Supporting Information

Understanding the role of Rutile TiO_2 Surface Orientation on Molecular Hydrogen Activation

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The effect of U

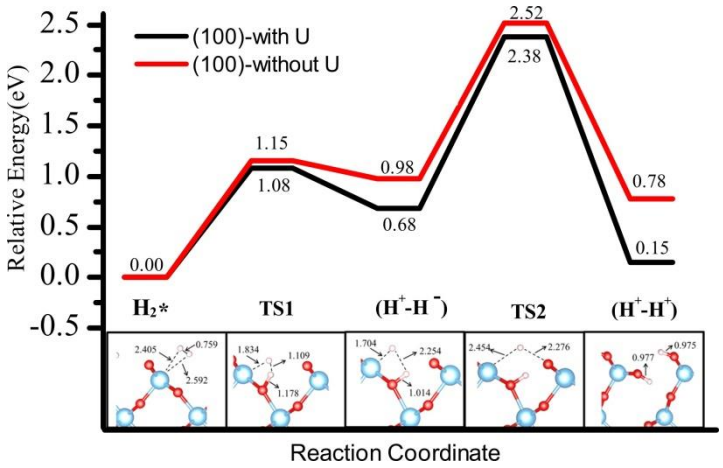

Figure S1. H_2 dissociation on rutile TiO_2 (100) facets with U= 4 eV and U = 0 eV.

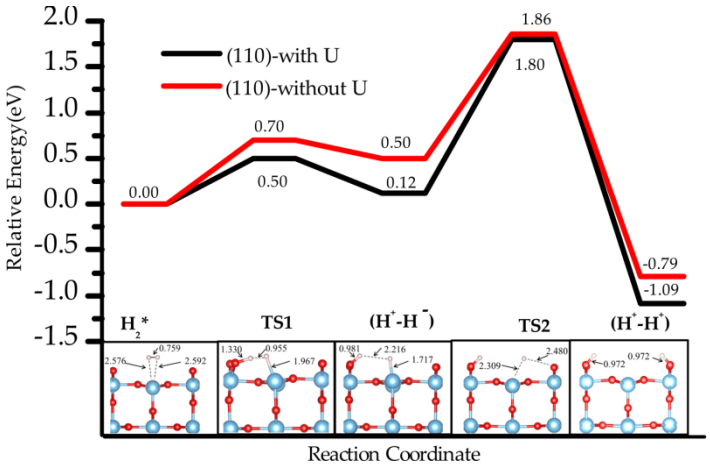

Figure S2. H_2 dissociation on Rutile TiO_2 (110) facets with U= 4 eV and U = 0 eV.

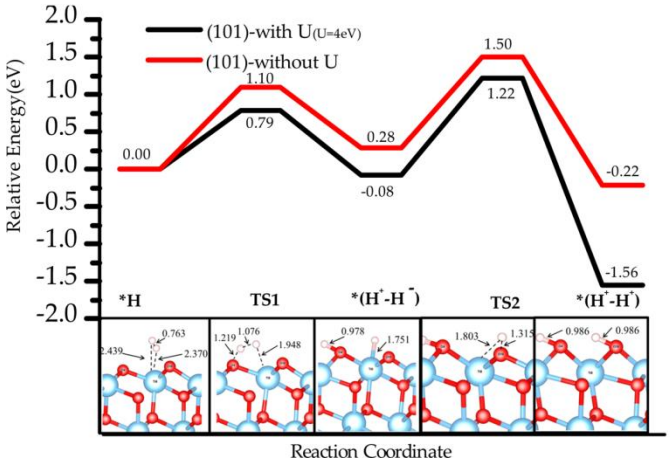

Figure S3. H_2 dissociation on Rutile TiO_2 (101) facets with U= 4 eV and U= 0 eV.

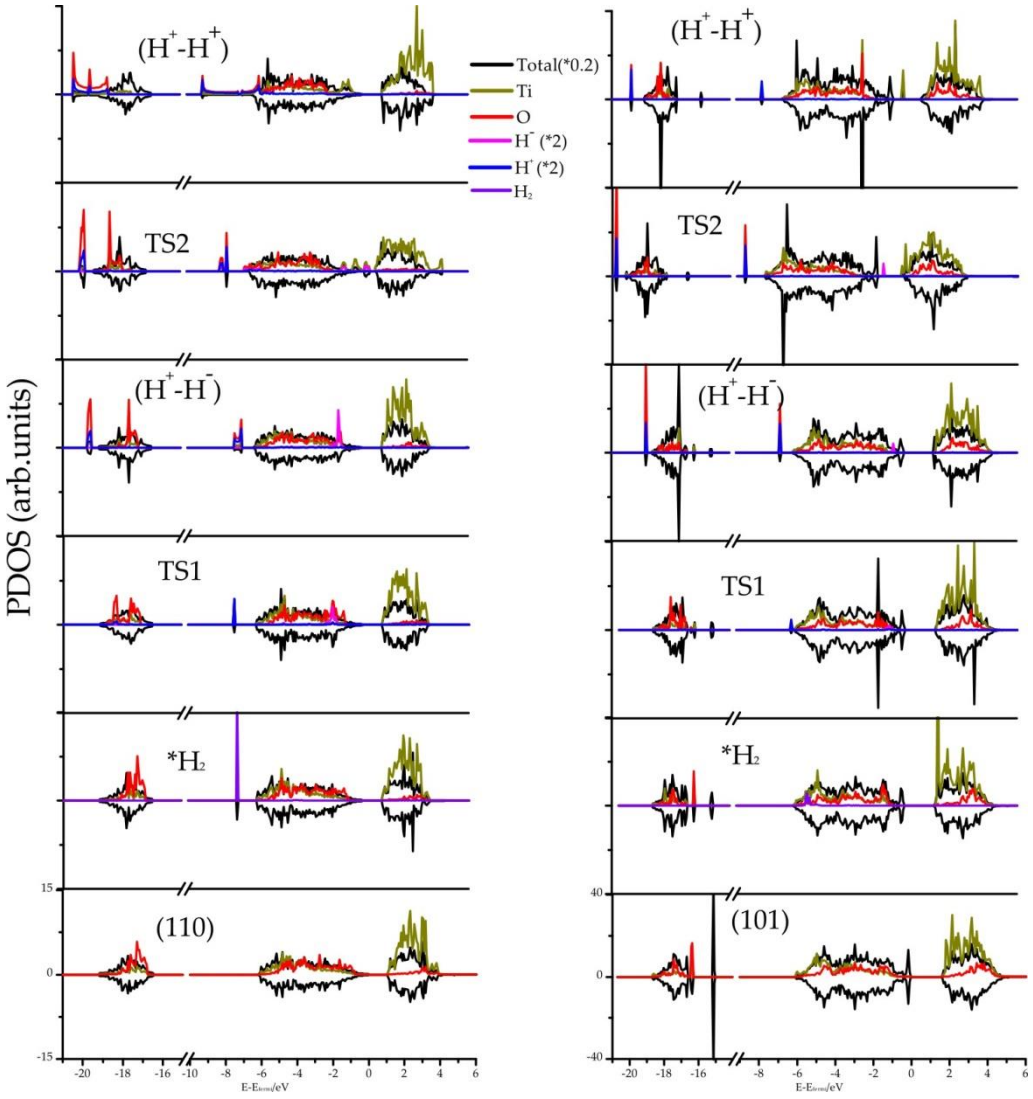

Figure S4. Total and Projected Density of State (PDOS) of the TiO_2 slab, $*H_2$, TS, and $*(H^+, H^-)$, $*(H^+\text{-}H^+)$ for the (110) (left) and (101) (right) surfaces. For the PDOS, only the Ti, O involved in the two processes are projected. Positive DOS correspond to spin up, negative to spin down.

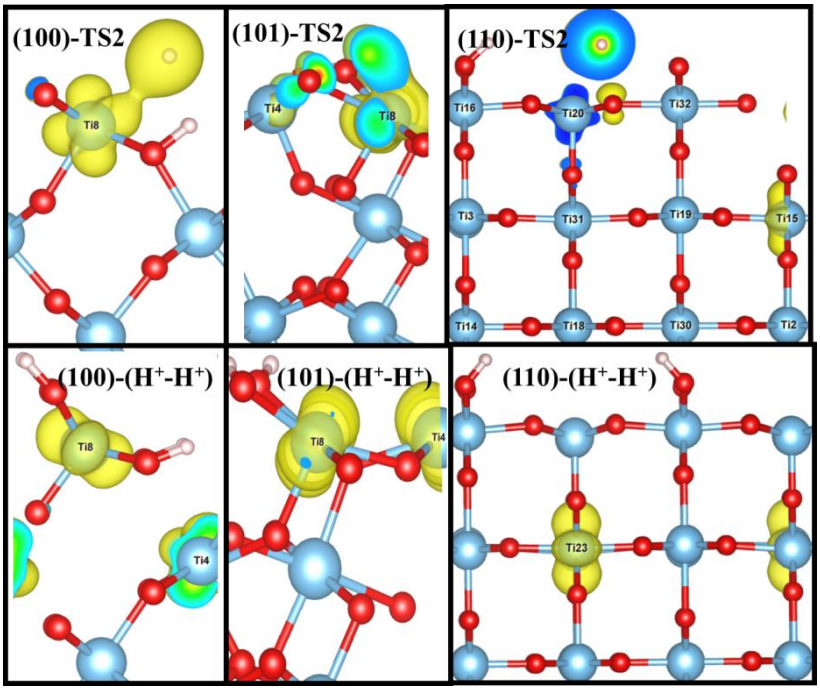

Figure S5. Spin Density of TS 2 and (H^+-H^+) species indicating the distribution of unpaired electrons on rutile TiO_2 (100), (101) and (110) facets.

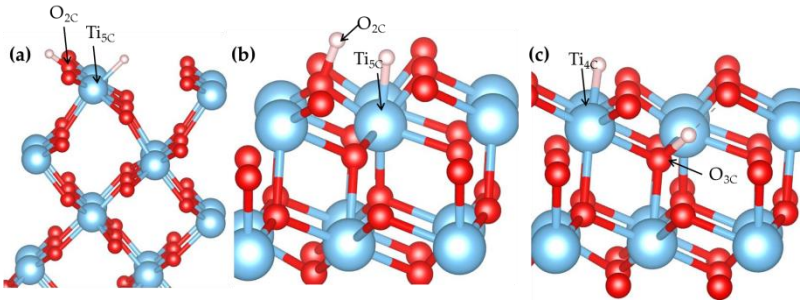

Figure S6. Structures of (H^+-H^-) for the other adsorption modes considered on (100) facet (a) and (101) facet(b,c).

Tests on IR frequency calculations

Table 1. Computed IR frequencies for (110) TiO_2-(H^+, H^-) species as a function of the functional, cut-off, U test and with dipole corrections.

system	test	method	υ(OH)/cm^{-1}	υ(Ti-H)/cm^{-1}
(110)	functional	PBE+U(4eV)-400eV	3606.5	1653.8
		LDA+U(4eV)-400eV	3607.8	1638.9
		PW91+U(4eV)-400eV	3608.1	1648.7
		PBE-Sol+U(4eV)-400eV	3631.8	1665.0
	cut-off test	300 eV	3486.2	1644.1
		400 eV	3606.5	1653.87
		500 eV	3610.9	1652.3
		600 eV	3603.0	1642.9
		700 eV	3612.8	1655.8
	choice of U	U=3eV	3605.6	1658.4
		U=4eV	3606.5	1653.8
		U=5eV	3606.2	1640.3
		U=6eV	3607.6	1630.6
		U=7eV	3609.4	1609.0
	with dipole corrections	PBE+U(4eV)-400eV	3604.8	1610.3

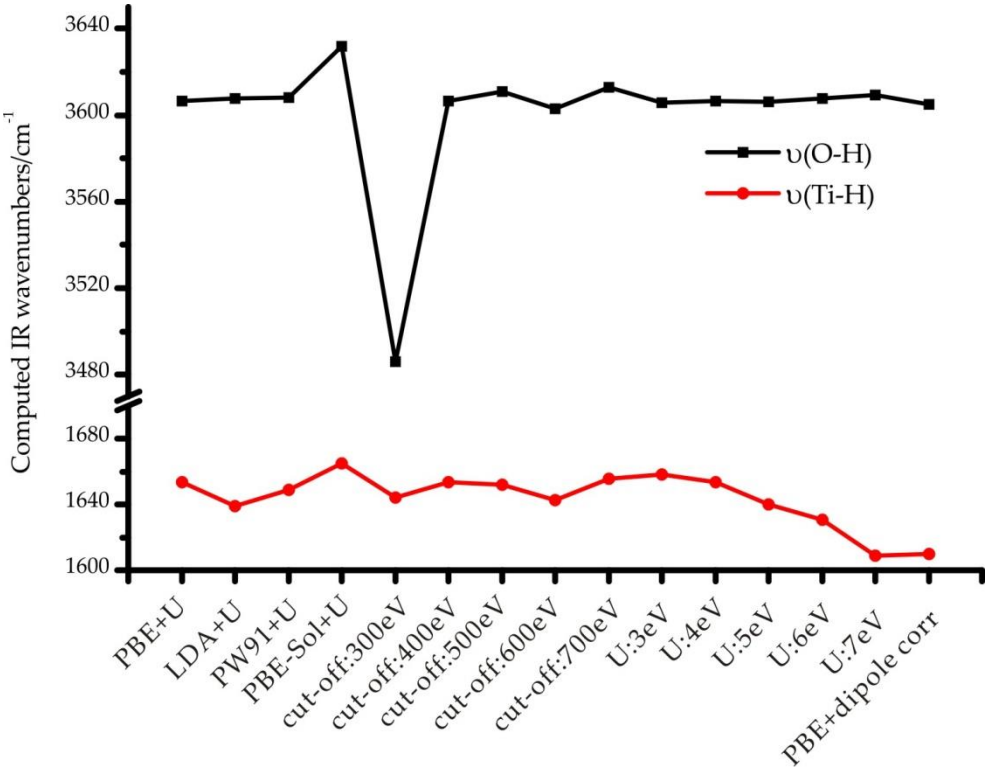

Figure S7. Computed IR vibrations of Ti-H and O-H in (H^+, H^-) species for the (110) termination as a function of the functional, plane wave cut-off, choice of U, and with dipole corrections.

Table S2. Computed IR frequencies for (100) TiO_2-(H^+, H^-) species as a function of the functional, cut-off, U test and with dipole corrections.

system	test	method	υ(OH)	υ(Ti-H)
(100)	functional	PBE+U(4eV)-400eV	2976.5	1768.7
		LDA+U(4eV)-400eV	2954.5	1718.6
		PW91+U(4eV)-400eV	2956.1	1724.3
		PBE-Sol+U(4eV)-400eV	2990.0	1736.2
	cut-off	300 eV	2810.3	1721.3
		400 eV	2976.5	1768.7
		500 eV	2955.8	1726.9
		600 eV	2957.8	1723.8
		700 eV	2949.0	1714.6
	choice of U	U=3eV	2958.6	1732.2
		U=4eV	2976.5	1768.7
		U=5eV	2949.6	1719.0
		U=6eV	2945.1	1710.3
		U=7eV	2940.9	1699.4
	with dipole corrections	PBE+U(4eV)-400eV	2945.0	1726.1

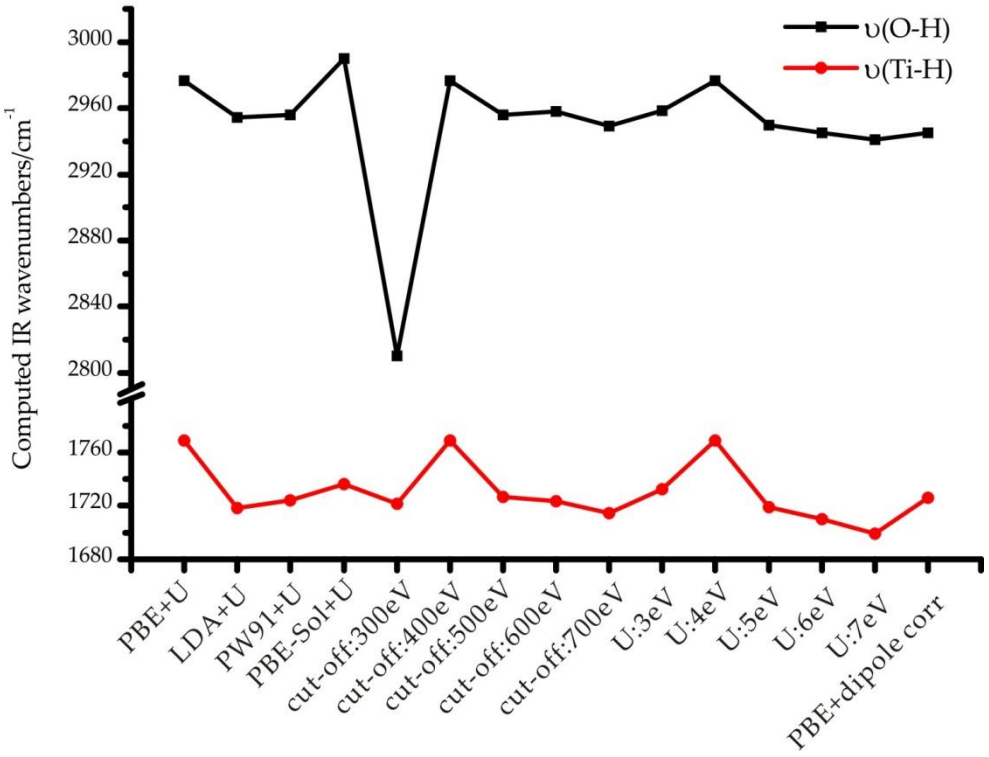

Figure S8. Computed IR vibrations of Ti-H and O-H in (H^+, H^-) species for the (100) termination as a function of the functional, plane wave cut-off, choice of U, and with dipole corrections..

Table S3. Computed IR frequencies for (001) TiO_2-(H^+, H^-) species as a function of the functional, cut-off, U test and with dipole corrections.

system	test	method	υ(OH)	υ(Ti-H)
(001)	functional	PBE+U(4eV)-400eV	3742.9	1644.8
		LDA+U(4eV)-400eV	3745.9	1649.3
		PW91	3746.8	1653.8
	cut-off	300 eV	3628.3	1646.6
		400 eV	3742.9	1644.8
		500 eV	3743.1	1645.2
		600 eV	3750.2	1651.3
		700 eV	3745.0	1641.8
	choice of U	U=3eV	3743.9	1648.2
		U=4eV	3742.9	1644.8
		U=5eV	3744.0	1656.8
		U=6eV	3744.0	1660.5
		U=7eV	3744.2	1663.7
	with dipole corrections	PBE+U(4eV)-400eV	3728.71	1623.37

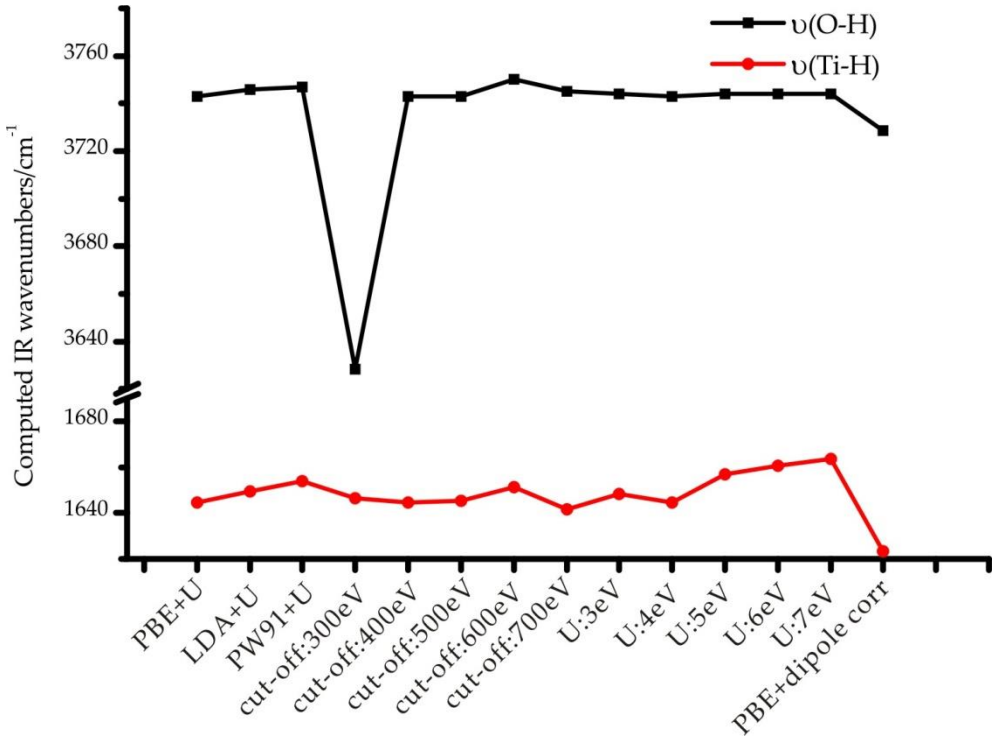

Figure S9. Computed IR vibrations of Ti-H and O-H in (H^+, H^-) specie for the (001) termination as a function of the functional, plane wave cut-off, choice of U, and with dipole corrections.

Table S4. Computed IR frequencies for (101) TiO_2-(H^+, H^-) species as a function of the functional, cut-off, U test and with dipole corrections.

system	test	method	υ(OH)	υ(Ti-H)
(101)	functional	PBE+U(4eV)-400eV	3622.4	1577.5
		LDA+U(4eV)-400eV	3618.3	1581.2
		PW91	3620.2	1586.1
	cut-off	300 eV	3496.0	1585.1
		400 eV	3622.4	1577.5
		500 eV	3623.9	1584.0
		600 eV	3625.4	1580.0
		700 eV	3619.2	1570.2
	choice of U	U=3eV	3617.5	1589.8
		U=4eV	3622.4	1577.5
		U=5eV	3617.9	1586.0
		U=6eV	3618.1	1582.3
		U=7eV	3618.2	1577.5
	with dipole corrections	PBE+U(4eV)-400eV	3615.5	1566.5

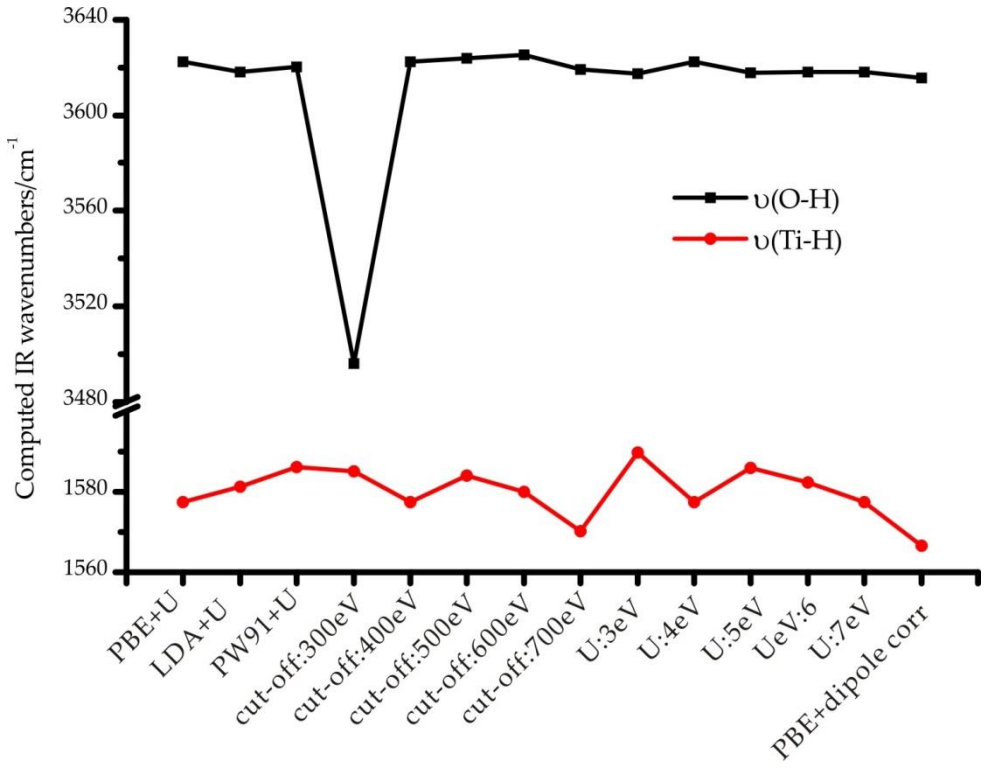

Figure S10. Computed IR vibrations of Ti-H and O-H in (H^+, H^-) specie for the (101) termination as a function of the functional, plane wave cut-off, choice of U, and with dipole corrections.

Table 5. Selected previous studies of experimental and calculated stretching frequencies of various OH in TiO_2 systems, and Ti-H supported on silica.

	System	Method	υ(OH)/cm^{-1}	υ(Ti-H)/cm^{-1}
Experimental data[1-6]	TiO_2(110) single crystal	HREELS	3690	
	TiO_2(110)	IRAS	3711	
	rutile (110)	Infrared spectroscopic techniques	3410 and 3650	

	rutile (100)	Infrared spectroscopic techniques	3550	
	rutile (101)	Infrared spectroscopic techniques	3680 and 3610	
	rutile (110)	Infrared spectroscopic techniques	3655 and 3410	
	Silica-Supported Titanium Hydrides	Infrared spectroscopic techniques		1706, 1692, 1679, and 1647 cm^{-1}
	anatase TiO_2	FT-IR	3640-3735	
Theoretical data[7,8]	rutile (110)	The vibrational frequencies were calculated numerically	3700	
	anatase (001): Ti_V-μ1OH	finite difference approach +anharmonicity corrections (71–73 cm^{-1})	3760(3746–3751)	
	anatase (110): Ti_V- μ1OH		3728	
	anatase (100): Ti_{VI}-μ1OH		3688	

Table S6. Comparison of computed IR wavenumbers (cm^{-1}) of Ti–H and O–H Stretching Modes of (H^+,H^-) Species for the four terminations studied with and without grimme D3 corrections using Finite Differences (FD) method.

	υ(Ti-H)/cm^{-1}		υ(OH)/cm^{-1}	
Slab	**FD-PBE-U**	FD-PBE-U-D3	FD-PBE-U	FD-PBE-U-D3
(001)	1656.94	1656.47	3763.85	3766.78
(100)	1726.98	1718.94	2959.92	2958.67
(110)	1654.55	1659.93	3618.55	3623.73
(101)	1570.11	1583.89	3626.45	3625.28

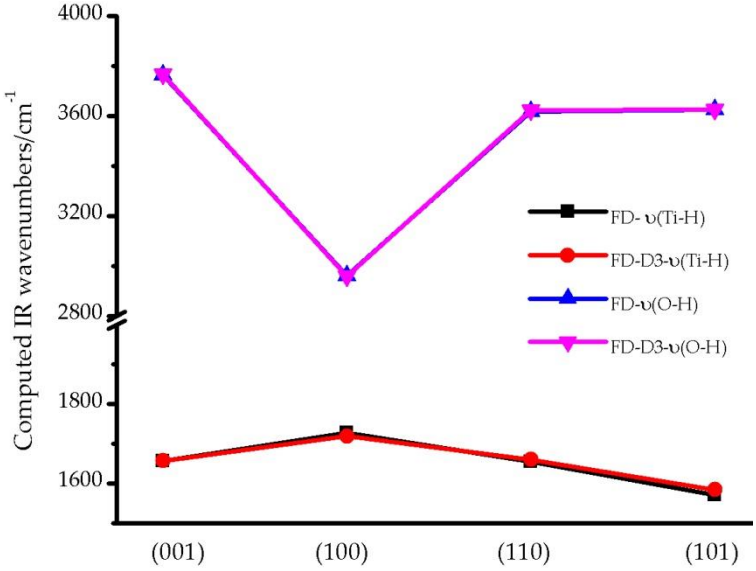

Figure S11. Comparison of computed IR wavenumbers (cm^{-1}) of Ti–H and O–H Stretching Modes of (H^+,H^-) Species for the four terminations studied with and without grimme D3 corrections using Finite Differences (FD) method.

Grimme D3 dispersion correction

Table 7. Relative energy (eV) of adsorption of molecular hydrogen on four surfaces and subsequent heterolytic dissociation generating (H^+-H^-) species (in parentheses, the D3 corrected values). ΔE(eV) is the reaction energy for heterolytic dissociation of adsorbed hydrogen ΔE=E(H^+-H^-)-E(*H_2). The reference is taken as the sum of dihydrogen and the bare slab.

	(001)	(100)	(110)	(101)
slab+H_2	0.00(0.00)	0.00(0.00)	0.00(0.00)	0.00(0.00)
*H_2	-0.13(-0.21)	-0.08(-0.23)	0.10(-0.24)	-0.14(-0.25)
TS1	0.43(0.32)	1.00(0.62)	0.60(0.29)	0.65(0.53)
$E^{\neq}$	0.56(0.53)	1.08(0.85)	0.50(0.54)	0.79(0.79)
(H^+-H^-)	-0.21(-0.36)	0.60(0.38)	0.22(-0.18)	-0.22(-0.35)
ΔE	-0.08(-0.15)	0.68(0.61)	0.12(0.06)	-0.08(-0.10)

Figure S12. The energy profile of the adsorption of molecular hydrogen on four surfaces and subsequent heterolytic dissociation generating (H^+-H^-) species.(a) without D3 correction; (b) with D3 correction.

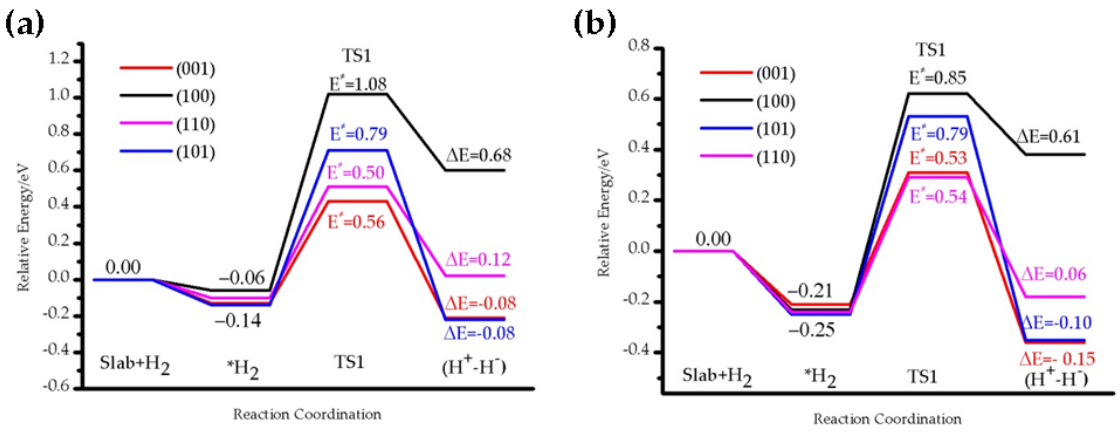

Figure S12. The energy profile of the adsorption of molecular hydrogen on four surfaces and subsequent heterolytic dissociation generating (H^+-H^-) species.(a) without D3 correction; (b) with D3 correction.

References:

1. Primet, M.; Pichat, P.; Mathieu, M.V. Infrared study of the surface of titanium dioxides. I. Hydroxyl groups. *The Journal of Physical Chemistry* **1971**, *75*, 1216-1220, doi: org/10.1021/j100679a007
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8. Buchholz, M., Wöll, C., Interaction of carboxylic acids with rutile TiO_2(110): IR-investigations of terephthalic and benzoic acid adsorbed on a single crystal substrate, *Surf. Sci.* **2016**, 643, 117–123. doi: org/10.1016/j.susc.2015.08.006

Structures (POSCAR format)

A. Surfaces

※ (002)-bare

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4.6612049999999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.6612049999999998 0.0000000000000000
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Ti O
8 16
Selective dynamics
Direct

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0.0000000000000000	0.1955000000000027	0.0975400000000022	F	F	F
-0.0000000000000000	0.1955000000000027	0.1993034740869846	T	T	T
-0.0000000000000000	0.1955000000000027	0.3050444256455350	T	T	T
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0.5000000000000000	0.6955000100000035	0.1463100100000005	F	F	F
0.5000000000000000	0.6955000100000035	0.2442446311049732	T	T	T
0.5000000000000000	0.6955000100000035	0.3402608140993794	T	T	T
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0.1955000000000027	0.0000000000000000	0.1463100100000005	F	F	F
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0.8044999899999965	0.3909999899999974	0.1463100100000005	F	F	F
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※ (002)-H_2

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0.0000000000000000 4.6612049999999998 0.0000000000000000

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H
8 16 2
Selective dynamics
Direct

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0.0000000000000000	0.1955000000000027	0.0975400000000022	F	F	F
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0.5000000000000000	0.6955000100000035	0.0487699999999975	F	F	F
0.5000000000000000	0.6955000100000035	0.1463100100000005	F	F	F
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※ (002)-H^+-H^-

1.00000000000000
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0.0000000000000000 4.6612049999999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.3668990000000001
Ti O H
8 16 2
Selective dynamics
Direct

0.0000000000000000	0.1955000000000027	0.0000000000000000	F	F	F
0.0000000000000000	0.1955000000000027	0.0975400000000022	F	F	F

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0.1955000000000027	0.0000000000000000	0.1463100100000005	F	F	F
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0.1919120687838471	0.0035879312161485	0.3476074538817706	T	T	T
0.8044999899999965	0.3909999899999974	0.0487699999999975	F	F	F
0.8044999899999965	0.3909999899999974	0.1463100100000005	F	F	F
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0.8481420228767608	0.3473579671232412	0.3781473132712567	T	T	T

※(002)-TS1

1.00000000000000

4.6612049999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612049999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.3668990000000001

Ti	O	H
8	16	2

Selective dynamics

Direct

0.0000000000000000	0.1955000000000027	0.0000000000000000	F	F	F
0.0000000000000000	0.1955000000000027	0.0975400000000022	F	F	F
0.0029315047703022	0.1923962380738615	0.1987680999377446	T	T	T
0.0129490893627846	0.1815129450191506	0.3028467571756508	T	T	T
0.5000000000000000	0.6955000100000035	0.0487699999999975	F	F	F
0.5000000000000000	0.6955000100000035	0.1463100100000005	F	F	F
0.5083464289270054	0.6868500021500026	0.2454658464781900	T	T	T
0.4968415925365832	0.6969536835015404	0.3432798047643502	T	T	T
0.3045000199999990	0.5000000000000000	0.0000000000000000	F	F	F

0.3045000199999990	0.5000000000000000	0.0975400000000022	F	F	F
0.3080515012668670	0.4961412396507541	0.1971978156690213	T	T	T
0.3120245992706927	0.4875123126502956	0.2972783294904460	T	T	T
0.6955000100000035	0.8909999700000029	0.0000000000000000	F	F	F
0.6955000100000035	0.8909999700000029	0.0975400000000022	F	F	F
0.6993556229011375	0.8870331730338208	0.1972123040480867	T	T	T
0.7071128583042068	0.8827008320723522	0.2973504825444166	T	T	T
0.1955000000000027	0.0000000000000000	0.0487699999999975	F	F	F
0.1955000000000027	0.0000000000000000	0.1463100100000005	F	F	F
0.2006493968332705	0.9944586296223648	0.2484949492699826	T	T	T
0.2149698336780546	0.9801454310131632	0.3477866526819398	T	T	T
0.8044999899999965	0.3909999899999974	0.0487699999999975	F	F	F
0.8044999899999965	0.3909999899999974	0.1463100100000005	F	F	F
0.8111794933839889	0.3836149945824445	0.2484943492055720	T	T	T
0.8028071329038369	0.3930010702668199	0.3508866220536788	T	T	T
0.5755420711312880	0.6146375082375641	0.4043939959586424	T	T	T
0.7307048329368229	0.4620423458252034	0.3850134762888047	T	T	T

※(002)-TS2

Ti O H

1.00000000000000

4.6612049999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612049999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.3668990000000001

Ti O H

8 16 2

Selective dynamics

Direct

0.0000000000000000	0.1955000000000027	0.0000000000000000	F	F	F
0.0000000000000000	0.1955000000000027	0.0975400000000022	F	F	F
0.0014144947563292	0.1942695914033768	0.1969018884841363	T	T	T
0.0131419094772985	0.1838458462935561	0.2991890948084995	T	T	T
0.5000000000000000	0.6955000100000035	0.0487699999999975	F	F	F
0.5000000000000000	0.6955000100000035	0.1463100100000005	F	F	F
0.5078118400777977	0.6879438836518873	0.2465143813797936	T	T	T
0.4997077692445395	0.7015386969253092	0.3440972050684749	T	T	T
0.3045000199999990	0.5000000000000000	0.0000000000000000	F	F	F
0.3045000199999990	0.5000000000000000	0.0975400000000022	F	F	F
0.3027676998291667	0.4924805896389756	0.1957132738644561	T	T	T
0.3087327341576238	0.4823672657997402	0.3018454625371225	T	T	T
0.6955000100000035	0.8909999700000029	0.0000000000000000	F	F	F
0.6955000100000035	0.8909999700000029	0.0975400000000022	F	F	F
0.7023974472116524	0.8937524593196613	0.1957226972832722	T	T	T

0.7110907121797380	0.8940060786288412	0.3010656090988665	T	T	T
0.1955000000000027	0.0000000000000000	0.0487699999999975	F	F	F
0.1955000000000027	0.0000000000000000	0.1463100100000005	F	F	F
0.1977546628673606	0.9972353125704696	0.2501518904465682	T	T	T
0.2124229399124736	0.9824116327712601	0.3543991688411517	T	T	T
0.8044999899999965	0.3909999899999974	0.0487699999999975	F	F	F
0.8044999899999965	0.3909999899999974	0.1463100100000005	F	F	F
0.8177487190049216	0.3820948882413980	0.2509380156491487	T	T	T
0.7980172509590243	0.3966353037439359	0.3555235080921110	T	T	T
0.3422298880560332	0.8431005951391592	0.3973964980107870	T	T	T
0.9102695681205897	0.3476295934271332	0.3814356058955297	T	T	T

※ (002)-H^+-H^+

1.00000000000000

4.6612049999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612049999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.3668990000000001

Ti O H

8 16 2

Selective dynamics

Direct

0.0000000000000000	0.1955000000000027	0.0000000000000000	F	F	F
0.0000000000000000	0.1955000000000027	0.0975400000000022	F	F	F
0.0008991255129241	0.1941854902610489	0.1955384765382058	T	T	T
0.9841096108057232	0.2177716849690477	0.2953473048046902	T	T	T
0.5000000000000000	0.6955000100000035	0.0487699999999975	F	F	F
0.5000000000000000	0.6955000100000035	0.1463100100000005	F	F	F
0.4901023615959322	0.7047154981339698	0.2487783966066029	T	T	T
0.5452948608506497	0.6575641937988884	0.3513917446843169	T	T	T
0.3045000199999990	0.5000000000000000	0.0000000000000000	F	F	F
0.3045000199999990	0.5000000000000000	0.0975400000000022	F	F	F
0.2974552157874973	0.4976191530653293	0.1957285401376275	T	T	T
0.2993419694637933	0.4791965148217639	0.3052342266230700	T	T	T
0.6955000100000035	0.8909999700000029	0.0000000000000000	F	F	F
0.6955000100000035	0.8909999700000029	0.0975400000000022	F	F	F
0.6974884826882275	0.8984278820719411	0.1957367419946908	T	T	T
0.7133910673243825	0.8999812949247767	0.3060068617729105	T	T	T
0.1955000000000027	0.0000000000000000	0.0487699999999975	F	F	F
0.1955000000000027	0.0000000000000000	0.1463100100000005	F	F	F
0.1837970380593047	0.0094269417779553	0.2504856047695752	T	T	T
0.2682007344631050	0.6710994920279780	0.4006332555110219	T	T	T
0.8044999899999965	0.3909999899999974	0.0487699999999975	F	F	F
0.8044999899999965	0.3909999899999974	0.1463100100000005	F	F	F

0.8011299692717132 0.3963460315465338 0.2484721548243076 T T T
0.8526190593269185 0.3466495310596264 0.3598800119923815 T T T
0.2247208243921673 0.8258368972598110 0.4209339939032165 T T T
0.0060085779327261 0.4438878718643945 0.3773978289724536 T T T

※(100)-bare

1.00000000000000
4.6612049999999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 2.9619610000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 37.4114300000000028
Ti O
8 16
Selective dynamics
Direct
0.9907484399999973 0.0000000000000000 0.0225501800000032 F F F
0.9933728500000001 0.0000000000000000 0.1430838499999965 F F F
0.0012269971612176 0.0000000000000000 0.2647141009436588 T T T
-0.0018283757240420 0.0000000000000000 0.3928539551519645 T T T
0.4921791399999975 0.5000000000000000 0.0828389200000004 F F F
0.4956807800000007 0.5000000000000000 0.2028307400000031 F F F
0.4995269288052293 0.5000000000000000 0.3285231949641199 T T T
0.4901137428157775 0.5000000000000000 0.4552154979437046 T T T
0.6989695600000019 0.0000000000000000 0.0618577799999969 F F F
0.6879715600000011 0.0000000000000000 0.1802123200000025 F F F
0.7045681285534378 0.0000000000000000 0.3043387373218517 T T T
0.7400515282680256 0.0000000000000000 0.4341148286857447 T T T
0.2021347599999999 0.5000000000000000 0.0441403499999993 F F F
0.1872477100000012 0.5000000000000000 0.1657281499999996 F F F
0.2037295507440408 0.5000000000000000 0.2889997247748871 T T T
0.2189177591657117 0.5000000000000000 0.4159365337338155 T T T
0.2957171099999982 0.0000000000000000 0.1053988299999986 F F F
0.3054150199999981 0.0000000000000000 0.2256907800000008 F F F
0.2994912162793038 0.0000000000000000 0.3525671043798094 T T T
0.3636547152586171 0.0000000000000000 0.4824267100281232 T T T
0.8587117053733961 0.5000000000000000 0.9949993661784378 T T T
0.7982593600000030 0.5000000000000000 0.1207107099999973 F F F
0.8054150199999981 0.5000000000000000 0.2397132700000029 F F F
0.7980335084283420 0.5000000000000000 0.3689380857514415 T T T

※(100)-H_2

1.00000000000000000000
4.6612049999999998 0.0000000000000000 0.0000000000000000

```
      0.0000000000000000      2.9619610000000001      0.0000000000000000
      0.0000000000000000      0.0000000000000000     37.4114300000000028
   Ti     O       H
    8      16      2
Selective dynamics
Direct
   0.9907499999999985   0.0000000000000000   0.0225500000000025   F   F   F
   0.9933699899999979   0.0000000000000000   0.1430799899999968   F   F   F
   0.0011511493819829   0.9997153200669053   0.2647869129927501   T   T   T
  -0.0014265615683368   0.9981281881137597   0.3930085992793760   T   T   T
   0.4921799899999968   0.5000000000000000   0.0828399999999974   F   F   F
   0.4956800100000009   0.5000000000000000   0.2028299999999987   F   F   F
   0.4996069148683389   0.4987067722457575   0.3286485838782707   T   T   T
   0.4901062517385200   0.4970146591202269   0.4555935839960930   T   T   T
   0.6989700000000028   0.0000000000000000   0.0618600000000029   F   F   F
   0.6879699699999975   0.0000000000000000   0.1802099900000016   F   F   F
   0.7039735738810442   0.9989428063694372   0.3043548202183810   T   T   T
   0.7350952976424762   0.9974703056654657   0.4341070940504281   T   T   T
   0.2021300099999976   0.5000000000000000   0.0441399999999987   F   F   F
   0.1872499999999988   0.5000000000000000   0.1657300099999972   F   F   F
   0.2030984750866620   0.4995572868863244   0.2890965087855573   T   T   T
   0.2173234647253838   0.4979193825196236   0.4161306338403511   T   T   T
   0.2957200099999966   0.0000000000000000   0.1054000099999968   F   F   F
   0.3054200199999997   0.0000000000000000   0.2256900100000010   F   F   F
   0.2999582358232483   0.9986237744110973   0.3527968686578333   T   T   T
   0.3468667978206949   0.9969864696525212   0.4818350674703918   T   T   T
   0.8585603044367173   0.4999872570055785   0.9949570312406069   T   T   T
   0.7982599899999983   0.5000000000000000   0.1207100000000025   F   F   F
   0.8054199700000026   0.5000000000000000   0.2397100100000031   F   F   F
   0.7990343289414876   0.4982302764667723   0.3689261578577177   T   T   T
   0.7765188257365757   0.5414039214344972   0.5089706755750172   T   T   T
   0.8992154533541895   0.4308940201813546   0.4988714975453386   T   T   T
```

※(100)-TS1

```
   1.00000000000000
    4.6612049999999998      0.0000000000000000      0.0000000000000000
      0.0000000000000000      2.9619610000000001      0.0000000000000000
      0.0000000000000000      0.0000000000000000     37.4114300000000028
   Ti     O       H
    8      16      2
Selective dynamics
Direct
   0.9907499999999985   0.0000000000000000   0.0225500000000025   F   F   F
```

0.9933699899999979 0.0000000000000000 0.1430799899999968 F F F
0.0018038990704596 0.0002620724453308 0.2643382250692738 T T T
0.0016205539087153 0.0017548325033800 0.3909208291919626 T T T
0.4921799899999968 0.5000000000000000 0.0828399999999974 F F F
0.4956800100000009 0.5000000000000000 0.2028299999999987 F F F
0.4998615424596764 0.5018755811449154 0.3275669937626944 T T T
0.4620918208947060 0.5151408140896336 0.4579377846614179 T T T
0.6989700000000028 0.0000000000000000 0.0618600000000029 F F F
0.6879699699999975 0.0000000000000000 0.1802099900000016 F F F
0.7037982023940472 0.0012943396288634 0.3036130107132777 T T T
0.7328805229582045 0.9991352036723171 0.4341170729260853 T T T
0.2021300099999976 0.5000000000000000 0.0441399999999987 F F F
0.1872499999999988 0.5000000000000000 0.1657300099999972 F F F
0.2041953209258267 0.5005706287545308 0.2882855490015857 T T T
0.2137728171667064 0.5007290549457224 0.4136168878109956 T T T
0.2957200099999966 0.0000000000000000 0.1054000099999968 F F F
0.3054200199999997 0.0000000000000000 0.2256900100000010 F F F
0.2927532639385220 0.0015328570561834 0.3508650172517136 T T T
0.2999872892940516 0.0090589013168980 0.4808550853154188 T T T
0.8598053460369073 0.4999808220000190 0.9949306060429564 T T T
0.7982599899999983 0.5000000000000000 0.1207100000000025 F F F
0.8054199700000026 0.5000000000000000 0.2397100100000031 F F F
0.7904414219344176 0.5025807954442456 0.3678845921804310 T T T
0.7960928346601648 0.4058587488487788 0.4828899611994686 T T T
0.8277949756085121 0.1735990875776636 0.4603100085256742 T T T

※(100)- H^+-H^-

1.00000000000000
4.6612049999999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 2.9619610000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 37.4114300000000028
Ti O H
8 16 2
Selective dynamics
Direct
0.9907499999999985 0.0000000000000000 0.0225500000000025 F F F
0.9933699899999979 0.0000000000000000 0.1430799899999968 F F F
0.0028612912214862 -0.0003139182572888 0.2646537534876320 T T T
0.0075179961818691 0.0016217905795053 0.3922282357808965 T T T
0.4921799899999968 0.5000000000000000 0.0828399999999974 F F F
0.4956800100000009 0.5000000000000000 0.2028299999999987 F F F
0.5013659490549415 0.5009381176514922 0.3287214737514866 T T T
0.4572240503787776 0.5026287258795973 0.4635927348634230 T T T

0.6989700000000028	0.0000000000000000	0.0618600000000029	F	F	F
0.6879699699999975	0.0000000000000000	0.1802099900000016	F	F	F
0.7051776296254213	0.0009813330521925	0.3047521000339962	T	T	T
0.7460826771206351	0.0023133635429394	0.4409974401710334	T	T	T
0.2021300099999976	0.5000000000000000	0.0441399999999987	F	F	F
0.1872499999999988	0.5000000000000000	0.1657300099999972	F	F	F
0.2051097555116824	0.5003782406052510	0.2887056790170166	T	T	T
0.2158324872999103	0.5020301233631420	0.4141551074964343	T	T	T
0.2957200099999966	0.0000000000000000	0.1054000099999968	F	F	F
0.3054200199999997	0.0000000000000000	0.2256900100000010	F	F	F
0.2880123085966793	0.0013762638593044	0.3515434686439303	T	T	T
0.2431394598492825	0.0024409933610196	0.4798526231953872	T	T	T
0.8586838442427086	0.4999970547835936	0.9950164769692075	T	T	T
0.7982599899999983	0.5000000000000000	0.1207100000000025	F	F	F
0.8054199700000026	0.5000000000000000	0.2397100100000031	F	F	F
0.7815875060260047	0.5017104061256668	0.3702404206528291	T	T	T
0.7060286485094713	0.5028286457710119	0.4969524636444890	T	T	T
0.9077771586233044	0.0024058628624221	0.4591490725146786	T	T	T

※(100)-TS2

1.00000000000000

4.6612000278999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	2.9619999359199998	0.0000000000000000
0.0000000000000000	0.0000000000000000	37.4113999047799979

Ti O H

8 16 2

Selective dynamics

Direct

0.9907500011999986	0.0000000000000000	0.0225499993999989	F	F	F
0.9933699882000013	0.0000000000000000	0.1430799911999969	F	F	F
1.0065753520514304	-0.0039540959581146	0.2662879722223821	T	T	T
1.0117362574670539	0.9881273796521503	0.3939707473291828	T	T	T
0.4921799906000004	0.5000000000000000	0.0828400011999975	F	F	F
0.4956800076000007	0.5000000000000000	0.2028300011999988	F	F	F
0.5059013986845746	0.4917725149001270	0.3303600207251394	T	T	T
0.4714563826126399	0.4756629571246567	0.4616632698823036	T	T	T
0.6989700000000028	0.0000000000000000	0.0618599981999992	F	F	F
0.6879699694000010	0.0000000000000000	0.1802099912000017	F	F	F
0.7155179046476188	-0.0074488152290255	0.3070149762210121	T	T	T
0.7794178644219498	0.9703288390535164	0.4438074019764706	T	T	T
0.2021300106000012	0.5000000000000000	0.0441399999999987	F	F	F
0.1872499999999988	0.5000000000000000	0.1657300070000005	F	F	F
0.2162462710057747	0.4952221026899619	0.2895423194966213	T	T	T
0.2276903027985095	0.4879542736667680	0.4148340087892447	T	T	T

0.2957200069999999 0.0000000000000000 0.1054000070000001 F F F
0.3054200187999996 0.0000000000000000 0.2256900129999977 F F F
0.2895011411011921 0.9909245094493176 0.3525730008305497 T T T
0.2416459462686801 0.0060527056234896 0.4815691975516501 T T T
0.8754863946555957 0.5000181453155008 0.9947862472162683 F F F
0.7982599911999984 0.5000000000000000 0.1207100017999991 F F F
0.8033227002211365 0.4967750363497078 0.2425001014965980 T T T
0.7830783869731850 0.4884531178845889 0.3725803937872272 T T T
0.8681144244501643 0.4074716950344824 0.5044365991464141 T T T
0.9610823736187631 0.9826207396238967 0.4609091027796508 T T T

※(100)-H^+-H^+

1.00000000000000
4.6612000278999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 2.9619999359199998 0.0000000000000000
0.0000000000000000 0.0000000000000000 37.4113999047799979
Ti O H
8 16 2
Selective dynamics
Direct
0.9907499999999985 0.0000000000000000 0.0225500000000025 F F F
0.9933699899999979 0.0000000000000000 0.1430799899999968 F F F
0.0026473327852120 -0.0006428428863722 0.2648929265493196 T T T
-0.0022779047899394 0.0178110152487355 0.3910305092372965 T T T
0.4921799899999968 0.5000000000000000 0.0828399999999974 F F F
0.4956800100000009 0.5000000000000000 0.2028299999999987 F F F
0.5011300894905220 0.4974382234831806 0.3291300498520111 T T T
0.4415607510879175 0.5174481499705975 0.4620546563707937 T T T
0.6989700000000028 0.0000000000000000 0.0618600000000029 F F F
0.6879699699999975 0.0000000000000000 0.1802099900000016 F F F
0.7086628511967378 -0.0028969033187366 0.3053849874004011 T T T
0.7415713187662428 0.0179491445823724 0.4524695667777170 T T T
0.2021300099999976 0.5000000000000000 0.0441399999999987 F F F
0.1872499999999988 0.5000000000000000 0.1657300099999972 F F F
0.2060088778815594 0.4986398066246913 0.2886131140239399 T T T
0.1990788008317071 0.5265578074961974 0.4225180759289424 T T T
0.2957200099999966 0.0000000000000000 0.1054000099999968 F F F
0.3054200199999997 0.0000000000000000 0.2256900100000010 F F F
0.2851090474285306 -0.0045813832243775 0.3515583058957079 T T T
0.2890403607519770 0.0159104678864128 0.4968432095202697 T T T
0.8607111823592581 0.4999970462218259 0.9946754526871907 T T T
0.7982599899999983 0.5000000000000000 0.1207100000000025 F F F
0.8054199700000026 0.5000000000000000 0.2397100100000031 F F F
0.7500466249400053 0.5040745747767843 0.3726971790233209 T T T

0.1526931598909132 0.0144835270470761 0.5163804034822491 T T T
0.9382620017255254 0.0168969252990854 0.4614896726355668 T T T

※(110)-bare

1.00000000000000
6.0177998542999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 13.0965995788999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.1138000488000017
Ti O H
24 48 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0533199999999994 F F F
0.0000000000000000 0.2500000000000000 0.1896899999999988 F F F
-0.0000775868934326 -0.0000449116615511 0.3224592158902428 T T T
0.2500000000000000 0.2500000000000000 0.0533199999999994 F F F
0.2500000000000000 0.0000000000000000 0.1896899999999988 F F F
0.2500242127595584 0.2499296515469911 0.3320854445773209 T T T
0.5000000000000000 0.0000000000000000 0.0533199999999994 F F F
0.5000000000000000 0.2500000000000000 0.1896899999999988 F F F
0.4999211604893551 -0.0000100350950193 0.3224813362258777 T T T
0.7499999799999983 0.2500000000000000 0.0533199999999994 F F F
0.7499999799999983 0.0000000000000000 0.1896899999999988 F F F
0.7497436096257363 0.2498910599700177 0.3320373240029290 T T T
0.0000000000000000 0.5000000000000000 0.0533199999999994 F F F
0.0000000000000000 0.7500000200000017 0.1896899999999988 F F F
-0.0001328749367197 0.4998189772262316 0.3234387110501082 T T T
0.2500000000000000 0.7500000200000017 0.0533199999999994 F F F
0.2500000000000000 0.5000000000000000 0.1896899999999988 F F F
0.2499780792751334 0.7500160253872313 0.3320507282559009 T T T
0.5000000000000000 0.5000000000000000 0.0533199999999994 F F F
0.5000000000000000 0.7500000200000017 0.1896899999999988 F F F
0.4998679542952505 0.5000605795961403 0.3219445985191813 T T T
0.7499999799999983 0.7500000200000017 0.0533199999999994 F F F
0.7499999799999983 0.5000000000000000 0.1896899999999988 F F F
0.7497627628562566 0.7499824373313994 0.3320961156682768 T T T
0.0000000000000000 0.2500000000000000 0.0000000000000000 F F F
0.0000000000000000 0.0000000000000000 0.1363700100000003 F F F
-0.0000162360318745 0.2489313673895272 0.2722441947647348 T T T
0.0000000000000000 0.2500000000000000 0.1066399999999987 F F F
0.0000000000000000 0.0000000000000000 0.2430100099999990 F F F
-0.0001677786159065 0.2515317151768287 0.3794957991374647 T T T
0.2500000000000000 0.0977499999999978 0.0533199999999994 F F F
0.2500000000000000 0.3477499899999970 0.1896899999999988 F F F

0.2498296843677858	0.0928635635564961	0.3345720014163551	T	T	T
0.2500000000000000	0.4022499900000014	0.0533199999999994	F	F	F
0.2500000000000000	0.1522500100000030	0.1896899999999988	F	F	F
0.2509582757255849	0.4066425968300953	0.3330954285475348	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.1363700100000003	F	F	F
0.4998805006601356	0.2490429658581801	0.2722458571491644	T	T	T
0.5000000000000000	0.2500000000000000	0.1066399999999987	F	F	F
0.5000000000000000	0.0000000000000000	0.2430100099999990	F	F	F
0.4999544299450802	0.2505324306464229	0.3794995748743392	T	T	T
0.7499999799999983	0.0977499999999978	0.0533199999999994	F	F	F
0.7499999799999983	0.3477499899999970	0.1896899999999988	F	F	F
0.7499991492872813	0.0928679610103199	0.3345115521690589	T	T	T
0.7499999799999983	0.4022499900000014	0.0533199999999994	F	F	F
0.7499999799999983	0.1522500100000030	0.1896899999999988	F	F	F
0.7488357898696016	0.4066147145335462	0.3330509239332731	T	T	T
0.0000000000000000	0.7500000200000017	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1363700100000003	F	F	F
-0.0001349711397927	0.7509903184172017	0.2722503796817322	T	T	T
0.0000000000000000	0.7500000200000017	0.1066399999999987	F	F	F
0.0000000000000000	0.5000000000000000	0.2430100099999990	F	F	F
-0.0000727791357524	0.7485802246195683	0.3795065520610351	T	T	T
0.2500000000000000	0.5977500099999986	0.0533199999999994	F	F	F
0.2500000000000000	0.8477499899999970	0.1896899999999988	F	F	F
0.2505897701763727	0.5932497279834770	0.3331916698765112	T	T	T
0.2500000000000000	0.9022500299999976	0.0533199999999994	F	F	F
0.2500000000000000	0.6522499699999997	0.1896899999999988	F	F	F
0.2498895558456996	0.9070717771939633	0.3344683798625074	T	T	T
0.5000000000000000	0.7500000200000017	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.1363700100000003	F	F	F
0.4999417224554515	0.7507899612361756	0.2722539450926812	T	T	T
0.5000000000000000	0.7500000200000017	0.1066399999999987	F	F	F
0.5000000000000000	0.5000000000000000	0.2430100099999990	F	F	F
0.4998195438077417	0.7494291119886612	0.3795003596775239	T	T	T
0.7499999799999983	0.5977500099999986	0.0533199999999994	F	F	F
0.7499999799999983	0.8477499899999970	0.1896899999999988	F	F	F
0.7490837630986528	0.5932286853378935	0.3332070211372793	T	T	T
0.7499999799999983	0.9022500299999976	0.0533199999999994	F	F	F
0.7499999799999983	0.6522499699999997	0.1896899999999988	F	F	F
0.7499312977603746	0.9070771776207694	0.3345327753749677	T	T	T
-0.0042302189024367	0.4700569025728925	0.4247191666850267	T	T	T
0.0026501448102331	0.5281293111552626	0.4243659912613063	T	T	T

※(110)-H_2

```
1.00000000000000
  5.9239001273999996        0.0000000000000000        0.0000000000000000
  0.0000000000000000       13.1838998795000002        0.0000000000000000
  0.0000000000000000        0.0000000000000000       27.4654006957999997
 Ti     O       H
 32     64      2
Selective dynamics
Direct
  0.0000000000000000  0.2500000000000000  0.0469200009999966  F  F  F
  0.0000000000000000  0.0000000000000000  0.1669299980000005  F  F  F
  0.9997650858038083  0.2490600211728926  0.2927006030425817  T  T  T
  0.9992658344881975  0.9981279234079629  0.4059138792555976  T  T  T
  0.2500000000000000  0.0000000000000000  0.0469200009999966  F  F  F
  0.2500000000000000  0.2500000000000000  0.1669299980000005  F  F  F
  0.2499334687660536  0.9993231366774450  0.2871316267217316  T  T  T
  0.2496607065985710  0.2480240089055323  0.4167822305416769  T  T  T
  0.5000000000000000  0.2500000000000000  0.0469200009999966  F  F  F
  0.5000000000000000  0.0000000000000000  0.1669299980000005  F  F  F
  0.4998662191178251  0.2490542756406270  0.2926426775613734  T  T  T
  0.4992973668871166  0.9982693640878324  0.4059670051882403  T  T  T
  0.7499999799999983  0.0000000000000000  0.0469200009999966  F  F  F
  0.7499999799999983  0.2500000000000000  0.1669299980000005  F  F  F
  0.7499282320393709  0.9992206645134259  0.2871374574831126  T  T  T
  0.7493639256728251  0.2480293747344503  0.4167819844882731  T  T  T
  0.0000000000000000  0.7500000180000015  0.0469200009999966  F  F  F
  0.0000000000000000  0.5000000000000000  0.1669299980000005  F  F  F
  0.9996719373999641  0.7492240825315264  0.2928066441877181  T  T  T
  0.9994580539621433  0.4977240258756412  0.4069636877245465  T  T  T
  0.2500000000000000  0.5000000000000000  0.0469200009999966  F  F  F
  0.2500000000000000  0.7500000180000015  0.1669299980000005  F  F  F
  0.2494124282086289  0.4992386752848635  0.2873315036755278  T  T  T
  0.2495869481742814  0.7482791385336788  0.4169879134529866  T  T  T
  0.5000000000000000  0.7500000180000015  0.0469200009999966  F  F  F
  0.5000000000000000  0.5000000000000000  0.1669299980000005  F  F  F
  0.4995162060676895  0.7491070393005802  0.2927446239993722  T  T  T
  0.4994089060862924  0.4985217599301655  0.4053834679768203  T  T  T
  0.7499999799999983  0.5000000000000000  0.0469200009999966  F  F  F
  0.7499999799999983  0.7500000180000015  0.1669299980000005  F  F  F
  0.7504666681165306  0.4993993231117726  0.2872781562580295  T  T  T
  0.7494868334290736  0.7482757226412560  0.4169848188796969  T  T  T
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2500000000000000  0.1199999930000004  F  F  F
  0.9999962666725211  0.9991573209725171  0.2419738856406450  T  T  T
  0.9995150022765417  0.2469926757516491  0.3632156529767125  T  T  T
```

0.0000000000000000	0.0000000000000000	0.0938400009999967	F	F	F
0.0000000000000000	0.2500000000000000	0.2138500029999975	F	F	F
0.9999048746915419	0.9993772947307722	0.3372718965976630	T	T	T
-0.0005463160526877	0.2501423831261776	0.4587326134730140	T	T	T
0.2500000000000000	0.3477499910000006	0.0469200009999966	F	F	F
0.2500000000000000	0.0977499999999978	0.1669299980000005	F	F	F
0.2497504481245396	0.3483918295849674	0.2895921833093652	T	T	T
0.2490829628458540	0.0919735871918489	0.4179436473028913	T	T	T
0.2500000000000000	0.1522500089999994	0.0469200009999966	F	F	F
0.2500000000000000	0.4022499909999979	0.1669299980000005	F	F	F
0.2497913915732324	0.1498643462842565	0.2888768902446301	T	T	T
0.2511832223328789	0.4036356195618541	0.4158384979932339	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.1199999930000004	F	F	F
0.4999831565566761	0.9991767673997415	0.2419768490303311	T	T	T
0.4995083462627366	0.2469115952708215	0.3631840544269974	T	T	T
0.5000000000000000	0.0000000000000000	0.0938400009999967	F	F	F
0.5000000000000000	0.2500000000000000	0.2138500029999975	F	F	F
0.4998933904405592	0.9994720366429661	0.3373133977395505	T	T	T
0.4995358806162480	0.2489727336543812	0.4586904490992542	T	T	T
0.7499999799999983	0.3477499910000006	0.0469200009999966	F	F	F
0.7499999799999983	0.0977499999999978	0.1669299980000005	F	F	F
0.7498007817841316	0.3484499037354407	0.2896174084198049	T	T	T
0.7495732567814199	0.0919584981490583	0.4179217449541984	T	T	T
0.7499999799999983	0.1522500089999994	0.0469200009999966	F	F	F
0.7499999799999983	0.4022499909999979	0.1669299980000005	F	F	F
0.7498194296971029	0.1498474714003933	0.2888836216453887	T	T	T
0.7476951641718634	0.4036094434595020	0.4157974268043468	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.7500000180000015	0.1199999930000004	F	F	F
-0.0000448389187090	0.4992126818894966	0.2420589608039601	T	T	T
0.9996064287166728	0.7486741496251210	0.3633197651052458	T	T	T
0.0000000000000000	0.5000000000000000	0.0938400009999967	F	F	F
0.0000000000000000	0.7500000180000015	0.2138500029999975	F	F	F
-0.0000890334075733	0.4996594657759940	0.3376431479224771	T	T	T
0.9996064706453784	0.7482270360083831	0.4588554360635816	T	T	T
0.2500000000000000	0.8477499910000006	0.0469200009999966	F	F	F
0.2500000000000000	0.5977500090000021	0.1669299980000005	F	F	F
0.2497584005125647	0.8486815260342111	0.2894953752524000	T	T	T
0.2498896856640215	0.5921205521821447	0.4174478640818243	T	T	T
0.2500000000000000	0.6522499729999964	0.0469200009999966	F	F	F
0.2500000000000000	0.9022500270000009	0.1669299980000005	F	F	F
0.2495210381179040	0.6500953349099871	0.2890469488499843	T	T	T
0.2495017174046688	0.9042054850570821	0.4172294036888083	T	T	T

0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.7500000180000015	0.1199999930000004	F	F	F
0.4998418646592696	0.4992190668372994	0.2420548263457651	T	T	T
0.4995186264254389	0.7483439584264190	0.3632851256806771	T	T	T
0.5000000000000000	0.5000000000000000	0.0938400009999967	F	F	F
0.5000000000000000	0.7500000180000015	0.2138500029999975	F	F	F
0.4999779760805734	0.4999574701246471	0.3369274740327676	T	T	T
0.4996132304908417	0.7485978839721052	0.4588308033821569	T	T	T
0.7499999799999983	0.8477499910000006	0.0469200009999966	F	F	F
0.7499999799999983	0.5977500090000021	0.1669299980000005	F	F	F
0.7494996080983114	0.8486257433421768	0.2894934210937400	T	T	T
0.7490246148849302	0.5921213526122594	0.4174244621491003	T	T	T
0.7499999799999983	0.6522499729999964	0.0469200009999966	F	F	F
0.7499999799999983	0.9022500270000009	0.1669299980000005	F	F	F
0.7498591085225698	0.6501454313357538	0.2890434313198271	T	T	T
0.7492470899703237	0.9042226211613336	0.4172431251987817	T	T	T
0.9978870385086049	0.5066522534583000	0.5012362159394096	T	T	T
0.9982894426571359	0.4494964413405536	0.4978527311914962	T	T	T

※(110)-TS1

1.00000000000000

6.0177998542999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	13.0965995788999994	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.1138000488000017

Ti	O	H
24	48	2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0533199999999994	F	F	F
0.0000000000000000	0.2500000000000000	0.1896899999999988	F	F	F
0.0002089637339929	-0.0000977958285672	0.3225969244433243	T	T	T
0.2500000000000000	0.2500000000000000	0.0533199999999994	F	F	F
0.2500000000000000	0.0000000000000000	0.1896899999999988	F	F	F
0.2497499552764376	0.2504748403313298	0.3324158002131151	T	T	T
0.5000000000000000	0.0000000000000000	0.0533199999999994	F	F	F
0.5000000000000000	0.2500000000000000	0.1896899999999988	F	F	F
0.5002131218235776	0.9964856211066111	0.3228576931278021	T	T	T
0.7499999799999983	0.2500000000000000	0.0533199999999994	F	F	F
0.7499999799999983	0.0000000000000000	0.1896899999999988	F	F	F
0.7508721785560344	0.2504816900276063	0.3324070205424114	T	T	T
0.0000000000000000	0.5000000000000000	0.0533199999999994	F	F	F
0.0000000000000000	0.7500000200000017	0.1896899999999988	F	F	F
0.0002960431490128	0.5050917388910623	0.3289442821809787	T	T	T
0.2500000000000000	0.7500000200000017	0.0533199999999994	F	F	F

0.2500000000000000	0.5000000000000000	0.1896899999999988	F	F	F
0.2562288601055870	0.7469808158820171	0.3308722075453917	T	T	T
0.5000000000000000	0.5000000000000000	0.0533199999999994	F	F	F
0.5000000000000000	0.7500000200000017	0.1896899999999988	F	F	F
0.5002780979295649	0.4939037004308185	0.3213559720595240	T	T	T
0.7499999799999983	0.7500000200000017	0.0533199999999994	F	F	F
0.7499999799999983	0.5000000000000000	0.1896899999999988	F	F	F
0.7443289431532552	0.7469803137551428	0.3308713275245191	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.1363700100000003	F	F	F
0.0001954020651905	0.2480181465142305	0.2725164325447149	T	T	T
0.0000000000000000	0.2500000000000000	0.1066399999999987	F	F	F
0.0000000000000000	0.0000000000000000	0.2430100099999990	F	F	F
0.0002706154947082	0.2454870652229588	0.3797359210344537	T	T	T
0.2500000000000000	0.0977499999999978	0.0533199999999994	F	F	F
0.2500000000000000	0.3477499899999970	0.1896899999999988	F	F	F
0.2536413181583054	0.0904722294046555	0.3338087251873418	T	T	T
0.2500000000000000	0.4022499900000014	0.0533199999999994	F	F	F
0.2500000000000000	0.1522500100000030	0.1896899999999988	F	F	F
0.2453401905555347	0.4068227623919187	0.3360740498061241	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.1363700100000003	F	F	F
0.5001639119703116	0.2515798287499724	0.2725122822769552	T	T	T
0.5000000000000000	0.2500000000000000	0.1066399999999987	F	F	F
0.5000000000000000	0.0000000000000000	0.2430100099999990	F	F	F
0.5002913677788581	0.2487172654475941	0.3795443958677045	T	T	T
0.7499999799999983	0.0977499999999978	0.0533199999999994	F	F	F
0.7499999799999983	0.3477499899999970	0.1896899999999988	F	F	F
0.7468215085587422	0.0904882536850501	0.3337594403846654	T	T	T
0.7499999799999983	0.4022499900000014	0.0533199999999994	F	F	F
0.7499999799999983	0.1522500100000030	0.1896899999999988	F	F	F
0.7552342366320510	0.4068212183254600	0.3360667500512839	T	T	T
0.0000000000000000	0.7500000200000017	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1363700100000003	F	F	F
0.0001610918095229	0.7547922126991045	0.2742774418484362	T	T	T
0.0000000000000000	0.7500000200000017	0.1066399999999987	F	F	F
0.0000000000000000	0.5000000000000000	0.2430100099999990	F	F	F
0.0002921814837595	0.7202773184683646	0.3829758556771187	T	T	T
0.2500000000000000	0.5977500099999986	0.0533199999999994	F	F	F
0.2500000000000000	0.8477499899999970	0.1896899999999988	F	F	F
0.2652317859665242	0.5951857855773882	0.3260684573073142	T	T	T
0.2500000000000000	0.9022500299999976	0.0533199999999994	F	F	F
0.2500000000000000	0.6522499699999997	0.1896899999999988	F	F	F
0.2453715751558663	0.9036678462050919	0.3370325862030191	T	T	T

0.5000000000000000	0.7500000200000017	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.1363700100000003	F	F	F
0.5002236885318732	0.7551735084497868	0.2734083878233091	T	T	T
0.5000000000000000	0.7500000200000017	0.1066399999999987	F	F	F
0.5000000000000000	0.5000000000000000	0.2430100099999990	F	F	F
0.5002550371319117	0.7478695412809507	0.3799151674323549	T	T	T
0.7499999799999983	0.5977500099999986	0.0533199999999994	F	F	F
0.7499999799999983	0.8477499899999970	0.1896899999999988	F	F	F
0.7353177368763789	0.5951770657988338	0.3261101304375507	T	T	T
0.7499999799999983	0.9022500299999976	0.0533199999999994	F	F	F
0.7499999799999983	0.6522499699999997	0.1896899999999988	F	F	F
0.7551026778127897	0.9036832627014063	0.3370768611424558	T	T	T
0.0006623935799739	0.5514926494804819	0.4023646153079649	T	T	T
0.0003488726262579	0.6376438524312051	0.3965269767189566	T	T	T

※(110)-H^+-H^-

1.00000000000000

5.9239001273999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	13.1838998795000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.4654006957999997

Ti	O	H
32	64	2

Selective dynamics

Direct

0.0000000000000000	0.2500000000000000	0.0469200009999966	F	F	F
0.0000000000000000	0.0000000000000000	0.1669299980000005	F	F	F
0.9995565857383447	0.2493468578939986	0.2918126320895935	T	T	T
0.9993328654396552	0.0004812233239241	0.4057343306699323	T	T	T
0.2500000000000000	0.0000000000000000	0.0469200009999966	F	F	F
0.2500000000000000	0.2500000000000000	0.1669299980000005	F	F	F
0.2498692386614911	0.9990581073085216	0.2870275492720356	T	T	T
0.2582671929860709	0.2509161327629215	0.4131518448789995	T	T	T
0.5000000000000000	0.2500000000000000	0.0469200009999966	F	F	F
0.5000000000000000	0.0000000000000000	0.1669299980000005	F	F	F
0.4995753486783842	0.2497776319650068	0.2885377638009195	T	T	T
0.4993637742615585	0.0014618540835418	0.4060623880585330	T	T	T
0.7499999799999983	0.0000000000000000	0.0469200009999966	F	F	F
0.7499999799999983	0.2500000000000000	0.1669299980000005	F	F	F
0.7498630433694259	0.9990574260464297	0.2870216872410089	T	T	T
0.7407178456129812	0.2509812449119457	0.4131955864700477	T	T	T
0.0000000000000000	0.7500000180000015	0.0469200009999966	F	F	F
0.0000000000000000	0.5000000000000000	0.1669299980000005	F	F	F
0.9992555222175911	0.7500641977506025	0.2928696696904650	T	T	T

0.9995000311580589	0.4998878355072344	0.4165098201341251	T	T	T
0.2500000000000000	0.5000000000000000	0.0469200009999966	F	F	F
0.2500000000000000	0.7500000180000015	0.1669299980000005	F	F	F
0.2442321004110299	0.5006302712040016	0.2878028406242842	T	T	T
0.2499820008418389	0.7495816417430687	0.4167549123719901	T	T	T
0.5000000000000000	0.7500000180000015	0.0469200009999966	F	F	F
0.5000000000000000	0.5000000000000000	0.1669299980000005	F	F	F
0.4992743752044106	0.7495602683807324	0.2924570720138106	T	T	T
0.4994173137002954	0.5006132235642539	0.4040201863499905	T	T	T
0.7499999799999983	0.5000000000000000	0.0469200009999966	F	F	F
0.7499999799999983	0.7500000180000015	0.1669299980000005	F	F	F
0.7548721347103915	0.5005839050907225	0.2878718359582669	T	T	T
0.7488295570817286	0.7495260597599886	0.4168192779440017	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.1199999930000004	F	F	F
0.9998671907452136	0.0003763918261373	0.2418687553233969	T	T	T
0.9994825419740055	0.2455725384027994	0.3642070175147331	T	T	T
0.0000000000000000	0.0000000000000000	0.0938400009999967	F	F	F
0.0000000000000000	0.2500000000000000	0.2138500029999975	F	F	F
0.9996951035556001	0.0010387420740635	0.3371985349155315	T	T	T
0.9995661289876421	0.2546552349172050	0.4620643850994453	T	T	T
0.2500000000000000	0.3477499910000006	0.0469200009999966	F	F	F
0.2500000000000000	0.0977499999999978	0.1669299980000005	F	F	F
0.2501186720803887	0.3467430306893728	0.2894398352389493	T	T	T
0.2471513884357007	0.0963686485120344	0.4181429155451463	T	T	T
0.2500000000000000	0.1522500089999994	0.0469200009999966	F	F	F
0.2500000000000000	0.4022499909999979	0.1669299980000005	F	F	F
0.2497450139817370	0.1504368709711711	0.2887661267518151	T	T	T
0.2549646466648331	0.4022178640637506	0.4139793382898996	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.1199999930000004	F	F	F
0.4998552382904468	0.0005094730778820	0.2418874576212909	T	T	T
0.4995133191607571	0.2462894495281459	0.3628781114318650	T	T	T
0.5000000000000000	0.0000000000000000	0.0938400009999967	F	F	F
0.5000000000000000	0.2500000000000000	0.2138500029999975	F	F	F
0.4997538752110946	0.0016326996775446	0.3374698354733018	T	T	T
0.4994609203776937	0.2503438827017231	0.4572455867082867	T	T	T
0.7499999799999983	0.3477499910000006	0.0469200009999966	F	F	F
0.7499999799999983	0.0977499999999978	0.1669299980000005	F	F	F
0.7490177006978649	0.3467371186911862	0.2894783505796648	T	T	T
0.7517688730922100	0.0963882392617540	0.4181655821999574	T	T	T
0.7499999799999983	0.1522500089999994	0.0469200009999966	F	F	F
0.7499999799999983	0.4022499909999979	0.1669299980000005	F	F	F
0.7494875479971574	0.1504444600677109	0.2887521417270710	T	T	T

0.7438068089171176	0.4022375164755360	0.4139847844386021	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.7500000180000015	0.1199999930000004	F	F	F
0.9995213403287211	0.4991331313022979	0.2409210428253425	T	T	T
0.9995487192621908	0.7518194475634309	0.3631764915131205	T	T	T
0.0000000000000000	0.5000000000000000	0.0938400009999967	F	F	F
0.0000000000000000	0.7500000180000015	0.2138500029999975	F	F	F
0.9996306026375934	0.4992937722719606	0.3354604981038723	T	T	T
0.9995343553415337	0.7512149388659458	0.4583845984316541	T	T	T
0.2500000000000000	0.8477499910000006	0.0469200009999966	F	F	F
0.2500000000000000	0.5977500090000021	0.1669299980000005	F	F	F
0.2497602520275417	0.8502395172353756	0.2890530442629781	T	T	T
0.2548103296139705	0.5945252980689278	0.4171394481894884	T	T	T
0.2500000000000000	0.6522499729999964	0.0469200009999966	F	F	F
0.2500000000000000	0.9022500270000009	0.1669299980000005	F	F	F
0.2493451862227850	0.6522067597756912	0.2888514555459056	T	T	T
0.2503883418778848	0.9079549323376861	0.4172326432666439	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.7500000180000015	0.1199999930000004	F	F	F
0.4997361310698453	0.4988652133845698	0.2417172676019049	T	T	T
0.4994634476424157	0.7511842973495553	0.3630414304693202	T	T	T
0.5000000000000000	0.5000000000000000	0.0938400009999967	F	F	F
0.5000000000000000	0.7500000180000015	0.2138500029999975	F	F	F
0.4994735907623767	0.5009818350812076	0.3360729279489701	T	T	T
0.4993816112934268	0.7528888846419253	0.4586304612033421	T	T	T
0.7499999799999983	0.8477499910000006	0.0469200009999966	F	F	F
0.7499999799999983	0.5977500090000021	0.1669299980000005	F	F	F
0.7492220796117871	0.8502401512964882	0.2890458104133445	T	T	T
0.7439440993981972	0.5945110305660567	0.4171238936343420	T	T	T
0.7499999799999983	0.6522499729999964	0.0469200009999966	F	F	F
0.7499999799999983	0.9022500270000009	0.1669299980000005	F	F	F
0.7495420304899537	0.6522002061257116	0.2888975759983724	T	T	T
0.7484891514690305	0.9079268510622199	0.4172354699344965	T	T	T
0.9992579809210048	0.4823501826443620	0.4784356804782550	T	T	T
0.9996131222680479	0.3145367613598974	0.4832433638949959	T	T	T

※(110)-TS2

1.00000000000000

6.0177998542999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	13.0965995788999994	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.1138000488000017

Ti	O	H
24	48	2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0533199999999994	F	F	F
0.0000000000000000	0.2500000000000000	0.1896899999999988	F	F	F
0.0002288837862940	1.0001168831409133	0.3224239425003571	T	T	T
0.2500000000000000	0.2500000000000000	0.0533199999999994	F	F	F
0.2500000000000000	0.0000000000000000	0.1896899999999988	F	F	F
0.2502409915849837	0.2511197457191681	0.3321755549030255	T	T	T
0.5000000000000000	0.0000000000000000	0.0533199999999994	F	F	F
0.5000000000000000	0.2500000000000000	0.1896899999999988	F	F	F
0.5002314128377023	-0.0014701325104042	0.3228050198743537	T	T	T
0.7499999799999983	0.2500000000000000	0.0533199999999994	F	F	F
0.7499999799999983	0.0000000000000000	0.1896899999999988	F	F	F
0.7504241557920955	0.2511259928027766	0.3321536502947823	T	T	T
0.0000000000000000	0.5000000000000000	0.0533199999999994	F	F	F
0.0000000000000000	0.7500000200000017	0.1896899999999988	F	F	F
0.0002459192146160	0.5020287062659298	0.3323402063087090	T	T	T
0.2500000000000000	0.7500000200000017	0.0533199999999994	F	F	F
0.2500000000000000	0.5000000000000000	0.1896899999999988	F	F	F
0.2541031792855828	0.7463495369370556	0.3327126941045070	T	T	T
0.5000000000000000	0.5000000000000000	0.0533199999999994	F	F	F
0.5000000000000000	0.7500000200000017	0.1896899999999988	F	F	F
0.5002487634402222	0.4974877071210034	0.3211612703614409	T	T	T
0.7499999799999983	0.7500000200000017	0.0533199999999994	F	F	F
0.7499999799999983	0.5000000000000000	0.1896899999999988	F	F	F
0.7467279330520291	0.7463420062047744	0.3327636313584037	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.1363700100000003	F	F	F
0.0002279877525782	0.2478440247175018	0.2723056408963246	T	T	T
0.0000000000000000	0.2500000000000000	0.1066399999999987	F	F	F
0.0000000000000000	0.0000000000000000	0.2430100099999990	F	F	F
0.0002698121726911	0.2489940174267014	0.3794229122402276	T	T	T
0.2500000000000000	0.0977499999999978	0.0533199999999994	F	F	F
0.2500000000000000	0.3477499899999970	0.1896899999999988	F	F	F
0.2522068689423617	0.0913229305625688	0.3341981789268046	T	T	T
0.2500000000000000	0.4022499900000014	0.0533199999999994	F	F	F
0.2500000000000000	0.1522500100000030	0.1896899999999988	F	F	F
0.2499974546358778	0.4067381017972547	0.3344985466201389	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.1363700100000003	F	F	F
0.5001551179017308	0.2493462584879908	0.2722985307930571	T	T	T
0.5000000000000000	0.2500000000000000	0.1066399999999987	F	F	F
0.5000000000000000	0.0000000000000000	0.2430100099999990	F	F	F
0.5003357188890823	0.2486327722151670	0.3793975240498482	T	T	T
0.7499999799999983	0.0977499999999978	0.0533199999999994	F	F	F

0.7499999799999983 0.3477499899999970 0.1896899999999988 F F F
0.7482945982649055 0.0913508783183441 0.3341133968103486 T T T
0.7499999799999983 0.4022499900000014 0.0533199999999994 F F F
0.7499999799999983 0.1522500100000030 0.1896899999999988 F F F
0.7505737078025769 0.4067319177861359 0.3344370330647163 T T T
0.0000000000000000 0.7500000200000017 0.0000000000000000 F F F
0.0000000000000000 0.5000000000000000 0.1363700100000003 F F F
0.0001880206977217 0.7540940225121394 0.2759122878974769 T T T
0.0000000000000000 0.7500000200000017 0.1066399999999987 F F F
0.0000000000000000 0.5000000000000000 0.2430100099999990 F F F
0.0004219771187809 0.7120113423882795 0.3865689712178133 T T T
0.2500000000000000 0.5977500099999986 0.0533199999999994 F F F
0.2500000000000000 0.8477499899999970 0.1896899999999988 F F F
0.2615806913825752 0.5946689475519912 0.3295422270702251 T T T
0.2500000000000000 0.9022500299999976 0.0533199999999994 F F F
0.2500000000000000 0.6522499699999997 0.1896899999999988 F F F
0.2460417329743605 0.9041692475298998 0.3360452886810831 T T T
0.5000000000000000 0.7500000200000017 0.0000000000000000 F F F
0.5000000000000000 0.5000000000000000 0.1363700100000003 F F F
0.5002689742006776 0.7515633557257689 0.2744713233956783 T T T
0.5000000000000000 0.7500000200000017 0.1066399999999987 F F F
0.5000000000000000 0.5000000000000000 0.2430100099999990 F F F
0.5003234499874591 0.7505395890516074 0.3808140142049066 T T T
0.7499999799999983 0.5977500099999986 0.0533199999999994 F F F
0.7499999799999983 0.8477499899999970 0.1896899999999988 F F F
0.7389384083663514 0.5946823938400954 0.3295554270182576 T T T
0.7499999799999983 0.9022500299999976 0.0533199999999994 F F F
0.7499999799999983 0.6522499699999997 0.1896899999999988 F F F
0.7544968371241941 0.9041985229564391 0.3361286314692927 T T T
1.0000227620727358 0.5391938407351967 0.4075556369225718 T T T
0.0003903057272182 0.6290694961522478 0.4016733791121966 T T T

※(110)-H^+-H^+

1.00000000000000
6.0177998542999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 13.0965995788999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.1138000488000017
Ti O H
24 48 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0533200030000032 F F F
0.0000000000000000 0.2500000000000000 0.1896900010000024 F F F
-0.0000427489681594 0.0000640850535770 0.3209621480107626 T T T

0.2500000000000000	0.2500000000000000	0.0533200030000032	F	F	F
0.2500000000000000	0.0000000000000000	0.1896900010000024	F	F	F
0.2584098721422534	0.2505105061284917	0.3313310969801091	T	T	T
0.5000000000000000	0.0000000000000000	0.0533200030000032	F	F	F
0.5000000000000000	0.2500000000000000	0.1896900010000024	F	F	F
0.4998571052880277	-0.0000396882681792	0.3213039786235906	T	T	T
0.7500000200000017	0.2500000000000000	0.0533200030000032	F	F	F
0.7500000200000017	0.0000000000000000	0.1896900010000024	F	F	F
0.7390340656745266	0.2512658910852243	0.3314030660970853	T	T	T
0.0000000000000000	0.5000000000000000	0.0533200030000032	F	F	F
0.0000000000000000	0.7500000000000000	0.1896900010000024	F	F	F
-0.0002553110377566	0.4999742626215292	0.3263848539588211	T	T	T
0.2500000000000000	0.7500000000000000	0.0533200030000032	F	F	F
0.2500000000000000	0.5000000000000000	0.1896900010000024	F	F	F
0.2605731838846220	0.7486522863157082	0.3313298780870391	T	T	T
0.5000000000000000	0.5000000000000000	0.0533200030000032	F	F	F
0.5000000000000000	0.7500000000000000	0.1896900010000024	F	F	F
0.4999703023110693	0.5001623419575443	0.3225327787204949	T	T	T
0.7500000200000017	0.7500000000000000	0.0533200030000032	F	F	F
0.7500000200000017	0.5000000000000000	0.1896900010000024	F	F	F
0.7413456263442851	0.7495139483356582	0.3313665120289309	T	T	T
0.0000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.1363700030000032	F	F	F
-0.0008048378871461	0.2503121864983393	0.2775228052241938	T	T	T
0.0000000000000000	0.2500000000000000	0.1066400059999992	F	F	F
0.0000000000000000	0.0000000000000000	0.2430100079999988	F	F	F
-0.0008547978228902	0.2463846688338250	0.3866771506994539	T	T	T
0.2500000000000000	0.0977499999999978	0.0533200030000032	F	F	F
0.2500000000000000	0.3477500190000029	0.1896900010000024	F	F	F
0.2491951322625126	0.0942431077330185	0.3342256169336110	T	T	T
0.2500000000000000	0.4022499809999971	0.0533200030000032	F	F	F
0.2500000000000000	0.1522500089999994	0.1896900010000024	F	F	F
0.2564159975397615	0.4044264974331243	0.3378836266218612	T	T	T
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.1363700030000032	F	F	F
0.4980678460923964	0.2495293581477632	0.2751196014204284	T	T	T
0.5000000000000000	0.2500000000000000	0.1066400059999992	F	F	F
0.5000000000000000	0.0000000000000000	0.2430100079999988	F	F	F
0.4979654351584898	0.2454880243195163	0.3818253828757168	T	T	T
0.7500000200000017	0.0977499999999978	0.0533200030000032	F	F	F
0.7500000200000017	0.3477500190000029	0.1896900010000024	F	F	F
0.7500672981554641	0.0941688576203212	0.3342017247568521	T	T	T
0.7500000200000017	0.4022499809999971	0.0533200030000032	F	F	F
0.7500000200000017	0.1522500089999994	0.1896900010000024	F	F	F

0.7333917854009885	0.4024735086781243	0.3370793745525392	T	T	T
0.0000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1363700030000032	F	F	F
0.0007900947995292	0.7493341626993224	0.2775076548035470	T	T	T
0.0000000000000000	0.7500000000000000	0.1066400059999992	F	F	F
0.0000000000000000	0.5000000000000000	0.2430100079999988	F	F	F
0.0007348866916859	0.7542216192244234	0.3867026599411620	T	T	T
0.2500000000000000	0.5977500190000029	0.0533200030000032	F	F	F
0.2500000000000000	0.8477499820000034	0.1896900010000024	F	F	F
0.2659972025787686	0.5975069842366930	0.3375202426639918	T	T	T
0.2500000000000000	0.9022500179999966	0.0533200030000032	F	F	F
0.2500000000000000	0.6522500179999966	0.1896900010000024	F	F	F
0.2496127580136867	0.9057182543145648	0.3338758905009757	T	T	T
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.1363700030000032	F	F	F
0.5017151411283456	0.7496969350761772	0.2751177257356573	T	T	T
0.5000000000000000	0.7500000000000000	0.1066400059999992	F	F	F
0.5000000000000000	0.5000000000000000	0.2430100079999988	F	F	F
0.5018226112661559	0.7551469327857456	0.3817606953565996	T	T	T
0.7500000200000017	0.5977500190000029	0.0533200030000032	F	F	F
0.7500000200000017	0.8477499820000034	0.1896900010000024	F	F	F
0.7437137480862499	0.5956097553567790	0.3384148205703031	T	T	T
0.7500000200000017	0.9022500179999966	0.0533200030000032	F	F	F
0.7500000200000017	0.6522500179999966	0.1896900010000024	F	F	F
0.7507239175983629	0.9056447372967853	0.3337539713799182	T	T	T
0.0012156652090079	0.2815334052956611	0.4221193755146013	T	T	T
-0.0004124549021207	0.7182380881719480	0.4218866853636188	T	T	T

※(101)-bare

1.00000000000000

5.5226850000000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612049999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.3530349999999984

Ti O

8 16

Selective dynamics

Direct

0.0231342299999966	0.3381019999999992	0.0276814500000029	F	F	F
0.9956512099999983	0.9953572900000012	0.1147915199999971	F	F	F
0.0099299089697006	0.6776084152850740	0.2017730748388492	T	T	T
0.9526799730085348	0.3565620301880545	0.2857192583825442	T	T	T
0.4768657700000034	0.8381019999999992	0.0276814500000029	F	F	F
0.5043487900000017	0.4953572900000012	0.1147915199999971	F	F	F
0.4900700910302996	0.1776084152850741	0.2017730748388492	T	T	T

0.5473200269914652	0.8565620301880543	0.2857192583825442	T	T	T
0.6942687900000024	0.5390462800000009	0.0533909399999999	F	F	F
0.6888860199999982	0.2014475399999966	0.1424443100000019	F	F	F
0.6641690688406934	0.8326643606345397	0.2254899776376359	T	T	T
0.6684133517980543	0.5222471881598669	0.3115624886505791	T	T	T
0.1988094599999997	0.6164099100000016	0.0016000999999974	F	F	F
0.1904341199999990	0.2886050899999972	0.0893614800000009	F	F	F
0.1697858835153961	0.0064592048204837	0.1752014915343000	T	T	T
0.1494149219178352	0.6806262224977000	0.2626352756476690	T	T	T
0.3011905400000003	0.1164099100000016	0.0016000999999974	F	F	F
0.3095658800000010	0.7886050899999972	0.0893614800000009	F	F	F
0.3302141264846048	0.5064592048204838	0.1752014915343000	T	T	T
0.3505850780821648	0.1806262224977000	0.2626352756476690	T	T	T
0.8057312099999976	0.0390462800000009	0.0533909399999999	F	F	F
0.8111139800000018	0.7014475399999966	0.1424443100000019	F	F	F
0.8358309311593066	0.3326643606345394	0.2254899776376359	T	T	T
0.8315866482019457	0.0222471881598670	0.3115624886505791	T	T	T

***(101)-H_2**

1.00000000000000

5.5226998328999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612000465000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.3530006408999995

Ti	O	H
8	16	2

Selective dynamics

Direct

0.0231299989999982	0.3380999910000000	0.0276799999999966	F	F	F
0.9956499520000008	0.9953600139999992	0.1147900030000031	F	F	F
0.0054655434450658	0.6775277739893919	0.2013494812739868	T	T	T
0.9846508535543644	0.3409416763896612	0.2829106728778807	T	T	T
0.4768699819999966	0.8381000170000021	0.0276799999999966	F	F	F
0.5043500049999992	0.4953599629999985	0.1147900030000031	F	F	F
0.4886202470153407	0.1705648645615964	0.2021512172124643	T	T	T
0.5791716692513258	0.8652551829147739	0.2894077803506321	T	T	T
0.6942700279999983	0.5390499680000005	0.0533899989999966	F	F	F
0.6888899710000018	0.2014500020000014	0.1424400100000014	F	F	F
0.6726068487863864	0.8337774526421843	0.2270155342441172	T	T	T
0.6904090251257410	0.5171946336525594	0.3089993774829742	T	T	T
0.1988100049999986	0.6164100230000003	0.0016000000000034	F	F	F
0.1904299979999990	0.2886100039999988	0.0893600010000029	F	F	F
0.1741042216214712	0.0029206134665705	0.1748199042398473	T	T	T
0.1458045991873561	0.6815126933817330	0.2616119075710275	T	T	T

0.3011899950000014 0.1164099980000017 0.0016000000000034 F F F
0.3095700240000028 0.7886100039999988 0.0893600010000029 F F F
0.3344154806308295 0.5031966559800061 0.1757748457568185 T T T
0.3505594339180283 0.1748676134591436 0.2637105821581206 T T T
0.8057299720000017 0.0390500029999998 0.0533899989999966 F F F
0.8111099859999982 0.7014499889999968 0.1424400100000014 F F F
0.8461345602517906 0.3241631657801976 0.2244547879774966 T T T
0.8595290548290254 0.0246975355397191 0.3157381138380699 T T T
0.2837088635377858 0.9105357660974972 0.3509714544747282 T T T
0.4043356087368530 0.9208299031850584 0.3635080473168692 T T T

※(101)-H^+-H^-

1.00000000000000
5.5226998328999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.6612000465000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 29.3530006408999995
Ti O H
8 16 2
Selective dynamics
Direct
0.0231299989999982 0.3380999910000000 0.0276799999999966 F F F
0.9956499520000008 0.9953600139999992 0.1147900030000031 F F F
-0.0133845153635041 0.6905696752129385 0.2027441244750440 T T T
0.0217411438565838 0.3340919406241513 0.2826744369188228 T T T
0.4768699819999966 0.8381000170000021 0.0276799999999966 F F F
0.5043500049999992 0.4953599629999985 0.1147900030000031 F F F
0.4914725924769892 0.1688944737378878 0.2006040608132500 T T T
0.5500145316589903 0.8659907427762785 0.2919548814609807 T T T
0.6942700279999983 0.5390499680000005 0.0533899989999966 F F F
0.6888899710000018 0.2014500020000014 0.1424400100000014 F F F
0.6564092807019870 0.8293147495993528 0.2256009833238274 T T T
0.7401154831504491 0.5487819311211979 0.3196235867043034 T T T
0.1988100049999986 0.6164100230000003 0.0016000000000034 F F F
0.1904299979999990 0.2886100039999988 0.0893600010000029 F F F
0.1748107991820639 -0.0003560656934251 0.1751510277818074 T T T
0.1409177712769634 0.7030644161057198 0.2623478136236700 T T T
0.3011899950000014 0.1164099980000017 0.0016000000000034 F F F
0.3095700240000028 0.7886100039999988 0.0893600010000029 F F F
0.3337613353056375 0.4994834113796479 0.1749639027041181 T T T
0.3643398329946456 0.2065896195057450 0.2647121009803003 T T T
0.8057299720000017 0.0390500029999998 0.0533899989999966 F F F
0.8111099859999982 0.7014499889999968 0.1424400100000014 F F F
0.8610577853812895 0.3217097386819194 0.2261834115380096 T T T
0.8249251502178998 0.0554318987904823 0.3116392039829677 T T T

0.3620467467056658	0.9100567454701592	0.3394908168256388	T	T	T
0.6612563574744368	0.3822213251045740	0.3334004196422921	T	T	T

※(101)-TS1

1.00000000000000

5.5226998328999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612000465000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.3530006408999995

Ti	O	H
8	16	2

Selective dynamics

Direct

0.0231300000000019	0.3380999900000035	0.0276799999999966	F	F	F
0.9956499500000007	0.9953600099999989	0.1147899999999993	F	F	F
0.9879908249598156	0.6933098900291674	0.2023286975634172	T	T	T
0.9983945357848425	0.3536258874348959	0.2833029975715685	T	T	T
0.4768699800000036	0.8381000199999988	0.0276799999999966	F	F	F
0.5043500100000031	0.4953599600000018	0.1147899999999993	F	F	F
0.4825565114277861	0.1794008128658262	0.2014783880270676	T	T	T
0.5699757953493844	0.8968226165889474	0.2913550288801167	T	T	T
0.6942700299999984	0.5390499700000007	0.0533900000000003	F	F	F
0.6888899699999982	0.2014500000000012	0.1424400100000014	F	F	F
0.6581198205757859	0.8452381500748551	0.2271957680686524	T	T	T
0.6914552905265716	0.5352412873884327	0.3120650575284019	T	T	T
0.1988100100000025	0.6164100200000036	0.0016000000000034	F	F	F
0.1904299999999992	0.2886099999999985	0.0893599999999992	F	F	F
0.1698638289635281	0.0097808453016214	0.1751693578596006	T	T	T
0.1319424606088975	0.7063695124283963	0.2613986462413426	T	T	T
0.3011899899999975	0.1164100000000019	0.0016000000000034	F	F	F
0.3095700200000024	0.7886099999999985	0.0893599999999992	F	F	F
0.3334188524348053	0.5103326810906649	0.1752995717811499	T	T	T
0.3442329906288965	0.2002938308334896	0.2647856397129609	T	T	T
0.8057299700000016	0.0390500000000031	0.0533900000000003	F	F	F
0.8111099899999985	0.7014499900000004	0.1424400100000014	F	F	F
0.8447572888715337	0.3334532652407377	0.2260257419399775	T	T	T
0.8521317212916426	0.0487495948383092	0.3153698169477063	T	T	T
0.4047196945539994	0.7749368138522512	0.3466874474383832	T	T	T
0.5404406723227861	0.6156924976249000	0.3395443198980631	T	T	T

※(101)-TS2

1.00000000000000

5.5226998328999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.6612000465000003	0.0000000000000000

0.0000000000000000 0.0000000000000000 29.3530006408999995
Ti O H
8 16 2
Selective dynamics
Direct
0.0231299989999982 0.3380999910000000 0.0276799999999966 F F F
0.9956499520000008 0.9953600139999992 0.1147900030000031 F F F
0.0012370609502403 0.6874002393934214 0.2021449487084943 T T T
0.9833355381025782 0.3210374512065557 0.2841586953302587 T T T
0.4768699819999966 0.8381000170000021 0.0276799999999966 F F F
0.5043500049999992 0.4953599629999985 0.1147900030000031 F F F
0.4988270433065193 0.1803134500093971 0.2013118577798925 T T T
0.5053698836268093 0.8165037598118886 0.2840419592698382 T T T
0.6942700279999983 0.5390499680000005 0.0533899989999966 F F F
0.6888899710000018 0.2014500020000014 0.1424400100000014 F F F
0.6711161251537613 0.8437674403904147 0.2241860943504116 T T T
0.6869669745755336 0.5038128160944156 0.3181656158268557 T T T
0.1988100049999986 0.6164100230000003 0.0016000000000034 F F F
0.1904299979999990 0.2886100039999988 0.0893600010000029 F F F
0.1688439073041851 0.0086534784956768 0.1755108327791723 T T T
0.1647697018610439 0.6767516918017404 0.2628906090318323 T T T
0.3011899950000014 0.1164099980000017 0.0016000000000034 F F F
0.3095700240000028 0.7886100039999988 0.0893600010000029 F F F
0.3336670851484561 0.5075405058933770 0.1750322928036802 T T T
0.3519983386130924 0.1834896275432434 0.2637036771751098 T T T
0.8057299720000017 0.0390500029999998 0.0533899989999966 F F F
0.8111099859999982 0.7014499889999968 0.1424400100000014 F F F
0.8355983251432101 0.3407100890766023 0.2260236946808704 T T T
0.8520453088136665 -0.0035761351938422 0.3093469218394792 T T T
0.6198724810817277 0.0082574065251129 0.3334359117765278 T T T
0.5931568084899029 0.3301450654560142 0.3264860404818882 T T T

※ (101) -H^+-H^+

1.00000000000000
5.5226998328999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.6612000465000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 29.3530006408999995
Ti O H
8 16 2
Selective dynamics
Direct
0.0231299989999982 0.3380999910000000 0.0276799999999966 F F F
0.9956499520000008 0.9953600139999992 0.1147900030000031 F F F
0.9893154934300281 0.6874982160464927 0.2020638435250713 T T T

0.0103273647415964	0.2813095176669463	0.2833660452326817	T	T	T
0.4768699819999966	0.8381000170000021	0.0276799999999966	F	F	F
0.5043500049999992	0.4953599629999985	0.1147900030000031	F	F	F
0.5113245372966442	0.1876271715267699	0.2021055790048440	T	T	T
0.4911781791341317	0.7796265093388678	0.2833120185673110	T	T	T
0.6942700279999983	0.5390499680000005	0.0533899989999966	F	F	F
0.6888899710000018	0.2014500020000014	0.1424400100000014	F	F	F
0.6614141607878694	0.8356734547282445	0.2241130222598008	T	T	T
0.7212643820025448	0.5126665882576854	0.3211052926802438	T	T	T
0.1988100049999986	0.6164100230000003	0.0016000000000034	F	F	F
0.1904299979999990	0.2886100039999988	0.0893600010000029	F	F	F
0.1677672385154986	0.0024381722615969	0.1754921489313303	T	T	T
0.1354760306296870	0.7050570303840259	0.2660342467240259	T	T	T
0.3011899950000014	0.1164099980000017	0.0016000000000034	F	F	F
0.3095700240000028	0.7886100039999988	0.0893600010000029	F	F	F
0.3320573023291198	0.5022152312528652	0.1755588269366501	T	T	T
0.3658330278857834	0.2051166348790354	0.2661467692898015	T	T	T
0.8057299720000017	0.0390500029999998	0.0533899989999966	F	F	F
0.8111099859999982	0.7014499889999968	0.1424400100000014	F	F	F
0.8390533392369210	0.3358237442262950	0.2242147509364948	T	T	T
0.7793375628906906	0.0122859695963971	0.3205282630097958	T	T	T
0.8346579793999219	0.8296689283694365	0.3338805243138078	T	T	T
0.6655421903756396	0.3277749219851417	0.3336690210056010	T	T	T