Supplementary information

Thermodynamic and kinetic properties of interacting hydrogen defects in $SrTiO_3$ from density functional theory

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Appendix A

Phonon frequencies for a $2 \times 2 \times 2$ supercell $SrTiO_3$. No atoms are constrained. Units are cm^{-1} .

41	133	193	304	429	497
32	134	198	310	432	502
57	136	200	316	436	505
74	139	207	319	443	512
79	140	216	323	447	515
82	144	221	326	448	519
91	145	232	337	452	525
92	150	236	339	460	532
96	155	244	343	464	537
99	156	255	349	465	546
103	159	258	354	468	550
106	160	266	356	471	555
111	166	270	359	474	561
112	169	276	364	476	630
116	173	281	370	481	649
118	177	287	372	484	662
121	181	290	374	484	719
122	184	293	389	486	732
124	188	295	393	489	734
125	190	302	406	490	775

Appendix B

Phonon frequencies for singly hydrogenated $2 \times 2 \times 2$ supercells of $SrTiO_3$. The ground state structure is illustrated in Fig. 2. Only two transition states (TS) are possible. Units are cm^{-1} . All but 8 atoms are constrained. Activation energies and pre-exponential factors are shown in Table 1.

Ground state configuration	H jump TS	OH rot. TS
112	1116i	712i
128	118	129
136	121	135
141	132	136
145	142	158
170	143	161
231	182	179
248	244	192
260	251	240
265	263	263
302	280	287
303	285	303
315	292	318
346	355	345
353	365	358
374	373	365
431	436	387
472	452	440
540	468	494
572	519	538
664	615	580
957	723	674
1026	1391	931
3301	1802	3862

Appendix C

Phonon frequencies for doubly hydrogenated $2 \times 2 \times 2$ supercells of $SrTiO_3$. Units are cm^{-1} . All but 10 atoms are constrained. The ground state is illustrated in Fig. 4. Although positioned differently relative to the ground state, both transition states (TS) lead to the same end configuration. Activation energies and pre-exponential factors are shown in Table 3.

Ground state	${ m H}$ jump ${ m TS}$	OH rotation TS	End configuration
134	944.0i	553.4i	128
162	136	131	139
178	144	138	168
227	175	190	209
238	216	203	220
254	223	215	227
292	242	247	270
298	277	265	288
304	285	281	291
309	298	282	301
320	308	298	305
328	311	316	323
349	317	319	338
355	333	339	350
368	355	358	356
393	383	365	370
413	421	382	420
437	449	419	447
508	470	458	496
549	495	506	517
574	521	521	580
593	572	563	604
634	608	595	620
730	671	610	675
999	740	675	816
1091	949	792	971
1141	1022	1121	1171
1180	1464	1198	1270
3198	1745	2981	2870
3306	3573	3886	3708