

SUPPORTING INFORMATION

First-principles study of Na insertion at TiO₂ anatase surfaces: new hints for Na-ion battery design

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Structural models

TiO₂ anatase unit cell has tetragonal symmetry, belonging to *I4₁/amd* space group, and contains 4 formula units (*i.e.* 12 atoms). We perform geometry optimization on the bulk state at PBE+U level of theory by relaxing both atom positions and cell volume. The lattice constants are reported in Table S1.

Table S1. Lattice parameters of TiO₂ anatase minimum-energy structure obtained at both PBE+U and PBE levels of theory.

	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)
PBE+U	3.839	3.839	9.843
PBE	3.803	3.803	9.751
<i>exp. [S1]</i>	3.784	3.784	9.515

The calculated values are in good agreement with experimental data at room temperature (PBE+U values show a 1.5% deviation on *a* and *b* values and 3.4% on *c*; PBE results show 0.5% deviation on *a* and *b* and

2.4% deviation on c). Despite PBE minimum-energy structure is closer to experimental one, we choose PBE+U level of theory for the following calculations as it would provide a higher accuracy in describing electronic features of the Na-ion interacting with a transition metal-based oxide. However, comparison with migration barrier computed with PBE functional is provided in Figure S3.

In Figure S1 we report the anatase unit cell in order to highlight the [010] Na-diffusion channel and the (101), (100) and (001) lattice planes that have been selected to cleave the corresponding surfaces.

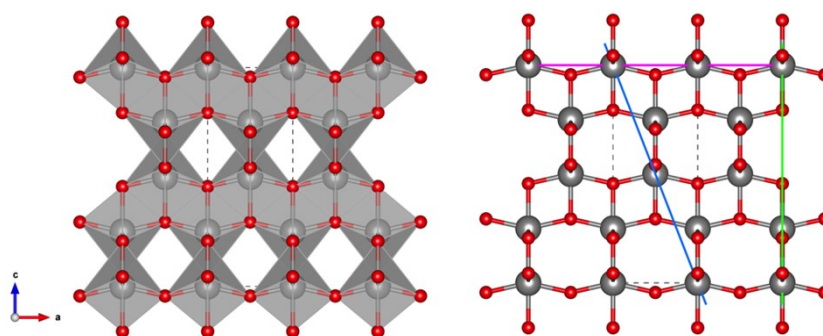


Figure S1. Structural model of TiO₂ anatase. Left: view of the Na-diffusion channel along the [010] direction. Right: view of the (101) (blue), (100) (green) and (001) (pink) lattice planes selected to cleave the surface models. Atoms are represented as spheres: Ti atoms in grey, O in red.

We built up 6-layers slabs to have 24 f.u.-containing cells of comparable exposed surface area by cleaving the bulk unit cell for (101), the 1x2x1 supercell for (100) and the 2x2x1 for (001) surface along the corresponding planes. 10Å of vacuum have been added along the c direction in order to avoid unfeasible interactions. We carried out geometry optimization of slab models at PBE+U level of theory by relaxing only atom positions thus assuming the lattice constants to be equal to the optimized bulk state. Figure S2 shows our slab models and the lattice parameters are listed in Table S2.

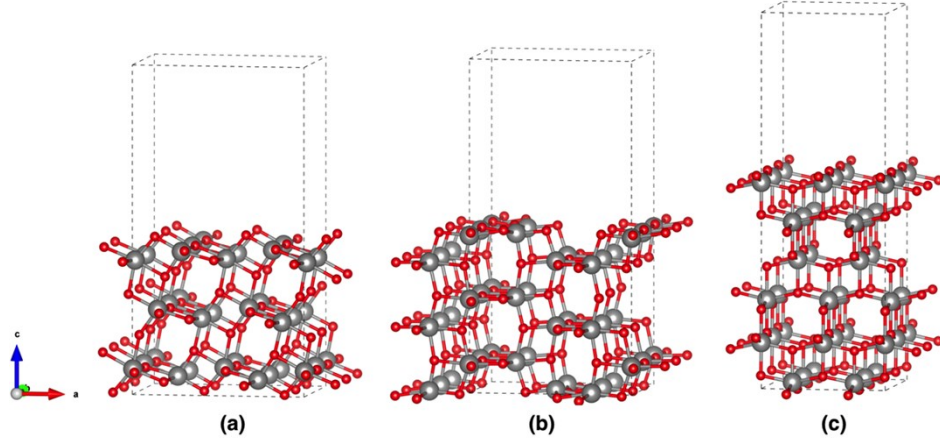


Figure S2. PBE+U minimum-energy structures of a) (101), b) (100) and c) (001) TiO₂ anatase surfaces. Colour code: Ti (grey), O (red).

Table S2. Lattice parameters of slab models for the three low-index surfaces of TiO₂ anatase, obtained from PBE+U minimum-energy structure of the bulk.

	a (Å)	b (Å)
(101)	10.566	7.678
(100)	9.843	7.678
(001)	7.678	7.678

Surface energy

In Table S3 we report the exposed surface area and the surface energy calculated by fully relaxation of layers at DFT-PBE+U level of theory. We calculate the surface energy as:

$$E_{surf} = \frac{E_{slab} - nE_{bulk}}{2S} \quad (S1)$$

where E_{slab} and E_{bulk} are, respectively, the total energy of the optimized slab model and the bulk unit cell, n is the ratio between formula units contained in the slab and in the bulk unit cell, and S is the exposed surface area. These results show that our models agree with the literature.

Table S3. Exposed surface area, S , and surface energy, E_{surf} , for each optimized slab model at PBE+U level of theory.

	$S (\text{\AA}^2)$	$E_{surf} (\text{J/m}^2)$	$E_{surf} (\text{J/m}^2) [S2]$
(101)	81.127	0.613	0.49
(100)	75.582	0.715	0.58
(001)	58.957	1.087	0.98

Oxygen vacancy defects

We investigated Na^+ adsorption and insertion energetics into the (101), (100) and (001) surface facets of TiO_2 by including oxygen vacancies, in order to see to what extent reduced titania could show different performances as NIB anode material. We introduced one oxygen vacancy in the 72-atoms cell (24 f.u.), which corresponds to $\sim 2\%$ of defect concentration. Each surface exposes two kind of oxygen atoms, differing for their coordination to titanium sites, *i.e.* the two-fold and three-fold coordinated oxygen, O_{2c} and O_{3c} respectively. Thus, two kind of vacancies have been considered for each surface and the vacancy formation energies computed at PBE+U level of theory are reported in Table S4 and are in agreement with literature [S3].

Table S4. Oxygen vacancy formation energies, ΔE_{form} , computed at PBE+U level of theory for each surface termination.

$\Delta E_{form} (\text{eV})$	O_{2c}	O_{3c}
(101)	4.364	5.578
(100)	4.216	5.506
(001)	3.693	4.958

As it can be observed in Table S5, the trends both for adsorption and insertion energies do not change if compared to pristine surfaces.

Table S5. Adsorption, E_{ads} , and insertion energies, E_{ins} , computed at PBE+U level of theory for each surface termination.

$E_{ads} (eV)$	<i>pristine</i>	O_{2c}	O_{3c}
(101)	-1.120	3.448	4.292
(100)	-1.554	2.396	3.144
(001)	-0.801	2.618	3.940
$E_{ins} (eV)$	<i>pristine</i>	O_{2c}	O_{3c}
(101)	0.266	4.394	5.632
(100)	0.460	4.311	4.993
(001)	0.364	3.262	4.152

36-atoms containing cells

In order to investigate different sodium coverage on the studied surfaces, we performed some preliminary tests on smaller cells (36 atoms, 12 f.u.) showing larger coverage. As it can be noted in Table S6, no change in the observed energetics was detected.

Table S6. Adsorption, E_{ads} , and insertion energies, E_{ins} , computed at PBE+U level of theory for each surface termination on 36-atoms cells corresponding to higher sodium coverage. Comparison with 2x-supercells is provided.

	$E_{ads} (eV)$		$E_{ins} (eV)$	
	36-atoms	72-atoms	36-atoms	72-atoms
(101)	-0.838	-1.120	-0.091	0.266
(100)	-1.452	-1.554	-0.789	0.460
(001)	-0.775	-0.801	0.021	0.364

Na migration path computed at PBE level of theory

We report the CI-NEB related to the MEPs of Na migration through (101), (100) and (001) surfaces computed at the PBE level of theory in order to compare energy barriers obtained for structures that are

closer to experimental ones. From Figure S3 it is clear that no change in the energy migration trend is detected when considering the PBE TiO₂ anatase minimum-energy structures.

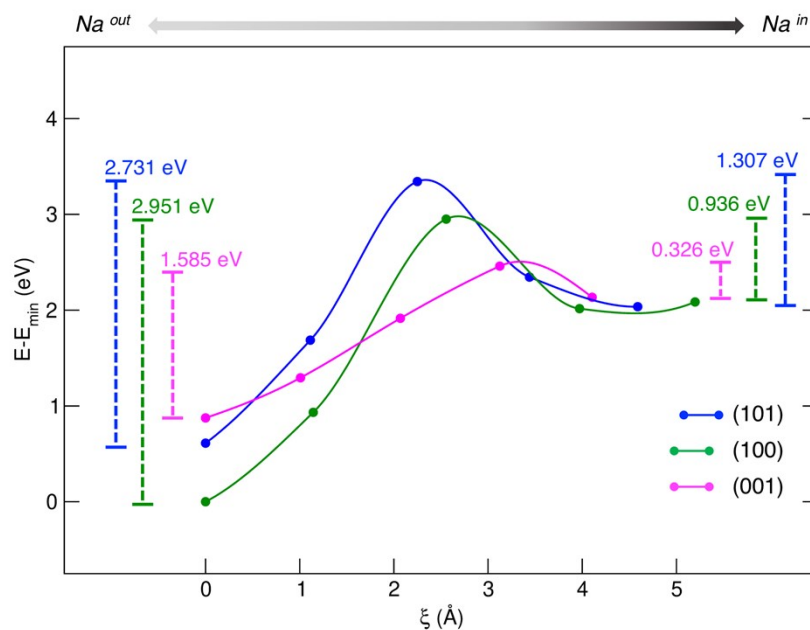


Figure S3. Energy variation along Na migration path computed for (101) (blue), (100) (green) and (001) (pink) surfaces at the PBE level of theory. Energy barriers at highest-energy points are calculated according to equations (4) and (5) for the in/out migration and are reported, respectively, to the right- and left-hand sides of the graph.

Coordinates of Na migration path computed at PBE+U level of theory for (101), (100) and (001) surfaces

- (101)

TiO2 anatase slab 101 6L Na out

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0.0000000000000000	0.0000000000000000	20.0000000000000000
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TiO2 anatase slab 101 6L Na -01

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Ti O Na
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TiO2 anatase slab 101 6L Na -02

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0.3460961061931670	0.2471092236063141	0.4496296456152585
0.3270746335083628	0.2495947811370071	0.1267106281883967
0.3275733696546327	0.7506491114049875	0.1263796650226958
0.4785678703610854	0.2513223959587766	0.3038638265005137
0.4796266429474866	0.7483766771112982	0.3032088642837441
0.6280576998308736	0.2460073473819371	0.4808450473345774
0.6273147154914226	0.7535117167451922	0.4811837260944695
0.8275311230807707	1.0002420047404146	0.1272592240034114
0.8277679223814587	0.4998140746474656	0.1272030514502268
0.1333009054494652	0.9973114667497713	0.4778430308781776
0.1418001307109037	0.5023038163344237	0.4811499788235984
0.1812062318164412	0.0000544602717415	0.0395948614966064
0.1813705609923203	0.5001940725933356	0.0397648063009586
0.3320899987866510	0.0000285062002681	0.2293353904048316
0.3320249460451025	0.5003039517660981	0.2286459682856307
0.4770272924943881	-0.0027245738151049	0.4057012995264465
0.4806122771182233	0.5018816744685685	0.4086069618201248
0.6818247839537485	0.2500533329976429	0.0401795509440853
0.6818487638615315	0.7501340697175006	0.0399079240963255
0.8325861992598945	0.2497495718271188	0.2309276679774777
0.8321720565786204	0.7502486949431514	0.2301086905550310
0.3857718083543974	0.2502295468138021	0.0055285149402807
0.3855069634971905	0.7499869860680830	0.0051277058148891
0.5416586698218806	0.2500356990560803	0.1811163797733613
0.5422322922754548	0.7502182015797307	0.1805050888621339
0.6915327035944977	0.2503362386064308	0.3594161814359961
0.6929742939488626	0.7500265622427734	0.3598069063664399
0.8860262129921133	0.0000960386991188	0.0060007434184325
0.8862591383630222	0.5001744701837691	0.0060180009837019
0.0419667605386247	1.0010333296023737	0.1816983538220678
0.0426716830806030	0.4994051284943980	0.1816065255523524
0.1968342856950674	1.0013368024785680	0.3593067553460698
0.2030780501710779	0.5004220097777289	0.3594796473638713
0.9657847200645876	0.7566483687522626	0.4074036286302108
0.9801762230346042	-0.0025847753894697	0.3045062624718626
0.9630949550789790	0.2431710182843513	0.4068985107046746
0.9803028861817825	0.5021617054294109	0.3039819008689515
0.3451855320129816	0.7517266478032145	0.4510897538206490
0.1548066429724273	0.2515168585475127	0.4251622098057070

TiO2 anatase slab 101 6L Na -03

1.0000000000000000		
10.5656501322887006	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
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0.7324223081999283	0.5000832476342979	0.0499170258579643
0.8723063253976483	0.0002237469865836	0.2265995982352942
0.8738654683819037	0.4994840741805382	0.2262873751338901
0.0145474637539076	0.9935956235797851	0.4101867039877765

0.0167256324102603	0.5077912118662214	0.4108689346872430
0.2312460396419782	0.2504224162772832	0.0496896364442800
0.2315366779315607	0.7500736784586717	0.0495688450928105
0.3727014359583459	0.2514114878790673	0.2252036720263658
0.3743692446993824	0.7498621219616378	0.2248979132091392
0.5170265657108800	0.2480574029150565	0.4074195208319878
0.5199747266143657	0.7487984377736639	0.4071522066344169
0.5018349974093151	0.2502821485781582	0.0770552413463486
0.5018352604927729	0.7499343754312700	0.0763115267950792
0.6481477606887983	0.2506550507810751	0.2592587784667672
0.6487301079418227	0.7491711896263854	0.2589645590941164
0.7878478014361019	0.2508055018972383	0.4350114235798591
0.7851828717595637	0.7491780434311675	0.4370358574817356
0.0018275927815156	1.0002479414604259	0.0773784076104199
0.0019622712408499	0.5002471749420755	0.0784876204996165
0.1484970119287867	0.9959592670983155	0.2583680136515736
0.1479163097707010	0.5078236395762257	0.2624329536287623
0.2938317793377841	0.9867305233308731	0.4388540766911880
0.2938876411158226	0.5089567053360492	0.4467547874383554
0.5423251513054473	0.0001361119753227	0.0748222073287827
0.5422921450156896	0.5000958823586640	0.0747273483729907
0.6882637435764291	-0.0001401386132157	0.2554846588648672
0.6877766355074350	0.4999578972057744	0.2548071618037178
0.8370758035719454	0.0005293159060991	0.4474645069684267
0.8349681350536566	0.4995300370329467	0.4474322318307111
0.0425640029035998	0.2501667657626508	0.0753716783779321
0.0429295494496009	0.7503802254232286	0.0759871814531428
0.1896310191324787	0.2505337094500529	0.2603463656709761
0.1879156744603927	0.7514879781253864	0.2515314087850296
0.3406081050113756	0.2377828618726990	0.4462002984259156
0.3264841591142737	0.2505900157593576	0.1265479548987102
0.3284676072374788	0.7500821357125281	0.1258486917289657
0.4777337828984251	0.2522404297858127	0.3037968380789628
0.4795263149992739	0.7471535233835087	0.3034096576891878
0.6332350390742986	0.2464447024545838	0.4792980788307089
0.6323389696207032	0.7518247699598414	0.4810079096076251
0.8278212206451748	-0.0001633267612681	0.1269441707066862
0.8272018784154205	0.5000612698328939	0.1267117499891016
0.1327098494142961	1.0019468385000039	0.4798720030622550
0.1248967562590946	0.4939862430088642	0.4825394191560209
0.1814962333713502	1.0001426247487548	0.0392125438641088
0.1815549662519114	0.5003406347671764	0.0395171301943743
0.3322982952234673	0.0007790113859132	0.2294032651012768
0.3311171572534478	0.5006986045870163	0.2299794863378726
0.4802370572945018	0.9970785502332907	0.4051070869730428
0.4780192131888130	0.4996794183678346	0.4107615630711572
0.6818852513246518	0.2499587114787579	0.0396980563502758
0.6820745591370347	0.7502217246804135	0.0393497016827631
0.8317691161245089	0.2493925897615618	0.2302037011361494
0.8324649212465177	0.7504647997232576	0.2301031044369207
0.3859612762945528	0.2501129160303598	0.0052588782170573
0.3858499069335834	0.7500974475456842	0.0046024286111473
0.5410997755531408	0.2500553922070169	0.1807544127686491
0.5421431518632096	0.7504480758021311	0.1804335478416907
0.6929037164052759	0.2506049828673291	0.3581373743637007
0.6935308303967933	0.7485821918956505	0.3590921745037115
0.8862136090909792	1.0000741776160997	0.0055764070685917
0.8870228865003525	0.5003747011330644	0.0058083736094337
0.0417214460716383	1.0027984121214280	0.1811672297150227
0.0412958099723589	0.4987001277843217	0.1819034002091332
0.1961672962174349	0.9770191567382580	0.3600450161695345
0.1872480946636679	0.5252821019743451	0.3609818245342029
0.9727391283941972	0.7511847747400993	0.4114805107290121
0.9812413670551987	0.9993757042906068	0.3045792640265340
0.9787107869698762	0.2487475769702137	0.4078615191150408
0.9764722492672538	0.5003394880021220	0.3044980240745129
0.3511044511774462	0.7579827729021756	0.4561489126994688
0.1847435680465167	0.2524044323983874	0.3713878097294543

TiO2 anatase slab 101 6L Na in

1.0000000000000000		
10.5656501322887006	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
24	48	1

Direct

0.7317057793936002	0.9997540961799558	0.0491596570235657
0.7323145414609655	0.5002117077271180	0.0485271674381451
0.8695210132906652	0.0004429357769524	0.2259123905388734
0.8700035287944914	0.4992909839045296	0.2253948381134805
0.0196015177035918	0.9977984040640706	0.4087729213758706
0.0209898836283031	0.5020765407931762	0.4095097926335569
0.2303872640119948	0.2501608095203878	0.0458400114459039
0.2316171174071755	0.7498526392457947	0.0489099950974961
0.3741303699682348	0.2504517119714507	0.2182003206710448
0.3716995483843277	0.7489594774956103	0.2258482552562171
0.5234105991635971	0.2475542983583736	0.4149725058298088
0.5182454265308323	0.7489976011095081	0.4093746195131089
0.5025076632307872	0.2502146475130971	0.0732420703388428

0.5013557764226491	0.7498151677287765	0.0769187101478224
0.6439632724649513	0.2504249609902942	0.2603103752873110
0.6459777629789585	0.7494128210462563	0.2597482213228304
0.7932597101728263	0.2506533091224910	0.4346705266841653
0.7888123482047362	0.7494562773181102	0.4346905494120037
0.0016498603607928	0.9998788072521876	0.0767700301813434
0.0017772456419536	0.5001977608046602	0.0777745664919749
0.1450179614389739	0.9987999066960782	0.2579360039221683
0.1432572772311573	0.5052715926821207	0.2614578392481945
0.2899589751957805	0.9922508171440683	0.4430136987642541
0.2891620305707789	0.5067003596083737	0.4512577885192997
0.5420131704096960	0.0002141321200995	0.0735675061647498
0.5420246809277174	0.4998077538016403	0.0732637246356447
0.6859804638704716	0.0003578664955199	0.2557563980039390
0.6852991193451814	0.4994165282617828	0.2550816142039878
0.8388403403370219	0.0000772490408991	0.4456593316761115
0.8360066064801188	0.4997580542660245	0.4449910491843596
0.0430805185187424	0.2499742147144346	0.0742720560129726
0.0429190255503755	0.7501565019582372	0.0750265890519017
0.1851646009940628	0.2506253681901995	0.2533206725714905
0.1870504802956319	0.7513522707178524	0.2550249949458632
0.3429111638460682	0.2369544001888784	0.4544133122818934
0.3271624315428170	0.2504502306225334	0.1223406289357598
0.3266010332266518	0.7494704568798696	0.1257171266381931
0.4748536303002950	0.2515114640622400	0.3010865370626945
0.4763856161134683	0.7469407029441300	0.3041792129777363
0.6400128459116914	0.2473240178249725	0.4835210643393779
0.6349489556397216	0.7508403890779149	0.4803255038504872
0.8267445797086381	0.0025138827015567	0.1260337395123017
0.8258495048748955	0.4972584168042147	0.1256189571388973
0.1300043190546702	0.9942847642325887	0.4824671238346241
0.1200665516194377	0.4995791688481930	0.4848784250168094
0.1810162670684647	0.9998957600950718	0.0373321829523405
0.1811085438428677	0.5001571395672713	0.0377495696674401
0.3304603320731303	0.0015082482995865	0.2283744445761045
0.3292247859579831	0.4989688119527003	0.2294196962753432
0.4794716287611536	0.9999660375444819	0.4071618973027427
0.4747539382876909	0.4964787856183008	0.4127739050203161
0.6814659219570203	0.2498333044330536	0.0366925936481195
0.6822339105968425	0.7501527730575432	0.0394734635252902
0.8293597639731374	0.2493023736439568	0.2303397752005196
0.8287276495793421	0.7505185621371098	0.2289900212344946
0.3858770072783457	0.2500191125734545	0.0016776328149817
0.3865075465694048	0.7500637571697979	0.0046214020184081
0.5424158542546422	0.2499765875066018	0.1782199523464598
0.5396027358142419	0.7500689020573219	0.1807240027080397
0.6893313050872223	0.2506004203539263	0.3603549574490899
0.6914043062509663	0.7488951297506219	0.3585397006841262
0.8863766190186695	0.9990211215333389	0.0047658662914287
0.8872580451821648	0.5010876871125447	0.0048459341607625
0.0398766501207390	0.9988756933189222	0.1802451460971426
0.0389493052673160	0.5021078725635491	0.1807710250944439
0.1960550971845763	0.9994754808049819	0.3617775474381801
0.1868103125869638	0.5067226976137533	0.3620500990536470
0.9759245349842942	0.7512852062922022	0.4087652990440489
0.9795077650551249	0.9995260163386348	0.303459777699020
0.9786173136017098	0.2483815273066412	0.4086318294785016
0.9741895852646110	0.5004886903613937	0.3030800668614191
0.3484116856637982	0.7587897333803468	0.4566622423147564
0.2821570764544390	0.2607344746782090	0.3485004404979932

- (100)

TiO2 anatase slab 100 6L Na out

1.0000000000000000		
9.8434554295713088	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
24	48	1

Direct

0.9992815942725173	0.9999980865693772	0.0858430767398772
0.9998254411258074	0.4999984088648048	0.0856322609369684
0.0018549550318383	0.9999922516726798	0.2803198148470898
0.0032470300707530	0.4999924868641870	0.2798535761059853
0.0011786614026761	0.9999863054658888	0.4713604552044828
0.9992255474082796	0.4999891542902404	0.4717324461171515
0.4987551535602393	0.2499827321350239	0.0043044614902499
0.4987545513786102	0.7500191656072701	0.0043048392351395
0.5016727574369639	0.2500510104291536	0.1946260487629914
0.5016743569387430	0.7499431767795315	0.1946267502517216
0.4988930700732084	0.2485031041769474	0.3881158132265696
0.4988920981742311	0.7514768179866422	0.3881168536213124
0.2522732777075376	0.2498457218081214	0.0861237917113584
0.2522738578844681	0.7501507738961379	0.0861250541894663
0.2506953044351974	0.2495809348552740	0.2807713497446755
0.2506956955676145	0.7504037995959436	0.2807714506980048
0.2511748070091357	0.2499970687390061	0.4717720470871711

0.2511748121146837	0.7499774434809652	0.4717733763305958
0.7523942268918304	0.0000004459425398	0.0044235542177518
0.7524011443143550	0.5000014463664542	0.0041509443305046
0.7506719442875962	0.9999977880583799	0.1949967328429878
0.7505189743835388	0.4999964900067084	0.1939480738546564
0.7546017624164207	0.9999900661581194	0.3894958810853311
0.7557503588728878	0.4999910869270323	0.3861915959663307
0.2058592253520430	0.9999980456669633	0.0888529351829774
0.2058718735880305	0.4999982034001675	0.0887683368153844
0.2077354282550985	0.9999923170862886	0.2820072798770852
0.2078511030895527	0.4999923601493421	0.2826238155694440
0.2126318222195991	0.9999878742062407	0.4897726850590161
0.2084444430321497	0.4999867745370068	0.4901451096723619
0.7074888982975551	0.2500941508504084	0.1935258932144492
0.7074906490434074	0.7498999555279227	0.1935262413598906
0.7061881873202367	0.2498212127308008	0.3862370341570127
0.7061867929676566	0.7501597411105649	0.3862390039204442
0.4683360616139893	0.2499386467675677	0.0950880212938117
0.4683369645292217	0.7500612148884187	0.0950884687530689
0.4546609379390745	0.2519289093029826	0.2890752915567205
0.4546613210699917	0.7480592701425550	0.2890760443136386
0.4421925935252986	0.2624416618087011	0.4813185723578286
0.4421921412335976	0.7375327835056211	0.4813196704804881
0.5447741822665080	0.9999970389765807	0.1938771169903646
0.5452517105779009	0.4999970230841839	0.1933114624930425
0.5449352724534862	0.9999901914051676	0.3885407171327842
0.5490547709019040	0.4999901179871387	0.3897875291024135
0.2991224209829397	0.2500702783314068	0.1870738619400498
0.2991245040869686	0.7499196639948451	0.1870742847802660
0.2853504342926954	0.2473190771003715	0.3808804356086952
0.2853486289870588	0.7526590712596217	0.3808813156740882
0.7834526155560653	0.9999992376862892	0.0951164036169416
0.7834925373349932	0.5000005848566218	0.0949419623995027
0.7989753779272917	0.9999940949684500	0.2887630226253464
0.7994595249829146	0.4999946980177157	0.2882549077324512
0.8126187299252123	0.9999928658101993	0.4799942449546748
0.8074204253028014	0.4999861668224597	0.4801735743838833
0.9533479157042137	0.0000017757966049	0.1867452755429397
0.9538342573812244	0.4999881632697409	0.1865497042344515
0.9687747323784066	0.9999779339164903	0.3804080743601403
0.9683651583477086	0.4999995035375733	0.3807122231781861
0.9396287243737760	0.9999960213647796	0.9956305678660726
0.0458644554865302	0.7500215028948816	0.0884918551675185
0.0458646581514017	0.2499747366147815	0.0884877433667697
0.9396650496192436	0.5000029055447897	0.9954943652252979
0.0454615591053908	0.7498935278505527	0.2820242624074893
0.0454609899375953	0.2500911010072002	0.2820309142512869
0.0417674191756561	0.7500379975516367	0.4893995943120686
0.0417672072191024	0.2499371494617861	0.4893935829394280
0.3114780479051262	0.2499484736169819	0.9958376818805945
0.5415738637171614	0.0000009782531407	0.9871801452305107
0.5415541844464329	0.5000008590501182	0.9870967597524114
0.7096115386117106	0.2500682539747530	0.9871777398006287
0.3114774273854977	0.7500504280442186	0.9958386753969393
0.7096102115331320	0.7499335838052374	0.9871774532799265
0.5744884075352275	0.4999828207197865	0.5183898786177110

TiO2 anatase slab 100 6L Na -01

1.0000000000000000		
9.8434554295713088	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
24	48	1

Direct

1.0019147993497501	1.0002070975925670	0.0859292993496666
1.0016735237431031	0.4998710136489998	0.0860878715719138
0.0038344673814090	1.0013333793005088	0.2801560008025048
0.0035933217581346	0.4995964276774882	0.2803843362158708
-0.0060107613763875	1.0020619258935100	0.4727325532872849
0.9977078654096225	0.5001561354089139	0.4716475148130421
0.4999739944432447	0.2499351117788316	0.0042050068359010
0.5007597593579112	0.7499046670270463	0.0044466583017541
0.5019265501332175	0.2497251948929854	0.1944601446571878
0.5032105868582434	0.7497844905914066	0.1944455417161131
0.4989328506106363	0.2424174722634725	0.3872859159580631
0.5007500006266977	0.7562067722242571	0.3859628157767491
0.2545072900378897	0.2501274026394717	0.0870734412991932
0.2540181333348332	0.7499881423764776	0.0863446109527725
0.2530760710251269	0.2509487995348017	0.2830247109409775
0.2497689731394909	0.7506017060180866	0.2804153560658849
0.2442000740446450	0.2381018623012892	0.4739671157966474
0.2425520291269203	0.7575877572029008	0.4699921742981613
0.7545503904752243	0.0001336337823902	0.0045748657205463
0.7544915107949540	0.4997672611278286	0.0046918171419962
0.7522489715405529	1.0002674087472603	0.1946303924757003
0.7520901792074028	0.4994184821300049	0.1949044766495547
0.7559362081294454	1.0006792511948615	0.3878639587331321
0.7539888043056786	0.4986106085190516	0.3882678994938507
0.2078873735424965	0.9999680977969823	0.0890217287481491

0.2077640216648439	0.5001871991472907	0.0890368014186180
0.2085017900766961	1.0006205352322557	0.2816395575378899
0.2082084406324057	0.5009832234838489	0.2815899329044977
0.1994687991877215	0.9907565421222310	0.4977746563578294
0.2114808034135703	0.5099665381340835	0.4919208688675740
0.7094892056030476	0.2497823095337718	0.1936923308717442
0.7090339913741690	0.7498771413191557	0.1939142189451894
0.7086791230440268	0.2497454731065166	0.3854060180412366
0.7071071292994360	0.7495323520187875	0.3859792169613597
0.4708212944323771	0.2499562270129230	0.0949072196721104
0.4704293893490150	0.7495737042893019	0.0952781900923129
0.4568193680560818	0.2487213563718448	0.2872991781788081
0.4537677325567226	0.7490126424647676	0.2884865580076255
0.4457428365594700	0.2272820423852528	0.4763051975132179
0.4360358013696697	0.7666293123807328	0.4767014807360061
0.5470814696299411	0.9992980779194555	0.1933370953556516
0.5469526613595496	0.5001941980698463	0.1937193887187193
0.5502852346273411	0.9980867005628100	0.3813581384291570
0.5455394247806394	0.5007376132902761	0.3891596477213663
0.3011172211148886	0.2506782914419975	0.1868432082948227
0.3006790061747501	0.7503635245275806	0.1867097085786212
0.2883909715600541	0.2540368196919519	0.3790866347583257
0.2790929435746928	0.7539170407182363	0.3792359658697007
0.7859496159661100	0.9996848228862848	0.0953246653194902
0.7857117740376903	0.5001255225735858	0.0954317755173140
0.8018091795489132	0.9993557597441625	0.2882787260412832
0.8006673171898294	0.5004534617462035	0.2886249610436893
0.8074543385611792	1.0005978090847076	0.4796255240456857
0.8095614997958467	0.4994812645150188	0.4794625556466178
0.9557812755526403	0.0007491402250652	0.1867942253062735
0.9553313437861997	0.4996396782646983	0.1869896829757148
0.9692277914663862	1.0033496951943530	0.3812312390847518
0.9695164575775497	0.4973677697728525	0.3807039137737213
0.9417523933284282	1.0002409383929372	0.9958582512832975
0.0477830215720094	0.7500373578957732	0.0888506914462068
0.0479424971282639	0.2500745804650980	0.0889904108131207
0.9416990594304658	0.4997868463466662	0.9960098602670079
0.0453384159800344	0.7505927180741588	0.2820221256980011
0.0465977846601656	0.2504878968404162	0.2824563669119666
0.0329112053152833	0.7494017309515414	0.4855661475527873
0.0369722868703983	0.2516031093762565	0.4908909765972885
0.3131811402823789	0.2500796643613831	0.9962641530578440
0.5437170434904411	-0.0002219327886490	0.9874450817281392
0.5437182903540607	0.5001137928076637	0.9874128345249966
0.7117486446631082	0.2499500746765469	0.9877374767541344
0.3136735608803988	0.7500393349136912	0.9960903947121685
0.7118080376507596	0.7499608819426541	0.9878713078428647
0.4498989100296515	0.4973009159754427	0.4933746755815775

TiO2 anatase slab 100 6L Na -02

1.0000000000000000		
9.8434554295713088	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
24	48	1

Direct

1.0013003137435741	1.0001886818140480	0.0854672677937793
1.0008512743066709	0.4998313884554659	0.0857968406315578
0.0034224082454482	1.0013137793222708	0.2794052064439467
0.0034715371068701	0.4994913734329389	0.2799596450511826
-0.0081293173785062	1.0021068962893793	0.4731614831936687
0.9977014864458751	0.5000359010863957	0.4715156371015360
0.4988316733315038	0.2499475637199415	0.0042685005864559
0.4997134431111658	0.7498244918587632	0.0045886127729911
0.5000887879133505	0.2497592702142425	0.1947242978211296
0.5016107069838044	0.7498010421923068	0.1949330154943059
0.5052934550612402	0.2383371067263974	0.3873625144847530
0.5079351498469292	0.7586311485793091	0.3867511325648080
0.2538490797164483	0.2501722651455671	0.0875564326033254
0.2533230461758980	0.7498831915726581	0.0866582699691842
0.2530171940504191	0.2500890165012398	0.2853467981878315
0.2495116338191318	0.7508947197287090	0.2820105921874314
0.2477253254792210	0.2329531380401713	0.4814205544940546
0.2416734384086260	0.7618678945614629	0.4744897072776785
0.7535120816973436	0.0001211147594643	0.0041629636374784
0.7535057291159439	0.4997069489395948	0.0044036402287244
0.7510840674824264	1.0003302849461786	0.1939545329147122
0.7513038125030299	0.4993368186563739	0.1946902144422618
0.7599877773906414	1.0010596195257262	0.3872159986518764
0.7556752382954440	0.4984001349416018	0.3881537651707263
0.2072174926784382	0.9999143969149741	0.0892221872892826
0.2070144090150731	0.5001726001041600	0.0892229981945377
0.2080999431378756	1.0003106592026221	0.2829263160696563
0.2088268789519016	0.5008684535409819	0.2829289336101014
0.1996711577429771	0.9889855449980071	0.5028263692586061
0.1999532103967195	0.5134738613572738	0.4973080047549894
0.7084792823365185	0.2497765758031212	0.1935068005229873
0.7078822052569858	0.7498601826657194	0.1937743646017691
0.7114134544803171	0.2478017982567459	0.3852314838719020

0.7104860055820241	0.7515743994430977	0.3862416127014091
0.4698602922623916	0.2501320347734920	0.0951538766162766
0.4691877455978940	0.7493579651174922	0.0955916714944457
0.4564818458289371	0.2458825480851557	0.2882852582716123
0.4527904132167379	0.7524517370864552	0.2896588716979908
0.4474327764489003	0.2434634498659448	0.4764689001291960
0.4377245616754012	0.7531896587762783	0.4759046428353125
0.5461832815714996	0.9993231129190456	0.1932568459864520
0.5456716379255456	0.5002078141777498	0.1944107120494553
0.5517228085601147	0.9984273446934132	0.3827239002551224
0.5530579711246052	0.5004464267358715	0.3818279586366792
0.3004487808055036	0.2507777990520357	0.1877258660678895
0.2997391560740820	0.7500631093072330	0.1876381817648775
0.2880523413637646	0.2551212295113349	0.3814004174882897
0.2754494311686845	0.7492006205097212	0.3820117069301360
0.7851221936146516	0.9996101776278783	0.0950206626068113
0.7846972225828167	0.5001246630696591	0.0952140615029385
0.8015462339447719	0.9991862409854460	0.2878145263320936
0.8014279051294124	0.5004852956357113	0.2881882598222231
0.8071174483751289	1.0019706743787196	0.4797635518286186
0.8099682689596840	0.4987669907645436	0.4789455487615505
0.9551991982062353	0.0008180316712802	0.1863847896699209
0.9548079898789512	0.4995220682828442	0.1865774668601693
0.9686471601957968	1.0041462017853013	0.3811549350841408
0.9704047514247757	0.4969277945564315	0.3803381014828505
0.9408253734742856	1.0002501739680258	0.9955324304033820
0.0470072371631470	0.7500427879663287	0.0885443804255886
0.0472245567616349	0.2500103522846673	0.0887155319945409
0.9407342944715482	0.4997214007463505	0.9957718998535138
0.0448927048841495	0.7506387306721430	0.2815725173416113
0.0464647783269489	0.2502300943603183	0.2821012950430107
0.0307556211106818	0.7527523092617907	0.4839835865650280
0.0387545898468619	0.2492575260417743	0.4899768693401359
0.3121292266074367	0.2500406712931449	0.9965822303381862
0.5426203813569792	-0.0002753703201037	0.9875792437545829
0.5426208868114515	0.5000956993307458	0.9875185828935114
0.7106667228238744	0.2498682969940877	0.9875288015967478
0.3126500572797625	0.7500121446393244	0.9963483146564457
0.7107118556875683	0.7499692257200192	0.9876912058632872
0.3715591687162389	0.4965675917109880	0.4355346026697458

TiO2 anatase slab 100 6L Na -03

1.0000000000000000		
9.8434554295713088	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
24	48	1

Direct

0.9998356465297922	0.0000486250605329	0.0853522173742762
-0.0002499026320662	0.4996739663043650	0.0855449526942683
-0.0000938127654494	0.0004295031777012	0.2794606877444771
1.0014012044105864	0.4986135523625987	0.2803163079160244
0.9954728100286246	0.0022318059871709	0.4728310782379468
0.9979146235954670	0.5008023641772276	0.4714529703983427
0.4979810711508570	0.2499948597862902	0.0042815529062263
0.4989084177305217	0.7499869725841162	0.0046240486970017
0.4994620807107780	0.2505878737131136	0.1953093480626339
0.5008992721459674	0.7493152883760724	0.1955426210327434
0.5031959227046788	0.2407668041181868	0.3909710455512558
0.5063501375434341	0.7573007006086617	0.3900944009961374
0.2528077913743395	0.2499571714278203	0.0869014480407797
0.2522400494104333	0.7497183968902710	0.0859595834974956
0.2523616301548415	0.2430493307952432	0.2837544434525066
0.2486169914228112	0.7539695754836175	0.2804922849650518
0.2530111380586781	0.2404085022858869	0.4824609309021579
0.2473089887785434	0.7626389062811162	0.4752938226617454
0.7524013533210987	0.0001937554035160	0.0039074458714468
0.7524933531897053	0.4997738668019169	0.0042395346887884
0.7493243417356098	0.0003994838219641	0.1938833834608749
0.7506633212993197	0.4994025494587936	0.1945984757831060
0.7583053664168087	0.0014017300752652	0.3883702643330429
0.7522482830687973	0.4985180989856675	0.3891903397004878
0.2060688820837912	0.9997046475412293	0.0890981826742069
0.2058278553442883	0.4999439512588164	0.0886138866580986
0.2052465579558964	0.9989225770612309	0.2782281719415002
0.2100349470362655	0.4996428265481159	0.2880826820604808
0.2009823605371878	0.9913776580303717	0.5024564400919289
0.2061747392470311	0.5124338605521837	0.4893801294812423
0.7072625561341258	0.2498918823245889	0.1932853414689381
0.7066503565401790	0.7498732985867850	0.1936433182137206
0.7098678598881001	0.2492102014727064	0.3855763336349056
0.7090021531077769	0.7505581822543621	0.3866656083936996
0.4682567815785978	0.2499398584388170	0.0950474919693074
0.4676497574335325	0.7500571563643598	0.0955148376878834
0.4551616722089702	0.2507720132016991	0.2884498730199205
0.4509366399178811	0.7491290011827406	0.2899287960248227
0.4484373841623093	0.2546030448304563	0.4787391162658385
0.4391234302803494	0.7484134540827756	0.4778346545760263
0.5442200474768466	0.9993945652088126	0.1938005025721265

0.5452293322780944	0.5004082076629307	0.1938419084011686
0.5515030200603591	0.9989915262218541	0.3855361025418199
0.5445965437821194	0.5007407146893350	0.3848939631857874
0.2990557500364399	0.2521178450310864	0.1874892333486376
0.2982659317376012	0.7467306575148116	0.1872617080728873
0.2882508526500540	0.2257666704112201	0.3811530583040676
0.2760372548994140	0.7729370031573773	0.3820279149087169
0.7833930374669712	0.9996528405496051	0.0947313250439440
0.7840580019493840	0.5002513002982242	0.0950746013891715
0.7993556447626088	0.9991809847621029	0.2878568132259707
0.8002619040875406	0.5002120016793929	0.2882561777204072
0.8092721921820670	0.0024816822075895	0.4797975517211805
0.8094052350779392	0.4989681841655347	0.4789725373549579
0.9527679680262150	0.0003641532438562	0.1861718714448498
0.9543204803660488	0.4991233057905290	0.1866911073679219
0.9686875697632494	0.0031646266607949	0.3807629180017010
0.9689548410259818	0.4975629029683611	0.3803875757464220
0.9397504207982784	0.0002109092735992	0.9953841585466742
0.0457865038796585	0.7499192124574054	0.0882804937014611
0.0459984988346000	0.2497748081941197	0.0884882549205059
0.9396751883801292	0.4996152445146709	0.9955194452503399
0.0440324983431693	0.7492983360201366	0.2811720985179096
0.0456590760906881	0.2495991684928390	0.2817515655441098
0.0326776588810016	0.7519412640921440	0.4858238665187702
0.0402416579550106	0.2511272415096804	0.4901754101287785
0.3111262260216425	0.2497801050524702	0.9961862602800842
0.5416566498952766	0.9997967390277933	0.9873994435273993
0.5416133039763525	0.5001660877299713	0.9875547450020277
0.7095756715603923	0.2500380206187217	0.9873245518555995
0.3117194353197010	0.7499862742070473	0.9959179597227102
0.7096409153797600	0.7499189692345153	0.9874782160895400
0.3125045775538510	0.4986209662382378	0.3912758500280120

TiO2 anatase slab 100 6L Na in

1.0000000000000000		
9.8434554295713088	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Ti	O	Na
24	48	1

Direct

0.9997559695232781	0.0001157154068494	0.0855701482793947
0.0003037787038167	0.4998242872992620	0.0844440917620091
0.0001849245908900	0.0005568148067283	0.2816961469433039
0.9981365861817793	0.4989696589791421	0.2782498479038580
0.9961820802297225	0.0017735787276010	0.4729443784519276
0.9898435942772110	0.5021677333151899	0.4761161351353138
0.4987011517456779	0.2500002859931101	0.0026795119159218
0.4997136380730893	0.7500654026821252	0.0031272426550260
0.5017376075834079	0.2494846714784771	0.1935977359574395
0.5025617983770516	0.7509104696912985	0.1939798568214997
0.4970302970395224	0.2476043849592600	0.3921765013479543
0.4989158861108365	0.7521670566708849	0.3908558054103679
0.2530277206565614	0.2496926532414037	0.0848008625608330
0.2525830790455785	0.7501573437624316	0.0840279774175485
0.2563260893176320	0.2421836198953855	0.2801587543427786
0.2522360648088693	0.7530692394627536	0.2776590563681580
0.2562835046895628	0.2439854998354534	0.4834306567810955
0.2527439001023026	0.7579077787177368	0.4769657505451477
0.7531727757898494	0.0002476603682098	0.0040526279658479
0.7526682041852908	0.4997512251440668	0.0036150697325255
0.7521293326444223	0.0003651369103679	0.1947438399906360
0.7492775229849116	0.4996473262912815	0.1938127441643118
0.7520293273278966	0.0011024534675030	0.3898589554214240
0.7493431660387699	0.4988865485497840	0.3892385104891432
0.2060249748536123	0.9998057194058063	0.0869714594116786
0.206258264839641	0.5000266275813559	0.0871799364517400
0.2069763726786462	0.9983948838215753	0.2793503179965029
0.2091202766590854	0.4991085916302680	0.2781107825663440
0.2030228614965850	0.9916851740150392	0.4984591164285561
0.2062548638478532	0.5130531366848814	0.4931899428043849
0.7085820606254813	0.2501207954176934	0.1928714514878607
0.7079658842219985	0.7499423235506839	0.1934628979043040
0.7076695684569216	0.2504461563499305	0.3854979521528676
0.7062035420212212	0.7497731058033921	0.3865335747524838
0.4687371519401324	0.2508877288971618	0.0932704311833135
0.4682032159926166	0.7493871512670367	0.0938564581691708
0.4559762859359608	0.2501917248638108	0.2860456075061961
0.4518827696146204	0.7501075157968202	0.2875395534444465
0.4505534353687395	0.2527212526380254	0.4809284390789728
0.4416983560126297	0.7539913646683374	0.4807507099900974
0.5461944727483754	0.9995299766983621	0.1919776466177225
0.5457495506293455	0.5006070877083175	0.1919054333293531
0.5469537395803314	0.9990181028938423	0.3862784510554604
0.5434889209282616	0.5013720116731974	0.3858939046046430
0.3000061658282434	0.2465423538049691	0.1850925036501891
0.2990807778895430	0.7521413291572756	0.1849897862572050
0.2912989886913451	0.2371070755504334	0.3808276466728771
0.2830347264297970	0.7565448558875261	0.3822642456515908
0.7848207581498841	0.9997515269227648	0.0948543952268395

0.7843460388399777	0.5002394797597702	0.0944297945079740
0.7991283681599270	0.9998036983182885	0.2884000740637020
0.7998228250556423	0.5000343446826037	0.2881337677594829
0.8088373440803238	0.0033176483918353	0.4802200877628806
0.8035910099421955	0.4983925930521877	0.4804266353837718
0.9541549776908695	0.0004049414571909	0.1870801295164455
0.9535950692102233	0.4994004059338621	0.1858757327842824
0.9682844023578170	0.0014595563880420	0.3812928624802581
0.9712015105211833	0.4991477500399739	0.3830629337685210
0.9401812631026161	0.0002754547467418	0.9953739483702080
0.0459558261725235	0.7498577398807456	0.0878666805554786
0.0461257662830263	0.2500479868918077	0.0881519708206113
0.9401231008541231	0.4997070038564289	0.9947340050136049
0.0455312378682393	0.7485458074178268	0.2828785474942208
0.0470143169282551	0.2502653114278885	0.2837192459124083
0.0320729017860799	0.7514684001077967	0.4885024407342442
0.0405201726534798	0.2523026345195660	0.4910983792288945
0.3115589305209099	0.2499916521339500	0.9943510169025487
0.5423999590689590	0.9998403172995154	0.9863535484889709
0.5426357622124272	0.5001872995198582	0.9858982905839895
0.7103155472764513	0.2499577150565884	0.9869374280020082
0.3123146963575465	0.7498794293941984	0.9942043111348511
0.7104521226474745	0.7500504486416588	0.9872603108694520
0.2058393760577673	0.4920431655227233	0.3840837047539978

- (001)

TiO2 anatase slab 001 6L Na out

1.0000000000000000		
7.6783716825835899	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.0000000000000000

Ti	O	Na
24	48	1

Direct

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0.0005397818381283	0.4959234486000739	0.1228992896524588
0.9975449100081661	0.9939174331825456	0.5456592438619481
0.9981519869396678	0.5021637083990242	0.5467576955664200
0.5005167145217300	0.9958421678841205	0.1228675535687387
0.5005133511398299	0.4959055710613498	0.1228927672626838
0.5042612743906432	0.0042172249685422	0.5488378351411427
0.5048648836958165	0.4977462313066283	0.5525512650351914
0.2504684583066705	0.2529723731540372	0.3372719464332974
0.2505897822891328	0.7501641840331672	0.3374911509509744
0.7506268052238880	0.2530101217571357	0.3364954453997768
0.7504758890699605	0.7505661801495833	0.3365270849621638
0.0008693206071300	0.2478169155850551	0.2300025454807297
0.0009491443563476	0.7478800407330866	0.2301109440565483
0.5001648844577176	0.2478207207600036	0.2300192708054709
0.5000648172719622	0.7478973396741111	0.2300641579667726
0.2505244502223789	0.0012627175873519	0.0186596606472875
0.2505281121779248	0.5012897060838952	0.0186731450092594
0.2523045123633807	0.0037878313055231	0.4437194833618392
0.2549048662335878	0.5033355928632801	0.4457957010100415
0.7505330711517146	0.0012994473321868	0.0186698391455451
0.7505292501472383	0.5012911877061015	0.0186800411337202
0.7485142022061737	0.0034124259413915	0.4423766581230097
0.7477247652435608	0.5036427722678880	0.4442496353449883
0.0007555471358529	0.9978567569404433	0.2107683551690087
0.0007890913698958	0.4978947571920500	0.2107345666549207
0.5002622843933295	0.9978715664091382	0.2107368911781649
0.5002350081635640	0.4978974988784017	0.2107183983826530
0.2507545884455169	0.2511442803004797	0.4249707996733747
0.2526842273854157	0.7510230451106423	0.4252207034245643
0.7509523891908998	0.2513081254175376	0.4240650538331110
0.7489105182210523	0.7514130292050680	0.4240653377495107
0.0007930176991948	0.2514192150149697	0.3177409053234399
0.0008084449972543	0.7514262577367603	0.3178933303471894
0.5002893377329656	0.2514074338911314	0.3177498425981256
0.5002466902428537	0.7514853945102402	0.3177548796199048
0.2505218601768746	0.0067943036588574	0.1041323568959811
0.2505226130293323	0.5069186108498940	0.1041434061545132
0.2479061094122414	0.0265346721611763	0.5325294124641786
0.2457717123820444	0.5166983666629648	0.5328662168184621
0.7505360586653751	0.0068777843836756	0.1041616540875623
0.7505353211962102	0.5068362553837176	0.1041745281899580
0.7525356865752357	0.0254817862219383	0.5293761428820218
0.7563271562953915	0.5238685400700334	0.5301511168311350
0.2507460025255455	0.0015249723269903	0.3563648579708598
0.2510060835811032	0.5014353036392123	0.3562996508649690
0.7500258020809483	0.0017317599275657	0.3550499005239089
0.7503585095540259	0.5016522255825464	0.3551246616557435
0.0007320039580705	0.2481984471210765	0.1419750115943401
0.0006707702765354	0.7482560202311035	0.1420308217782349
0.5003325893400259	0.2482090552385543	0.1419665154315197
0.5003876609326880	0.7482602938285439	0.1419864920746647
0.2505256624863677	0.2482693591748202	0.2488475177063165

0.2504946143027098	0.7477630239152546	0.2489698594590806
0.7505309705639078	0.2484172933135653	0.2484891780398826
0.7505391740251071	0.7478408391215368	0.2485462364398714
0.0005257028309913	0.9776214762067070	0.0356318962988169
0.0005328229548596	0.4776264649404496	0.0356348866751901
0.0008529685167389	0.9891923272707075	0.4612029554367965
0.0012447380940728	0.4929138086915970	0.4617638295808675
0.5005337090353024	0.9776291255059917	0.0356198183514138
0.5005264115707035	0.4776215529144281	0.0356281056096392
0.5000891130573422	0.9949133214485286	0.4623263773971118
0.5010027573989930	0.4937092377484760	0.4627483412558533
0.0003019818075103	0.2747045777973156	0.5774540550599596
0.4986160039868963	0.2547762584943527	0.5813113541043649
0.9993320243281261	0.7709439294997225	0.5722170935982263
0.5029774522811508	0.7848753031987172	0.5764940240310068
0.2505386938859715	0.2258190823315331	0.9937489610288139
0.2505351719190401	0.7258325047414971	0.9937962832568630
0.7505258890418816	0.2258584645081498	0.9938000190757919
0.7505293314710286	0.7258386212045664	0.9938483206144255
0.2458512871073069	0.2496779233416930	0.6259293162315913

TiO2 anatase slab 001 6L Na -01

1.0000000000000000		
7.6783716825835899	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.0000000000000000

Ti	O	Na
24	48	1

Direct

-0.0004791505204214	0.9967763086954206	0.1232102682792244
-0.0004781183757664	0.4963578239542115	0.1232418172625752
1.0003364046819858	0.9860156939998549	0.5465627809319342
0.9951120927662446	0.5053563616705817	0.5463079899263485
0.4995199210446983	0.9967862568444716	0.1231947184560044
0.4995205071686473	0.4963558235293200	0.1232365294543852
0.5145383512457495	0.0060243645374735	0.5498254718803586
0.5088682532252509	0.5412171455801166	0.5524598318127719
0.2501755077797661	0.2516651747356657	0.3375514643163779
0.2504034811122938	0.7500548965480984	0.3366254823219456
0.7502310744115397	0.2516267419672116	0.3369390521864605
0.7503415615929035	0.7498749653805679	0.3366373065520962
0.0002760520398607	0.2483736372474012	0.2304526717895078
0.0000135746286805	0.7484315311440778	0.2300358004899446
0.4998392180748258	0.2483530110114836	0.2304521704594634
0.5003616667314412	0.7484650776170584	0.2300124776391646
0.2494930710445123	0.0028988822629337	0.0190651896354564
0.2494977886519063	0.5029158554541980	0.0191054131681944
0.2561768605301591	0.0003538248292415	0.4435266900250359
0.2558856687732477	0.5033838366331153	0.4446170460762977
0.7495015647296649	0.0029891268500773	0.0190682150021429
0.7495028727643164	0.5028093346167671	0.0190951606832232
0.7521387535834008	0.0006160847948130	0.4423949168615066
0.7482317694584537	0.5013939423172757	0.4437646901445750
0.0001874079229289	0.9985841077648475	0.2112174675542817
0.0000913047820154	0.4983049348191316	0.2112399479293575
0.4999046004867160	0.9985913525371891	0.2111813542440388
0.4999955762859550	0.4983065623586742	0.2112337406662780
0.2533870363330711	0.2505554432570098	0.4259273674343140
0.2546038012710299	0.7512045441517622	0.4244312958936152
0.7518736846999386	0.2503158132750709	0.4248337071194473
0.7512263598417804	0.7508856920634329	0.4237803148256799
0.0004672775905127	0.2505312787186755	0.3184098629556599
0.0005146598854622	0.7507072805610319	0.3179307177088009
0.5000372694989974	0.2501176098867017	0.3183342749318911
0.5002423989906776	0.7511931759131699	0.3177891326637433
0.2495162997694050	0.0073517711174551	0.1046872804549292
0.2495197084486084	0.5074525613607040	0.1047301885720664
0.2529610616287247	0.0089420102067349	0.5325108591535703
0.2481463512897434	0.5158025278130365	0.5321171802678301
0.7495309639692834	0.0078449715169334	0.1046906714409918
0.7495343076242591	0.5069427671323447	0.1047302980169442
0.7583704695632825	0.0020268696595412	0.5290805141809131
0.7564897505278222	0.5229140297176892	0.5292346278705151
0.2508183259073038	0.0010210718537404	0.3561959167081409
0.2509203251398202	0.5008193246618092	0.3559657611682267
0.7507104229494612	0.0008878567393984	0.3552301669318422
0.7493839844575033	0.5005917661484677	0.3552077984947766
-0.0001524507140713	0.2488375463114869	0.1425493283709410
-0.0006779995260876	0.7488757239632549	0.1423263216589326
0.4991975083736329	0.2488461240996506	0.1425255949421773
0.4998470134384885	0.7488754756782521	0.1422897922877407
0.2500922253400949	0.2487170874829769	0.2494893354058763
0.2501978509819475	0.7485025627890128	0.2487719325209100
0.7501516561163478	0.2486584751004416	0.2491269664709338
0.7502720392996668	0.7485362733807897	0.2486151894338692
-0.0005132183453256	0.9795006990496102	0.0361624836707458
-0.0004779125170676	0.4791654287733247	0.0361952768014699
0.0051309325576784	0.9895212493567164	0.4617962156423986
0.0024960925318548	0.4975184562448098	0.4612216695958347
0.4995184204661337	0.9795027422646733	0.0361465196930567

0.4994885422474478	0.4791903551161570	0.0361862263310092
0.5041123735511664	0.9977801487236989	0.4627607880141653
0.5015579497211643	0.5035373607915621	0.4628577789879735
-0.0096691669685197	0.2704554126141401	0.5711118038026223
0.5261605187781804	0.2318135813916372	0.5769317960247459
1.0012124032864018	0.7625078195621260	0.5738583837625287
0.5077744916831173	0.7748900975828389	0.5813191907640934
0.2494702543716398	0.2277042815438174	0.9947121259495755
0.2494587433196592	0.7276875332333848	0.9947462102034512
0.7494883804455491	0.2277489532091814	0.9946709482396695
0.7495019672113573	0.7276247305539278	0.9947918613558249
0.2603721222518231	0.2633688056683745	0.5760822708958855

TiO2 anatase slab 001 6L Na -02

1.0000000000000000		
7.6783716825835899	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.0000000000000000

Ti O Na

24 48 1

Direct

-0.0000065631115847	0.9970115825090000	0.1227129166719683
-0.0000157459770832	0.4959070798600143	0.1227567148390781
1.0028083012626501	0.9898920365753877	0.5499574609304263
1.0039697964547707	0.5070460788063920	0.5483141055418750
0.5000299679428445	0.9969851415864337	0.1226915464953445
0.5000449532298558	0.4959344367535400	0.1227347314635576
0.5117574178243944	-0.0068441796202378	0.5539705764082450
0.5136144513293610	0.5089037962313249	0.5566057174671040
0.2504422550531381	0.2513282851409177	0.3373659933901996
0.2508652412943080	0.7503331125917574	0.3339314726662227
0.7502875043228517	0.2512994924692457	0.3378918693025474
0.7508848944552965	0.7500272771977933	0.3375056100961181
-0.0001562971763750	0.2482283287673008	0.2303729731542214
-0.0013937565514468	0.7483569489088495	0.2292907101325241
0.5007164715824511	0.2482216204820857	0.2303172620938214
0.5026699134821330	0.7483594969353093	0.2292811342644725
0.2499895794481972	0.0029088865280621	0.0185581447920915
0.2499895267840110	0.5029213335028446	0.0186217809100982
0.2531802423347258	-0.0057586364769216	0.4426411067989666
0.2550238156097153	0.5123672985684955	0.4428811449948771
0.7500019421334609	0.0029846773103374	0.0185385941179460
0.7500134702777091	0.5027344265471348	0.0185754291821268
0.7500321767860236	0.0019553115536788	0.4450590147224192
0.7480200284166787	0.5025344921549560	0.4457154645987389
0.0001666591723068	0.9985548128036067	0.2107725702281513
-0.0001549818822266	0.4981275608947560	0.2108708504967135
0.5006297721098524	0.9985508470033091	0.2107367924496215
0.5009573960018124	0.4981291886551635	0.2108387551538765
0.2536709895289995	0.2492503539896790	0.4262275959789797
0.2539086081843203	0.7519724900045240	0.4221921922291053
0.7494824647661937	0.2497384863304128	0.4257346577830707
0.7512725450975118	0.7511284714883013	0.4247177768560498
0.0004750819724450	0.2498191677319025	0.3184063340863272
0.0004411695132180	0.7512289746093539	0.3173319270611280
0.5003901790003066	0.2496993668479421	0.3182211638259913
0.5011846058147645	0.7513534542127835	0.3172228902634628
0.2500053781882931	0.0071882207468404	0.1042515428396609
0.2500115180033187	0.5073682629519805	0.1043197615932596
0.2545668480736307	-0.0077175816376020	0.5330707464239274
0.2498905327505510	0.5378419272256021	0.5304469400383556
0.7500241894025693	0.0078834617817256	0.1041960578505178
0.7500342768558936	0.5065887166105577	0.1042450555965173
0.7560266549969663	0.0131928332782883	0.5323980234310141
0.7619093172225132	0.5276385536420729	0.5304785045279767
0.2509300421191474	0.0004399825288874	0.3554113030414177
0.2515474139654028	0.5013371809274005	0.3546852610927150
0.7503730706263051	0.0006588637178541	0.3568643266528391
0.7502734211282729	0.5007231706777496	0.3560300558971229
0.0001529664624523	0.2487374776859796	0.1422597442467638
-0.0007711291097849	0.7487610309885340	0.1418372917027682
0.4997763251723473	0.2487391595601009	0.1421997057246926
0.5010064664718089	0.7487586483240264	0.1418046234709268
0.2503029014339993	0.2485389460197252	0.2493827433721461
0.2506409481942734	0.7485637933082920	0.2476107272114444
0.7503800967216243	0.2481072317984204	0.2493734570769488
0.7506983030365861	0.7488038435703278	0.2485086059462771
-0.0000067474833563	0.9796125093765253	0.0357189326401049
0.0000428421524520	0.4790351907075951	0.0357721150615822
0.0043311167786139	0.9912406291072989	0.4640750623944109
0.0051927050256939	0.4951206611453213	0.4616929869554151
0.5000076882836171	0.9795576399577318	0.0357025147667244
0.49999713737079315	0.4791197404193591	0.0357531675284718
0.5020531735920505	0.9920846014900092	0.4657668157455653
0.5013276742906618	0.4954922679492799	0.4641678563041835
0.0147778568343824	0.2710591561173411	0.5699999144093230
0.5100944291932679	0.2585457404900584	0.5778695509412977
0.9989457362757670	0.7672739088886282	0.5763478592033600
0.5126366394180344	0.7751654614273398	0.5826551506379720
0.2499965467776464	0.2277426912280128	0.9943660944897328

0.2499458090372349	0.7277211291529990	0.9943967886472493
0.7499822312342955	0.2277697676103976	0.9942701696223836
0.7500375021705228	0.7276156006720956	0.9944133130462665
0.2808907214076385	0.2609666312100952	0.5258160075650135

TiO2 anatase slab 001 6L Na -O3

1.0000000000000000		
7.6783716825835899	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6783716825835899	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.0000000000000000

Ti	O	Na
24	48	1

Direct

0.0004823097292284	0.9966656993125816	0.1220160869998065
0.0004264743995429	0.4958457689869898	0.1220714760913788
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TiO2 anatase slab 001 6L Na in

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Direct

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