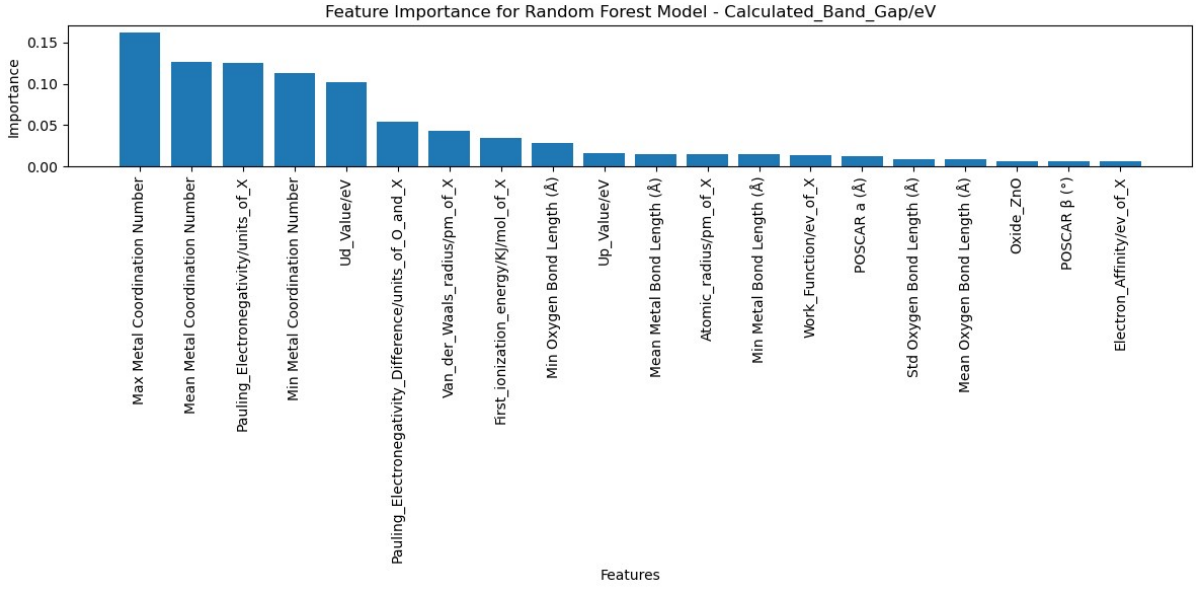

Figure S76. Feature importance analysis from the RFR Model for predicting the rPBE band gap across thirty-eight (38) metal oxides.

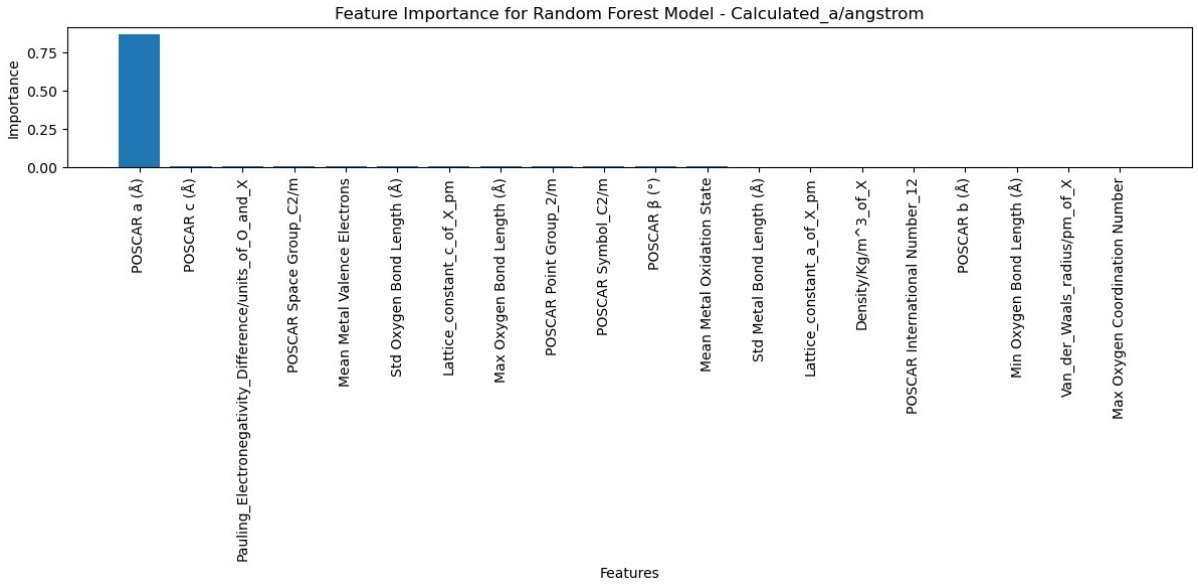

Figure S77. Feature importance analysis from the RFR Model for predicting the rPBE lattice constant (a) across thirty-eight (38) metal oxides.

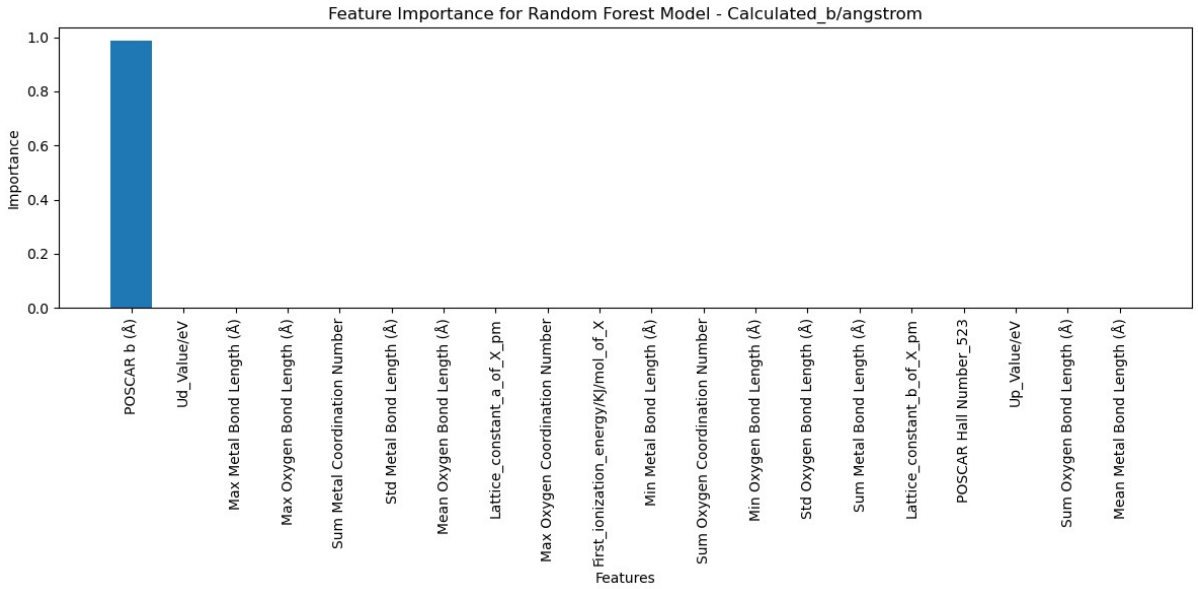

Figure S78. Feature importance analysis from the RFR Model for predicting the rPBE lattice constant (b) across thirty-eight (38) metal oxides.

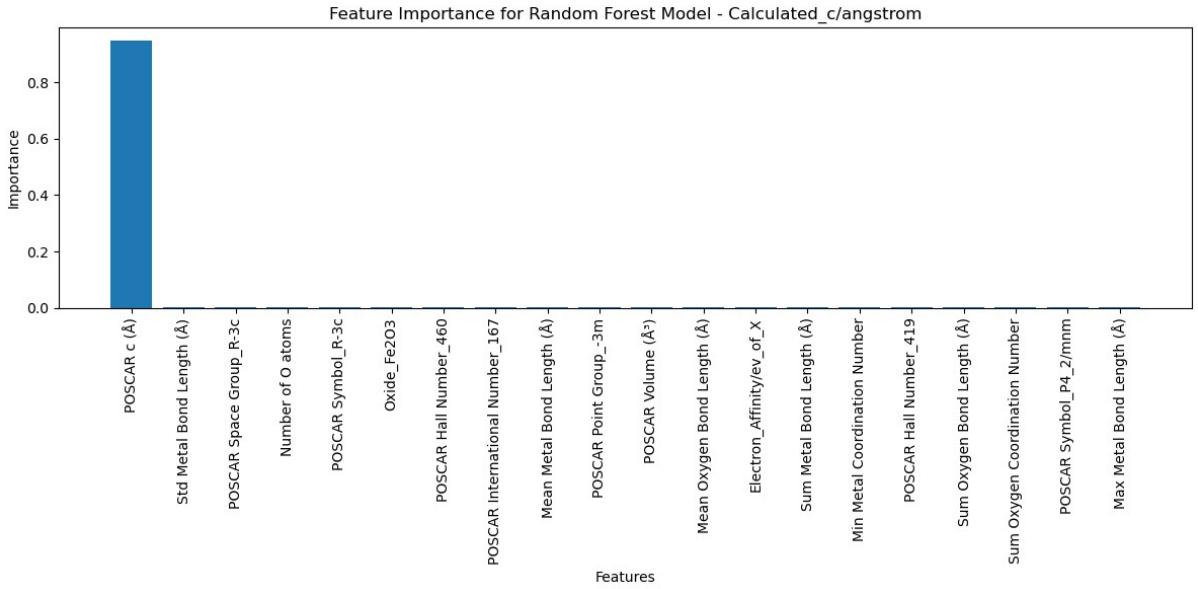

Figure S79. Feature importance analysis from the RFR Model for predicting the rPBE lattice constant (c) across thirty-eight (38) metal oxides.

MP-ID	Formula	Crystal System	Space Group	Space Group Number
mp-19128	CoO	Hexagonal	P6_3mc	186
mp-19770	Fe2O3	Trigonal	R-3c	167
mp-1986	*ZnO*	*Cubic*	*F-43m*	*216*
mp-20194	*CeO2*	*Cubic*	*Fm-3m*	*225*
mp-2133	ZnO	Hexagonal	P6_3mc	186
mp-2229	ZnO	Cubic	Fm-3m	225
mp-22408	CoO	Cubic	F-43m	216
mp-2574	ZrO2	Tetragonal	P4_2/nmc	137
mp-2657	*TiO2*	*Tetragonal*	*P4_2/mnm*	*136*
mp-1093993	ZnO	Tetragonal	P4_2/mnm	136
mp-1102744	ZnO2	Orthorhombic	P2_12_12_1	19
mp-1178232	FeO	Monoclinic	C2/m	12
mp-1178247	FeO	Trigonal	P31c	159
mp-1190186	ZrO2	Orthorhombic	Pbca	61
mp-1439	TiO2	Orthorhombic	Pbcn	60
mp-1565	*ZrO2*	*Cubic*	*Fm-3m*	*225*
mp-1840	TiO2	Orthorhombic	Pbca	61
mp-19009	NiO	Cubic	Fm-3m	225
mp-2858	ZrO2	Monoclinic	P2_1/c	14
mp-352	HfO2	Monoclinic	P2_1/c	14
mp-390	*TiO2*	*Tetragonal*	*I4_1/amd*	*141*
mp-715514	V2O3	Monoclinic	C2/c	15

mp-8484	*ZnO2*	*Cubic*	*Pa-3*	*205*
mp-720166	V2O5	Monoclinic	C2/m	12
mp-510568	V2O5	Monoclinic	P2_1/m	11
mp-754670	V2O5	Orthorhombic	Pmmn	59
mp-25279	V2O5	Orthorhombic	Pmmn	59
mp-19443	WO3	Tetragonal	P4/nmm	129
mp-636148	WO3	Monoclinic	P2_1/c	14
mp-545665	WO3	Hexagonal	P6/mmm	191
mp-19390	WO3	Cubic	Pm-3m	221
mp-19033	WO3	Monoclinic	P2_1/c	14
mp-2235359	WO3	Tetragonal	P-42_1m	113
mp-18773	WO3	Tetragonal	P4/ncc	130
mp-741	HfO2	Orthorhombic	Pnma	62
mp-550893	HfO2	Cubic	Fm-3m	225
mp-1018721	HfO2	Tetragonal	P4_2/nmc	137
mp-1858	HfO2	Orthorhombic	Pbca	61