

Intrinsic Oxygen Vacancy and Extrinsic Aluminium Dopant Interplay: A Route to the Restoration of Defective TiO₂

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Al doped TiO₂ GGA+U

Al	9.611882	1.907191	4.776339
Ti	11.409567	1.901207	7.190729
Ti	15.240633	0.000841	9.595639
Ti	3.817254	7.618020	9.604139
Ti	7.658216	7.601703	0.024405
Ti	11.424770	7.621303	0.001834
Ti	15.239506	3.810684	9.594054
Ti	3.814402	3.818209	9.601152
Ti	7.656263	3.838074	0.025510
Ti	11.422421	3.809050	0.005475
Ti	1.908565	0.000184	2.388861
Ti	5.730438	0.006809	2.385432
Ti	9.549016	0.026714	2.469434
Ti	13.344649	7.621585	2.396996
Ti	1.902787	3.812878	2.388419
Ti	5.722876	3.814761	2.383819
Ti	9.541622	3.783451	2.471220
Ti	13.340532	3.811513	2.396180
Ti	1.837695	1.906398	4.791504
Ti	5.602344	1.915402	4.773074
Ti	13.265193	1.904614	4.791937
Ti	1.896841	5.718994	4.792676
Ti	5.726642	5.726724	4.801340
Ti	9.525537	5.720884	4.799870
Ti	13.328959	5.714694	4.796182

Ti	15.235221	1.905774	7.190758
Ti	3.818762	1.904356	7.205741
Ti	7.678647	1.911331	7.278073
Ti	15.238440	5.718430	7.191814
Ti	3.812786	5.718041	7.187809
Ti	7.627461	5.723355	7.198086
Ti	11.424191	5.711005	7.205261
O	1.913856	0.011954	0.397580
O	5.729660	0.005726	0.414061
O	9.532717	0.012297	0.421668
O	13.341371	7.622325	0.402661
O	1.911966	3.800230	0.395044
O	5.728654	3.810827	0.413370
O	9.530980	3.800603	0.424991
O	13.340044	3.809592	0.403131
O	0.006739	0.002669	1.976279
O	3.815547	7.611660	1.981677
O	7.633377	0.011718	1.995805
O	11.440842	7.609045	1.991185
O	0.005856	3.808838	1.975069
O	3.812786	3.827782	1.978939
O	7.630892	3.803295	1.996967
O	11.439423	3.825343	1.993461
O	1.908627	1.907053	2.803384
O	5.673244	1.911300	2.783656
O	9.593432	1.906359	2.865573
O	13.340287	1.903485	2.801607

O	1.900897	5.718558	2.801981
O	5.713987	5.722142	2.818732
O	9.534563	5.719550	2.849034
O	13.350901	5.715723	2.804450
O	1.905516	0.000718	4.379537
O	5.778116	0.017536	4.393887
O	9.503563	0.022682	4.429433
O	13.336720	7.617675	4.380603
O	1.906066	3.813344	4.379460
O	5.759698	3.806360	4.395049
O	9.495605	3.791883	4.429039
O	13.344816	3.813161	4.379182
O	15.243730	1.904957	5.208438
O	3.795815	1.905704	5.194636
O	7.683480	1.915661	5.010046
O	0.000596	5.718819	5.204980
O	3.821599	5.726648	5.201283
O	7.616605	5.722219	5.229798
O	11.434711	5.708595	5.217188
O	1.914649	1.905522	6.785657
O	5.775937	1.907603	6.718541
O	9.498456	1.901131	6.696239
O	13.322783	1.905415	6.773969
O	1.910503	5.716654	6.779530
O	5.717036	5.718674	6.793062
O	9.527366	5.724148	6.808670
O	13.341493	5.716539	6.789134

O	15.241121	0.001626	7.603811
O	3.830746	0.004233	7.604176
O	7.626563	7.622060	7.618640
O	11.430822	0.000825	7.614875
O	15.239918	3.809541	7.603090
O	3.831647	3.808999	7.602341
O	7.633729	3.818758	7.617516
O	11.420729	3.806979	7.615961
O	15.239231	1.905576	9.178121
O	3.833613	1.906255	9.174087
O	7.653275	1.908618	9.182846
O	11.413775	1.904570	9.182337
O	0.009699	5.717714	9.181655
O	3.816110	5.718492	9.183172
O	7.636610	5.719666	9.212523
O	11.421568	5.715541	9.193132
O	11.430685	1.912055	5.181814