

SP-Info_O-vacancy

Electronic Energy and frequencies for formation of interface vacancy on Au₃/TiO₂ system.

The data could be used to reproduce the results using our papers as cited in the article.

electronic energy is in kJ/mol

Stoichiometric Au ₃ /TiO ₂			Reduced Au ₃ /TiO ₂		
Electronic Energy	-4550681.45		Electronic Energy	-4508473.57	
	Frequencies			Frequencies	
	[cm-1]	[THz]		[cm-1]	[THz]
1	0.39	0.0118	1	11.06	0.3314
2	9.6	0.2877	2	21.63	0.6484
3	33.48	1.0036	3	34.53	1.0352
4	54	1.619	4	75.28	2.2568
5	65.51	1.9639	5	92.83	2.7829
6	71.02	2.1291	6	96.67	2.898
7	99.6	2.986	7	119.13	3.5716
8	131.22	3.9337	8	146.76	4.3997
9	148.23	4.4438	9	172.8	5.1804
10	229.1	6.8683	10	231.6	6.9433
11	269.01	8.0647	11	237.51	7.1203
12	285.97	8.5732	12	244	7.315
13	293.13	8.7877	13	258.59	7.7523
14	304.95	9.142	14	264.63	7.9335
15	316.05	9.475	15	277.01	8.3047
16	319.94	9.5915	16	288.07	8.6361
17	328.32	9.8428	17	321.87	9.6494
18	335.3	10.052	18	331.72	9.9446
19	336.79	10.0966	19	340.22	10.1996
20	343.23	10.2898	20	348.79	10.4564
21	345.03	10.3438	21	365.94	10.9707
22	352.85	10.5781	22	380.22	11.3988
23	360.24	10.7996	23	385.45	11.5554
24	368.18	11.0379	24	395.98	11.8712
25	378.44	11.3455	25	403.24	12.0887
26	380.89	11.4188	26	425.48	12.7557
27	394.59	11.8294	27	433.53	12.9968
28	395.62	11.8605	28	442.52	13.2664
29	417.3	12.5104	29	482.84	14.4752
30	423.12	12.6848	30	486.35	14.5803
31	426.65	12.7907	31	493.1	14.7828
32	457.96	13.7292	32	503.54	15.0957
33	460.22	13.7969	33	508.34	15.2396
34	462.64	13.8695	34	520.2	15.5952
35	472.78	14.1735	35	529.51	15.8743
36	483.31	14.4893	36	532.33	15.9588
37	496.43	14.8826	37	702.11	21.0487
38	512.54	15.3655	38	707.15	21.1999
39	567.3	17.0072	39	726.09	21.7676
40	576.96	17.2968	40	737.23	22.1015
41	588.72	17.6493	41	748.04	22.4258
42	589.74	17.6799	42	769.48	23.0686

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43	599.14	17.9618	43	783.03	23.4746
44	606	18.1673	44	794.55	23.8199
45	616.72	18.4887	45	800.8	24.0074
46	618.4	18.5392	46	806.78	24.1867
47	624.69	18.7277	47	814.91	24.4304
48	629.96	18.8857	48	819.22	24.5596
49	630.6	18.9048	49	827.69	24.8135
50	637.77	19.1199	50	832.8	24.9667
51	645.63	19.3556	51	841.73	25.2343
52	650.02	19.4871	52	847.67	25.4125
53	666.85	19.9918	53	852.39	25.5539
54	674.38	20.2175	54	865.69	25.9528
55	677.28	20.3044	55	866.17	25.9673
56	703.79	21.0992	56	871.47	26.1259
57	707.12	21.1988	57	874.96	26.2306
58	711.62	21.3339	58	878.37	26.3328
59	713.81	21.3994	59	882.18	26.447
60	718.09	21.5277	60	886.48	26.5761
61	718.93	21.5529	61	892.01	26.7417
62	727.88	21.8212	62	894.45	26.8149
63	729.79	21.8785	63	901.97	27.0404
64	733.38	21.9862	64	913.07	27.3733
65	741.42	22.2272	65	916.03	27.462
66	742.01	22.245	66	920.87	27.6069
67	744.23	22.3114	67	930.56	27.8975
68	750.47	22.4987	68	936.01	28.0609
69	750.63	22.5034	69	942.2	28.2464
70	759.92	22.7818	70	949.52	28.466
71	760.84	22.8094	71	963.38	28.8813
72	762.55	22.8606	72	969.64	29.069
73	780.37	23.3949	73	971.86	29.1357
74	784.4	23.5158	74	981.89	29.4364
75	786.1	23.5667	75	992.87	29.7656
76	806.53	24.1792	76	995.09	29.832
77	819.94	24.5812	77	1003.32	30.0789
78	823.61	24.6913	78	1030.34	30.8889
79	826.51	24.7781	79	1038.17	31.1235
80	828.45	24.8362	80	1040.76	31.2011
81	838.69	25.1432	81	1051.77	31.5314
82	858.89	25.7487	82	1060.54	31.7942
83	896.66	26.8813	83	1083.09	32.4702
84	914.65	27.4205	84	1094.51	32.8127
85	919.15	27.5554	85	1125.09	33.7295
86	937.11	28.0939	86	1147.08	34.3885
87	951.06	28.5122	87	1173.24	35.1728
88	974.52	29.2155			
89	984.07	29.5017			
90	992.15	29.744			

O₂
Electronic Energy -83988.6561
Frequencies
[cm-1] 1484.81