

Ti_nO₂ 和 Ti_nO⁻₂ (n=1-10) 团簇的几何结构、电子和磁性质

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Structural, Electronic and Magnetic Properties of Ti_nO₂ and Ti_nO⁻₂ (n=1-10) Clusters

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Table S1 Cartesian coordinates and stable structures of Ti_nO_2 ($n=1-2$) clusters

	Coordinates (Å)			
TiO₂	1a, 0			
Ti1	-0.052910	-0.058969	0.079327	
O2	-0.992853	0.198017	1.422844	
O3	0.183381	-1.681003	-0.179967	
TiO₂	1b, 5.002			
Ti1	1.809041	-2.906830	-0.117108	
O2	1.028312	-1.652096	0.957131	
O3	2.589771	-4.161564	-1.191348	
TiO₂	1c, 5.511			
Ti1	1.072958	-1.724253	0.895064	
O2	1.817907	-2.920158	-0.127860	
O3	2.396504	-3.851473	-0.926234	
Ti₂O₂	2a, 0			
Ti1	1.207011	0.000532	-0.123285	
Ti2	-1.207016	-0.000535	-0.123498	
O3	-0.001317	1.338074	0.339316	
O4	0.001331	-1.338067	0.339336	
Ti₂O₂	2b, 0.307			
Ti1	0.930325	0.987613	0.000000	
Ti2	-0.930325	-0.987613	0.000000	
O3	0.930325	-0.875850	0.000000	
O4	-0.930325	0.875850	0.000000	
Ti₂O₂	2c, 2.242			
Ti1	0.000000	1.386399	0.000000	
Ti2	-0.799886	-1.132887	0.000000	
O3	0.575921	-1.999396	0.000000	
O4	1.623764	1.302238	0.000000	

Table S2 Cartesian coordinates and stable structures of Ti_3O_2 clusters

	Coordinates (Å)			Configuration
Ti_3O_2	3a, 0			
Ti1	1.314280	-1.022679	-0.000034	
Ti2	-0.000430	1.487310	-0.000078	
Ti3	-1.313700	-1.023356	0.000003	
O4	-1.708400	0.767879	0.000110	
O5	1.707988	0.768616	0.000189	
Ti_3O_2	3b, 0.124			
Ti1	0.000000	1.120037	-1.025354	
Ti2	0.000000	-1.120037	-1.025354	
Ti3	0.000000	0.000000	1.514341	
O4	0.000000	-1.666635	0.737505	
O5	0.000000	1.666635	0.737505	
Ti_3O_2	3c, 0.414			
Ti1	-0.885794	-1.212947	-0.182039	
Ti2	-0.527613	1.260982	-0.180280	
Ti3	1.581363	-0.565209	0.098267	
O4	1.291578	1.256704	0.046275	
O5	-1.753457	0.165523	0.679867	

Table S3 Cartesian coordinates and stable structures of Ti_4O_2 clusters

	Coordinates (Å)			Configuration
Ti_4O_2	4a, 0			
Ti1	-0.008780	1.563915	0.422877	
Ti2	1.388311	-0.562042	-0.843663	
Ti3	0.035751	-1.231709	1.255073	
Ti4	-1.428259	-0.572911	-0.724947	
O5	1.676587	1.126657	-0.211360	
O6	-1.657931	1.183698	-0.347530	
Ti_4O_2	4b, 0.124			
Ti1	-0.184941	1.462678	-0.000663	
Ti2	-1.315858	-0.958505	0.000741	
Ti3	0.790197	-0.490983	1.335128	
Ti4	0.789550	-0.492404	-1.334974	
O5	1.666069	0.533417	-0.000441	
O6	-1.883177	0.784420	-0.000196	
Ti_4O_2	4c, 0.414			
Ti1	-0.099324	1.439502	-0.803832	
Ti2	-1.144072	0.000376	1.135937	
Ti3	-0.095515	-1.440118	-0.805041	
Ti4	1.332728	0.000055	1.080278	
O5	-1.330584	-0.001701	-1.043336	
O6	1.335736	0.002453	-0.790887	

Table S4 Cartesian coordinates and stable structures of Ti_5O_2 clusters

	Coordinates (Å)			Configuration
Ti_5O_2	5a, 0			
Ti1	0.879011	-1.148445	0.547893	
Ti2	1.203585	1.075402	2.154752	
Ti3	0.873839	1.208568	-0.791858	
Ti4	-1.201760	0.883215	0.900059	
Ti5	-0.574155	-0.472061	2.783021	
O6	1.327782	-0.518171	-1.149157	
O7	0.286540	2.130575	0.869469	
Ti_5O_2	5b, 0.077			
Ti1	0.923073	-1.188624	0.761463	
Ti2	1.048955	1.289333	2.045902	
Ti3	0.796036	1.426748	-0.537859	
Ti4	-1.336623	0.443728	0.584695	
Ti5	2.038883	0.386441	0.694251	
O6	-0.137964	-0.380769	-0.639022	
O7	-0.458223	-0.666318	2.717787	
Ti_5O_2	5c, 0.086			
Ti	0.176693	-0.284607	1.483209	
Ti	-0.289256	1.339787	-0.614000	
Ti	2.164431	0.082165	-0.307800	
Ti	0.441059	-1.350247	-0.899316	
Ti	0.944096	1.341210	0.843007	
O	-2.102272	0.959354	-0.644256	
O	-2.063100	-0.612922	0.270773	
Ti_5O_2	5d, 0.177			
Ti1	0.888352	-1.273700	0.577696	
Ti2	0.675923	1.095422	1.901510	
Ti3	0.957807	1.280834	-0.687797	
Ti4	-1.521369	0.915795	0.719912	
Ti5	-0.484304	-0.840591	2.974142	
O6	1.169192	-0.434582	-1.112912	
O7	-0.017445	-2.221294	1.943883	

Table S5 Cartesian coordinates and stable structures of Ti_nO_2 ($n=6-8$) clusters

	Coordinates (Å)			Configuration
Ti₆O₂	6a, 0			
Ti1	0.816414	-0.013973	-1.857506	
Ti2	0.703170	-1.762520	0.161389	
Ti3	-1.770341	-0.613436	-0.435611	
Ti4	-0.542608	1.776121	-0.148908	
Ti5	1.705545	0.712381	0.611865	
Ti6	-0.261477	-0.007151	2.046141	
O7	-1.742194	0.582696	1.066696	
O8	-0.436485	-1.442426	-1.505058	
Ti₇O₂	7a, 0			
Ti1	-2.201406	-0.707507	-0.209825	
Ti2	0.002927	-2.240068	-0.017706	
Ti3	2.222290	-0.786538	-0.182211	
Ti4	1.314731	1.769087	-0.214643	
Ti5	-1.358700	1.786116	-0.189283	
Ti6	-0.002311	-0.138620	1.386401	
Ti7	0.041109	-0.085510	-1.504852	
O8	1.826284	0.549679	1.175861	
O9	-1.845599	0.491911	1.239371	
Ti₈O₂	8a, 0			
Ti1	0.017743	-0.040570	-0.014270	
Ti2	-0.132594	0.012756	2.962648	
Ti3	2.373971	0.005425	1.341284	
Ti4	0.898416	-2.003474	1.956555	
Ti5	2.049032	-2.059026	-0.545816	
Ti6	-0.564193	-2.765365	-0.020702	
Ti7	-2.138340	-1.164991	1.382917	
Ti8	-1.374414	-2.510297	3.188371	
O9	-1.193553	0.499186	1.432873	
O10	0.386748	-1.460333	-1.264184	

Table S6 Cartesian coordinates and stable structures of Ti_nO_2 ($n=9-10$) clusters.

	Coordinates (Å)			Configuration
Ti₉O₂	9a, 0			
Ti1	0.208655	-0.362663	-0.248705	
Ti2	-0.102479	0.189097	2.707750	
Ti3	2.242271	0.015575	1.397284	
Ti4	1.986217	2.214868	3.105623	
Ti5	3.452839	2.216654	0.964157	
Ti6	1.794471	4.044986	-0.317132	
Ti7	0.479144	1.969409	0.860560	
Ti8	2.209811	1.256940	-1.009133	
Ti9	-0.115926	2.502705	-1.731334	
O10	0.593274	4.179427	-1.718112	
O11	1.794743	3.443594	1.557356	
Ti₁₀O₂	10a, 0			
Ti1	-2.227737	0.871291	0.822951	
Ti2	-0.801946	2.948111	0.016459	
Ti3	0.599417	0.750309	1.169541	
Ti4	-0.899468	-1.543515	0.401329	
Ti5	-2.869892	-0.882345	-0.985755	
Ti6	-2.773723	2.008856	-1.555868	
Ti7	-0.177778	3.036305	-2.505817	
Ti8	1.662433	2.189943	-1.042759	
Ti9	1.391224	-0.577943	-0.860191	
Ti10	-0.699799	0.572122	-1.583420	
O11	1.006668	2.578911	0.689477	
O12	-0.936122	-0.251114	1.785640	

Table S7 Cartesian coordinates and stable structures of $Ti_nO_2^-$ ($n=1-6$) clusters.

	Coordinates (Å)			Configuration
TiO_2^-				
Ti1	-0.052423	-0.057992	0.078575	
O2	-1.007758	0.221002	1.443197	
O3	0.197799	-1.704965	-0.199567	
$Ti_2O_2^-$				
Ti1	1.378869	0.001048	0.108058	
Ti2	-1.378960	-0.001046	0.107808	
O3	-0.000827	1.286519	0.107992	
O4	0.000927	-1.286517	0.108011	
$Ti_3O_2^-$				
Ti1	0.220122	0.629572	2.407462	
Ti2	3.078765	0.203610	1.822830	
Ti3	1.050096	-0.407245	-0.225857	
O4	2.887535	-0.415200	0.096506	
O5	-0.443118	0.091352	0.774574	
$Ti_4O_2^-$				
Ti1	0.000819	1.537330	0.463716	
Ti2	1.440060	-0.580948	-0.782702	
Ti3	-0.024443	-1.254084	1.291661	
Ti4	-1.414601	-0.565924	-0.795354	
O5	1.655247	1.177706	-0.335626	
O6	-1.651403	1.193527	-0.291244	
$Ti_5O_2^-$				
Ti1	-0.315527	1.628252	0.047644	
Ti2	0.692270	-0.667754	1.441159	
Ti3	-1.992924	-0.623260	-0.015468	
Ti4	0.376911	-0.888343	-1.337509	
Ti5	2.189782	0.753964	-0.236299	
O6	-2.127764	1.206314	-0.092468	
O7	-0.423999	-1.742473	0.301108	
$Ti_6O_2^-$				
Ti1	0.768681	0.067772	-1.421553	
Ti2	0.662335	-1.776887	0.197902	
Ti3	-1.743677	-0.602144	-0.433411	
Ti4	-0.572285	1.731926	-0.230241	
Ti5	1.706019	0.630333	0.609929	
Ti6	-0.250154	0.029672	2.096929	
O7	-1.728583	0.572575	1.088593	
O8	-0.370313	-1.421553	-1.526918	

Table S8 Cartesian coordinates and stable structures of $Ti_nO_2^-$ ($n=7-9$) clusters.

	Coordinates (Å)			Configuration
$Ti_7O_2^-$				
Ti1	-2.224298	-0.713827	-0.235856	
Ti2	0.008747	-2.234090	-0.001451	
Ti3	2.205829	-0.775842	-0.190036	
Ti4	1.359083	1.829372	-0.177342	
Ti5	-1.321781	1.730364	-0.210982	
Ti6	-0.003165	-0.144958	1.367276	
Ti7	-0.032282	-0.108131	-1.522487	
O8	1.841124	0.553658	1.199124	
O9	-1.833933	0.502004	1.254865	
$Ti_8O_2^-$				
Ti1	0.069910	-0.048865	0.036346	
Ti2	-0.061512	0.005980	2.909973	
Ti3	2.290839	-0.055221	1.247722	
Ti4	0.875442	-2.160220	1.946987	
Ti5	2.092222	-1.847242	-0.445397	
Ti6	-0.605670	-2.752469	-0.059904	
Ti7	-2.127411	-1.159343	1.360131	
Ti8	-1.369223	-2.465061	3.254369	
O9	-1.223303	0.506916	1.395328	
O10	0.381521	-1.511164	-1.225879	
$Ti_9O_2^-$				
Ti1	0.282269	-0.369346	-0.283618	
Ti2	-0.120159	0.215526	2.706692	
Ti3	2.203367	0.005562	1.358153	
Ti4	1.992879	2.222211	3.133445	
Ti5	3.457248	2.208372	0.970447	
Ti6	1.794375	4.026973	-0.316172	
Ti7	0.475165	1.999058	0.894088	
Ti8	2.175673	1.261352	-1.027410	
Ti9	-0.117938	2.472489	-1.711815	
O10	0.589763	4.167511	-1.719277	
O11	1.810377	3.460885	1.563780	

Table S9 Cartesian coordinates and stable structures of $\text{Ti}_{10}\text{O}_2^-$ clusters

	Coordinates (Å)			Configuration
Ti₁₀O₂⁻				
Ti1	-2.213799	0.873272	0.785491	
Ti2	-0.809494	2.922615	-0.009293	
Ti3	0.587096	0.751507	1.153834	
Ti4	-0.850501	-1.554164	0.421155	
Ti5	-2.887088	-0.870407	-1.016242	
Ti6	-2.850052	2.060284	-1.554516	
Ti7	-0.207320	3.036907	-2.529432	
Ti8	1.697707	2.160934	-1.015952	
Ti9	1.423116	-0.591106	-0.825252	
Ti10	-0.724986	0.597281	-1.571219	
O11	1.031149	2.580704	0.704599	
O12	-0.922550	-0.266897	1.808414	

Table S10 The charge (Q , in e) and local magnetic moment (M , in μ_B) for per Ti atom and O atom of Ti_nO_2^- clusters

n	Ti-3d		Ti-4s		O-2s		O-2p	
	Q	M	Q	M	Q	M	Q	M
2	2.370	1.673	0.670	0.536	1.860	-0.005	5.150	-0.139
3	2.350	1.438	0.927	-0.202	1.850	0.001	5.160	-0.062
4	2.643	0.705	0.733	0.014	1.810	0	5.080	-0.002
5	2.698	0.824	0.664	0.026	1.790	0.001	5.145	0
6	2.778	0.147	0.585	0.002	1.760	0	5.165	0.004
7	2.876	0.067	0.544	0.004	1.745	0	5.140	0.010
8	2.909	0.538	0.527	0.012	1.735	0.001	5.130	-0.017
9	2.906	0.262	0.514	0.024	1.730	0.001	5.140	0.014
10	2.952	0.307	0.490	0	1.710	0.001	5.110	-0.001