

## Supporting information

# **Tetragonal-Zircon BiVO<sub>4</sub>: A better polymorph for the formation of coherent type-II heterostructures for water splitting application**

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**Table S1.** Valence and Conduction band edge positions of all lower index surfaces of different polymorphs of ZnO, TiO<sub>2</sub>, BiVO<sub>4</sub>, CdSe and ZnS.

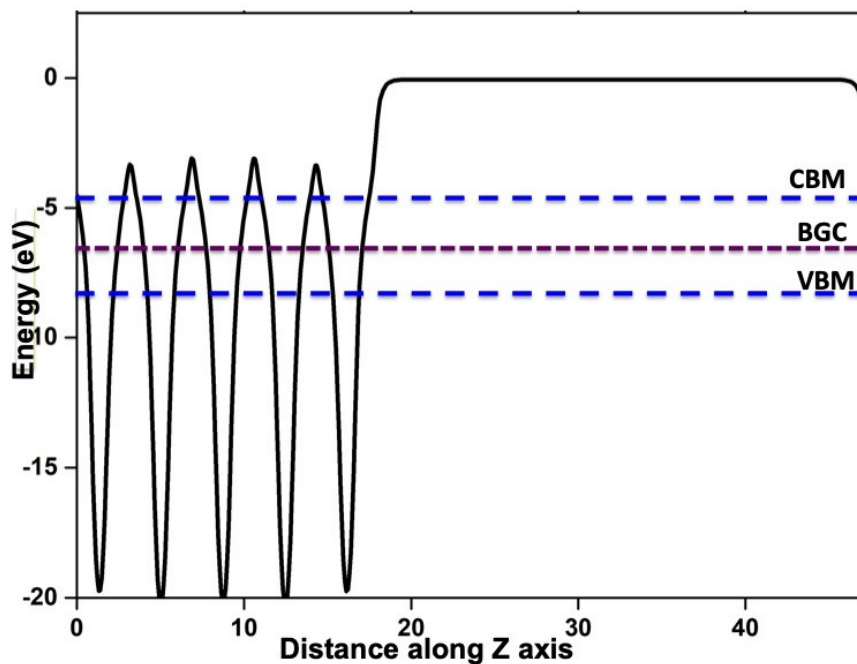
<b>Materials</b>	<b>Crystal structure</b>	<b>Surfaces</b>	<b>VBM</b>	<b>CBM</b>
<b>ZnO</b>	Wurtzite	(11 $\bar{1}$ 0)	-7.14	-3.78
	-	(11 $\bar{2}$ 0)	-7.3	-3.92
	Rocksalt	(100)	-6.79	-2.57
<b>TiO<sub>2</sub></b>	Zinblende	(110)	-6.98	-3.60
	Rutile	(110)	-8.2	-4.90
	Anatase	(101)	-8.59	-5.42
	Brookite	(201)	-5.93	-2.60
<b>BiVO<sub>4</sub></b>	-	(010)	-8.55	-5.19
	Monoclinic-scheelite	(010)	-7.56	-5.04
		(011)	-6.35	-3.82
	Tetragonal-scheelite	(001)	-7.84	-5.34
	Tetragonal-zircon	(010)	-7.61	-4.50
<b>CdSe</b>	Wurtzite	(10 $\bar{1}$ 0)	-6.17	-4.37
		(11 $\bar{2}$ 0)	-6.11	-4.31
	Zinblende	(110)	-6.0	-4.30
<b>ZnS</b>	Wurtzite	(10 $\bar{1}$ 0)	-6.72	-3.02
		(11 $\bar{2}$ 0)	-6.71	-3.01
	Zinblende	(110)	-6.83	-3.03

### Band gap centre calculation (BGC):

BGC for different surfaces has been calculated by using a 2D periodic slab model with the slab thickness and vacuum thickness of 20 Å. BGC is the average of conduction band maxima (CBM) and valence band minima (VBM) eigenvalues. Further, The position of the BGC relative to the vacuum has been calculated by the following equation:

$$\text{BGC relative to vacuum} = E_{\text{vac}} - E_{\text{BGC}}$$

Where,  $E_{\text{vac}}$  = Electrostatic potential energy in vacuum. The electrostatic potential of the surface is shown in Figure S1.



**Figure S1.** Average electrostatic potential of (100) surface of T-Z polymorph of BiVO<sub>4</sub> along the direction perpendicular to surface. The vacuum energy level is set to zero. The conduction band minimum and valence band maximum (CBM and VBM) along with the bandgap centre energy are shown with reference to the vacuum level.

**CONTCAR files of all low index surfaces of Tetragonal-zircon polymorph of BiVO<sub>4</sub>.**

**i) (001) surface**

CONTCAR\0\0\1)

1.0000000000000000

7.4005999564999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.4005999564999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 43.8110008239999971

O V Bi

48 12 12

Direct

0.0000000000000000 0.0615331102445088 0.0234945676658191

0.0000000000000000 0.0696064366801058 0.1710447523770812

0.0000000000000000 0.0675479978940993 0.3172391470655718

0.0000000000000000 0.9324520161058948 0.1121308469344264

0.0000000000000000 0.9303935863198927 0.2583252486229210

0.0000000000000000 0.9384668857554908 0.4058754353341834

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0.5000000000000000 0.9310756327072264 0.2448232855934742

0.5000000000000000 0.9253701827948433 0.3996931114159759

0.5000000000000000 0.0746298322051543 0.0296768825840223

0.5000000000000000 0.0689244122927738 0.1845467154065282

0.5000000000000000 0.0619715951789105 0.3318210297508286

0.1787772550057119 0.7500000000000000 0.0618304356150443

0.1816232442778035 0.7500000000000000 0.2079678702210679

0.1810839524267402 0.7500000000000000 0.3567045164928820

0.8189160475732595 0.2500000000000000 0.0726654995071179  
0.8183767407221989 0.2500000000000000 0.2214021307789345  
0.8212227299942833 0.2500000000000000 0.3675395723849552  
0.3200111214661119 0.2500000000000000 0.1340030454390036  
0.3207636522013214 0.2500000000000000 0.2823438817164928  
0.2896929321648500 0.2500000000000000 0.4292886630371010  
0.7103070678351499 0.7500000000000000 0.0000813199628998  
0.6792363477986785 0.7500000000000000 0.1470261192835022  
0.6799889385338859 0.7500000000000000 0.2953669855610012  
0.2896929321648500 0.7500000000000000 0.0000813199628998  
0.3207636522013214 0.7500000000000000 0.1470261192835022  
0.3200111214661119 0.7500000000000000 0.2953669855610012  
0.6799889385338859 0.2500000000000000 0.1340030454390036  
0.6792363477986785 0.2500000000000000 0.2823438817164928  
0.7103070678351499 0.2500000000000000 0.4292886630371010  
0.1810839524267402 0.2500000000000000 0.0726654995071179  
0.1816232442778035 0.2500000000000000 0.2214021307789345  
0.1787772550057119 0.2500000000000000 0.3675395723849552  
0.8212227299942833 0.7500000000000000 0.0618304356150443  
0.8183767407221989 0.7500000000000000 0.2079678702210679  
0.8189160475732595 0.7500000000000000 0.3567045164928820  
0.5000000000000000 0.5619715541789037 0.0975489932491756  
0.5000000000000000 0.5689243672927736 0.2448232855934742  
0.5000000000000000 0.5746298172051567 0.3996931114159759  
0.5000000000000000 0.4253701527948410 0.0296768825840223  
0.5000000000000000 0.4310755737072250 0.1845467154065282  
0.5000000000000000 0.4380283868210951 0.3318210297508286  
0.0000000000000000 0.4384668857554909 0.0234945676658191  
0.0000000000000000 0.4303935563198973 0.1710447523770812  
0.0000000000000000 0.4324519871058958 0.3172391470655718

0.0000000000000000 0.5675479838941052 0.1121308469344264  
0.0000000000000000 0.5696064136801073 0.2583252486229210  
0.0000000000000000 0.5615331142445092 0.4058754353341834  
0.0000000000000000 0.2500000000000000 0.0469213227346938  
0.0000000000000000 0.2500000000000000 0.1961915828038938  
0.0000000000000000 0.2500000000000000 0.3421612204984542  
0.0000000000000000 0.7500000000000000 0.0872087655015505  
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0.5000000000000000 0.7500000000000000 0.2692558973583898  
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0.5000000000000000 0.2500000000000000 0.1601140886416077  
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0.0000000000000000 0.7500000000000000 0.1600100674959987  
0.0000000000000000 0.7500000000000000 0.3081637199436017  
0.0000000000000000 0.2500000000000000 0.1212062810563934  
0.0000000000000000 0.2500000000000000 0.2693599335040038  
0.0000000000000000 0.2500000000000000 0.4118017388113424  
0.5000000000000000 0.2500000000000000 0.0898133807297054  
0.5000000000000000 0.2500000000000000 0.2358313572553322  
0.5000000000000000 0.2500000000000000 0.3941899815517879  
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0.5000000000000000 0.7500000000000000 0.1935386437446631  
0.5000000000000000 0.7500000000000000 0.3395566202702900

**ii) (100) surface**

CONTCAR\1\0\0

1.0000000000000000

7.4005999564999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 6.4674000740000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 47.4785995482999965

O V Bi

40 10 10

Direct

0.0672852520872153 0.2047139778350968 0.0277153098252947

0.0689018008293369 0.2042194262741419 0.1840851566043694

0.0673067227567901 0.2047338765532196 0.3403749089353625

0.9327147709127833 0.7952860371649010 0.0277153098252947

0.9310982221706616 0.7957805887258557 0.1840851566043694

0.9326933002432081 0.7952661384467781 0.3403749089353625

0.9304782906348615 0.7050230913444223 0.1057075625112381

0.9304944205204998 0.7049289895750436 0.2624270157692890

0.0695217323651365 0.2949769086555775 0.1057075625112381

0.0695056024794915 0.2950710104249566 0.2624270157692890

0.7500000000000000 0.4459852434268805 0.0565740961748561

0.7500000000000000 0.4542408305845029 0.2122473001360686

0.7500000000000000 0.4554571441035303 0.3673146986970668

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0.2500000000000000 0.5457045185662213 0.1559275668579684

0.2500000000000000 0.5542171003804959 0.3115419536416509

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0.5695055794795002 0.7049289895750436 0.2624270157692890  
0.4304782606348595 0.2949769086555775 0.1057075625112381  
0.4304943905205044 0.2950710104249566 0.2624270157692890  
0.4327147409127806 0.2047139778350968 0.0277153098252947  
0.4310981921706589 0.2042194262741419 0.1840851566043694  
0.4326932702432058 0.2047338765532196 0.3403749089353625  
0.5672852290872167 0.7952860371649010 0.0277153098252947  
0.5689017778293384 0.7957805887258557 0.1840851566043694  
0.5673066997567919 0.7952661384467781 0.3403749089353625  
0.2500000000000000 0.3741858584922539 0.0277387074058854  
0.2500000000000000 0.3748462639631511 0.1840874086866880  
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0.7500000000000000 0.6251537360368488 0.1840874086866880  
0.7500000000000000 0.6257248374190653 0.3403572588675672



0.7500000000000000 0.8761932661006676 0.1057878703234050  
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 0.2500000000000000 0.1238067338993323 0.1057878703234050  
 0.2500000000000000 0.1239769331387330 0.2623632736339408  
 0.7500000000000000 0.1462372802753252 0.0300654059452225  
 0.7500000000000000 0.1254695414074325 0.1841023648253917  
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**iii) (010) surface**

CONTCAR\0\1\0)

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6.4674000740000004 0.0000000000000000 0.0000000000000000  
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O V Bi

40 10 10

Direct

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 0.8040448531540295 -0.0000000000000000 0.0716666778981836  
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0.4542185769571574 0.1810847264316986 0.2331800010000009  
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0.5449708317552661 0.8195632047836939 0.1339112482660443  
0.5449708317552661 0.8195632047836939 0.3324487547339540  
0.9550291682447339 0.3195641887836904 0.1339112482660443  
0.9550291682447339 0.3195641887836904 0.3324487547339540  
0.0452107790109850 0.6827843972492634 0.0351209686487703  
0.0457814340428471 0.6810847564317011 0.2331800010000009  
0.0452107790109850 0.6827843972492634 0.4312390373512247  
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0.9550291682447339 0.6804367952163061 0.3324487547339540  
0.5449708317552661 0.1804358112163097 0.1339112482660443  
0.5449708317552661 0.1804358112163097 0.3324487547339540  
0.4547892249890153 0.8172156027507366 0.0351209686487703  
0.4542185769571574 0.8189152435682989 0.2331800010000009  
0.4547892249890153 0.8172156027507366 0.4312390373512247  
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0.7044206598401950 0.5000000000000000 0.1974904245750433  
0.6959551468459705 0.5000000000000000 0.3946933401018125  
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0.2991767960863910 0.5000000000000000 0.3680609968425860  
0.2067139127534974 -0.0000000000000000 0.1699639591362441

0.2008231889136114 -0.0000000000000000 0.3680609968425860  
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 0.7955793401598050 -0.0000000000000000 0.1974904245750433  
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 0.6241808519028594 -0.0000000000000000 0.0351364374676506  
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 0.8758191480971406 0.5000000000000000 0.0351364374676506  
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 0.1261535189581228 0.5000000000000000 0.1340073303344406  
 0.1261535189581228 0.5000000000000000 0.3323526726655577  
 0.1038109897639029 -0.0000000000000000 0.0381375847437819  
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 0.1038109897639029 -0.0000000000000000 0.4282224262562243  
 0.8716795312864438 -0.0000000000000000 0.1339948028281720  
 0.8716795312864438 -0.0000000000000000 0.3323652151718310  
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**iv) (011) surface**

CONTCAR\0\1\1)

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 7.4005999564999998 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 9.8283004761000008 0.0000000000000000

0.0000000000000000 0.0000000000000000 43.1627998351999977

O V Bi

64 12 16

Direct

-0.0000000000000000 0.1866361459717067 0.0776488032111565  
-0.0000000000000000 0.8136873396749030 0.1847675212477663  
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-0.0000000000000000 0.1119446372332884 0.3431710601888542  
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0.5000000000000000 0.7773987088502681 0.1960750299558696  
0.5000000000000000 0.3507361840557351 0.3186971444984937  
0.5000000000000000 0.7681197904312494 0.4309114231820805  
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0.5000000000000000 0.4131816268066358 0.1233771912925307  
0.5000000000000000 0.9851675231667528 0.2360422676557193  
0.5000000000000000 0.6119446262332915 0.3431710601888542

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-0.0000000000000000 0.8446408891656709 0.2246142313868236  
-0.0000000000000000 0.4116728842746882 0.3383004703714228  
-0.0000000000000000 0.8873186398752136 0.0824723177678924  
-0.0000000000000000 0.4544328568371847 0.1961783028065812  
-0.0000000000000000 0.0233340067965938 0.3092983049478962  
0.5000000000000000 0.7755697528300693 0.1114746905608156  
0.5000000000000000 0.3446408591656759 0.2246142313868236  
0.5000000000000000 0.9116728542746847 0.3383004703714228  
0.5000000000000000 0.3873186098752188 0.0824723177678924  
0.5000000000000000 0.9544328268371821 0.1961783028065812  
0.5000000000000000 0.5233340087965941 0.3092983049478962  
-0.0000000000000000 0.1451461048927886 0.0286998336119556  
-0.0000000000000000 0.6840212649948000 0.1400088294613585  
-0.0000000000000000 0.2346240720584528 0.2523271473740623  
-0.0000000000000000 0.7683752599136157 0.3700310722350663  
-0.0000000000000000 0.5306135243757373 0.0507092287378997  
-0.0000000000000000 0.0645225941267079 0.1683860907822271  
-0.0000000000000000 0.6151177064463103 0.2807664185999384  
-0.0000000000000000 0.1545873566438050 0.3920927713574623  
0.5000000000000000 0.6451461278927871 0.0286998336119556  
0.5000000000000000 0.1840212799948050 0.1400088294613585

0.5000000000000000 0.7346240720584536 0.2523271473740623  
0.5000000000000000 0.2683752299136136 0.3700310722350663  
0.5000000000000000 0.0306135243757381 0.0507092287378997  
0.5000000000000000 0.5645226011267050 0.1683860907822271  
0.5000000000000000 0.1151176764463152 0.2807664185999384  
0.5000000000000000 0.6545873416438003 0.3920927713574623

**v) (101) surface**

CONTCAR\1\0\1

1.0000000000000000

9.8283004761000008 0.0000000000000000 0.0000000000000000  
0.0000000000000000 7.4005999564999998 0.0000000000000000  
0.0000000000000000 0.0000000000000000 43.2620010376000010

O V Bi

64 16 16

Direct

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0.2113600497998362 0.0689395883768569 0.1215770930194751  
0.7772294229038366 0.0690072767149346 0.2340829974406944  
0.3465591723907977 0.0688201810561964 0.3466465869773145  
0.3852327304797782 0.9311293992415060 0.0754442223821528  
0.9550421417358734 0.9309670189048802 0.1880700879657908  
0.5204402165014770 0.9310572804879982 0.3004916043313202  
0.0956278208486907 0.9413233686876126 0.4124115752430271  
0.1365503688752625 0.9413178658854164 0.0097623437669156  
0.7113600347998386 0.9310604346231415 0.1215770930194751  
0.2772294229038366 0.9309927462850638 0.2340829974406944  
0.8465591723907977 0.9311798419438020 0.3466465869773145  
0.8852327004797758 0.0688706237584924 0.0754442223821528  
0.4550421417358663 0.0690330040951181 0.1880700879657908

0.0204402055014725 0.0689427425120002 0.3004916043313202  
0.5956278508486932 0.0586766543123858 0.4124115752430271  
0.6421543867573760 0.7500000000000000 0.0571402416742757  
0.2047690193891185 0.7500000000000000 0.1701884746614937  
0.7712015170641919 0.7500000000000000 0.2828948362531563  
0.3406635219571754 0.7500000000000000 0.3965982580027898  
0.3914699617275588 0.2500000000000000 0.0255521017180271  
0.9607812060622720 0.2500000000000000 0.1392055236590721  
0.5273691625388039 0.2500000000000000 0.2519657183485862  
0.0898802399509009 0.2500000000000000 0.3650164114295720  
0.9345391337447779 0.2500000000000000 0.0176205093587143  
0.5013250596181464 0.2500000000000000 0.1291371655590297  
0.0671852897143808 0.2500000000000000 0.2417368728365332  
0.6363042350010417 0.2500000000000000 0.3552292356850231  
0.0957239930061107 0.7500000000000000 0.0669306946591277  
0.6648484477059071 0.7500000000000000 0.1803589922328968  
0.2308376854286678 0.7500000000000000 0.2929870873611478  
0.7975163793537376 0.7500000000000000 0.4044962854136358  
0.8914699617275588 0.7500000000000000 0.0255521017180271  
0.4607812360622745 0.7500000000000000 0.1392055236590721  
0.0273691735388084 0.7500000000000000 0.2519657183485862  
0.5898802479509015 0.7500000000000000 0.3650164114295720  
0.1421544017573737 0.2500000000000000 0.0571402416742757  
0.7047690193891185 0.2500000000000000 0.1701884746614937  
0.2712014870641966 0.2500000000000000 0.2828948362531563  
0.8406634919571729 0.2500000000000000 0.3965982580027898  
0.5957239860061065 0.2500000000000000 0.0669306946591277  
0.1648484327059023 0.2500000000000000 0.1803589922328968  
0.7308377154286703 0.2500000000000000 0.2929870873611478  
0.2975163793537376 0.2500000000000000 0.4044962854136358



0.4345391337447779 0.7500000000000000 0.0176205093587143  
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0.5671852667143824 0.7500000000000000 0.2417368728365332  
0.1363042350010488 0.7500000000000000 0.3552292356850231  
0.1365503688752625 0.5586821341145836 0.0097623437669156  
0.7113600347998386 0.5689395653768585 0.1215770930194751  
0.2772294229038366 0.5690072537149362 0.2340829974406944  
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0.8852327004797758 0.4311293692415035 0.0754442223821528  
0.4550421417358663 0.4309669889048777 0.1880700879657908  
0.0204402055014725 0.4310572504879957 0.3004916043313202  
0.5956278508486932 0.4413233386876101 0.4124115752430271  
0.6365503828752637 0.4413178358854140 0.0097623437669156  
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0.3852327304797782 0.5688706007584940 0.0754442223821528  
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0.5716782435242607 0.2500000000000000 0.0264841746797018  
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0.2726150974130661 0.2500000000000000 0.3657865602619097  
0.4593603845827730 0.7500000000000000 0.0563125359440662  
0.0289679046314433 0.7500000000000000 0.1689905215851866  
0.5944627666473892 0.7500000000000000 0.2815591550402345  
0.1604523059908729 0.7500000000000000 0.3956752481605363  
0.0716782365242636 0.7500000000000000 0.0264841746797018  
0.6373893320130932 0.7500000000000000 0.1405430751354544

0.2032928019624407	0.7500000000000000	0.2531472518728748
0.7726150974130661	0.7500000000000000	0.3657865602619097
0.9593603845827730	0.2500000000000000	0.0563125359440662
0.5289679086314436	0.2500000000000000	0.1689905215851866
0.0944627436473908	0.2500000000000000	0.2815591550402345
0.6604522909908681	0.2500000000000000	0.3956752481605363
0.6742839310133704	0.7500000000000000	0.0071141272246322
0.2440570223401295	0.7500000000000000	0.1120940031392124
0.8097771291501203	0.7500000000000000	0.2252532256310644
0.3683008270510300	0.7500000000000000	0.3374235721515504
0.3632765576063761	0.2500000000000000	0.0848066454707919
0.9225425109407723	0.2500000000000000	0.1968711644150289
0.4875833516208985	0.2500000000000000	0.3098918891150220
0.0582767274206617	0.2500000000000000	0.4150654090662584
0.1742839460133681	0.2500000000000000	0.0071141272246322
0.7440570073401318	0.2500000000000000	0.1120940031392124
0.3097771291501203	0.2500000000000000	0.2252532256310644
0.8683008570510324	0.2500000000000000	0.3374235721515504
0.8632765876063715	0.7500000000000000	0.0848066454707919
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**vi) (110) surface**

CONTCAR(1\1\0)

1.0000000000000000

6.4674000740000004 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.4660997391000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 39.9757995605000005

O V Bi

## Direct

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0.7977146922610008	0.5339888490573633	0.1783109690514612
0.7971970482066666	0.0317364975313288	0.3091454204831946
0.7085678357082396	0.2848454592231637	0.1125153959510011
0.7057981129541810	0.7855096454032190	0.2437183727791994
0.7014750924592869	0.2919621731309107	0.3748233005465887
0.2985249075407133	0.7080377968690938	-0.0002033095465855
0.2942018870458186	0.2144903845967764	0.1309116162207995
0.2914321642917608	0.7151545107768416	0.2621046100489995
0.4419556491795817	0.2197645343191897	0.0465409629357407
0.4522853077389989	0.7160111509426367	0.1783109690514612
0.4528029517933334	0.2182635064686715	0.3091454204831946
0.5471970482066666	0.7817365235313239	0.0654745855168060
0.5477146922610008	0.2839888190573681	0.1963090369485394
0.5580443508204184	0.7802354956808054	0.3280790240642620
0.9514750924592869	0.5419622031309062	-0.0002033095465855
0.9557981129541810	0.0355096194032240	0.1309116162207995
0.9585678357082396	0.5348454892231584	0.2621046100489995
0.0414321492917630	0.4651545407768363	0.1125153959510011
0.0442018720458209	0.9644903545967810	0.2437183727791994
0.0485248925407155	0.4580378268690893	0.3748233005465887
0.0471970332066690	0.2817364935313286	0.0654745855168060
0.0477146772610033	0.7839888490573633	0.1963090369485394
0.0580443358204206	0.2802354656808105	0.3280790240642620
0.9419556491795816	0.7197645043191946	0.0465409629357406

0.9522853077389992 0.2160111809426320 0.1783109690514612  
0.9528029517933334 0.7182634764686761 0.3091454204831946  
0.5414321642917604 0.9651545107768416 0.1125153959510011  
0.5442018870458190 0.4644903845967764 0.2437183727791994  
0.5485249075407131 0.9580377968690938 0.3748233005465887  
0.4514750924592867 0.0419621771309110 -0.0002033095465855  
0.4557981129541814 0.5355096454032190 0.1309116162207995  
0.4585678357082392 0.0348454632231637 0.2621046100489995  
0.7028029517933334 0.4682635064686714 0.0654745855168060  
0.7022853077389992 0.9660111509426367 0.1963090369485394  
0.6919556491795816 0.4697645343191895 0.3280790240642620  
0.3080443508204183 0.5302354956808054 0.0465409629357407  
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0.2014751074592845 0.7919622031309062 0.3748233005465887  
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0.6250000000000000 0.6250000000000000 0.1545877230851692  
0.6250000000000000 0.1250000000000000 0.2855606051356830  
0.8750000000000000 0.3750000000000000 0.0890593998643211  
0.8750000000000000 0.8750000000000000 0.2200322679148267  
0.8750000000000000 0.3750000000000000 0.3519586522706398  
0.1250000000000000 0.6250000000000000 0.0226613367293560

0.1250000000000000	0.1250000000000000	0.1545877230851692
0.1250000000000000	0.6250000000000000	0.2855606051356830
0.1250000000000000	0.1250000000000000	0.0279221394815062
0.1250000000000000	0.6250000000000000	0.1556924021171630
0.1250000000000000	0.1250000000000000	0.2877565511438597
0.8750000000000000	0.8750000000000000	0.0868634538561446
0.8750000000000000	0.3750000000000000	0.2189275888828329
0.8750000000000000	0.8750000000000000	0.3466978495184894
0.6250000000000000	0.6250000000000000	0.0279221394815062
0.6250000000000000	0.1250000000000000	0.1556924021171630
0.6250000000000000	0.6250000000000000	0.2877565511438597
0.3750000000000000	0.3750000000000000	0.0868634538561446
0.3750000000000000	0.8750000000000000	0.2189275888828329
0.3750000000000000	0.3750000000000000	0.3466978495184894

**vii) (111) surface**

CONTCAR(1\1\1)

1.0000000000000000

9.8283004761000008 0.0000000000000000 0.0000000000000000

4.2557622364999999 8.8591183552999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 32.0139007567999982

O V Bi

48 12 12

Direct

0.8147043971436636 0.8888118409894527 0.0306457232028911

0.5264408270628217 0.5905516641375690 0.1588553119106423

0.1984043935331556 0.3106951172085424 0.2914855187300839

0.7067616118189189 0.5964645793628596 0.0838491577087948

0.3797939006762035 0.3157895628383289 0.2163817241067778

0.0923728966528778 0.0176306304856648 0.3445934109738252

0.3652397632728191 0.8102317710143913 0.0180270586172499  
0.0533546257674088 0.4968267370402227 0.1453385659688682  
0.7668497106004588 0.1831330355606192 0.2692205328336439  
0.1398803345420254 0.7233327120858042 0.1061410627642439  
0.8532932095748910 0.4094406617258871 0.2300191925954354  
0.5410857356365923 0.0966648647242987 0.3570864406722794  
0.9463500148935459 0.5336816822776788 0.0246292833517301  
0.6707199281456347 0.2386352056943362 0.1748236683005804  
0.3773858889719848 0.9365256597934163 0.3010118385613502  
0.5294549061863733 0.9694785239721737 0.0741429445157166  
0.2354671834937364 0.6678572222371355 0.2004435807766329  
0.9586757952004417 0.3735492867474798 0.3506627266580457  
0.0578496589093935 0.0045069991261078 0.0591740095892088  
0.7578739206436705 0.6998810640150734 0.1904196016158818  
0.4610258936434536 0.3727332778881910 0.3130122085910602  
0.4448693896074438 0.5338242638497651 0.0621562196720001  
0.1486619128712471 0.2062629008161141 0.1848107076033702  
0.8490396034714859 0.9022042918130099 0.3162836873190977  
0.3182508001679782 0.5677611731527397 0.9887346642483928  
0.8894435330418412 0.3194721452454208 0.1410378401316075  
0.5987283613866723 0.0041396175717061 0.2645477238481580  
0.3082310058759314 0.9020078032770902 0.1107573900428450  
0.0168321200735577 0.5871910506732616 0.2342598633491337  
0.5879108535703386 0.3392321266878663 0.3864081601093258  
0.7858290470052668 0.8572192489547660 0.1190266537793399  
0.4806675668600467 0.5675889842725099 0.2475626895282935  
0.2660068669446197 0.3417270117422743 0.3772835503375265  
0.6399564796851489 0.5649434583444080 0.9978800369296985  
0.4256156468147594 0.3387223015121830 0.1276258830768459  
0.1208217485388886 0.0491571797949613 0.2562088175438448

0.1686794552643711 0.2464500145748560 0.0955112335747864  
0.8823052913603818 0.9305045715967755 0.2251945786729012  
0.5721875260420360 0.6512405321883066 0.3537632401247817  
0.3361303449663018 0.2551906937371404 0.0217120515454175  
0.0245425102807570 0.9758443990552232 0.1502136760866789  
0.7376940235215850 0.6600636774725305 0.2797304078883115  
0.7094945761218052 0.1419080735839329 0.0749722879496636  
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0.8366411693722040 0.3240135761642184 0.0458820025286666  
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0.7890641171490625 0.5149859210989217 0.0365697097534368  
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0.1962955426784402 0.9465686106288120 0.3006504292044466  
0.4437132358035478 0.6223954267044468 0.0144154828722271  
0.0675392062492712 0.3191562747066449 0.1410817681655962  
0.7734650729258411 0.0072988565807195 0.2683470351952418  
0.1334419516643762 0.8991311250705791 0.1070435324567390  
0.8389170113263602 0.5872001356953966 0.2341815073187584  
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0.6434369769860969 0.4003443978380054 0.1124023170959729  
0.3448781816861533 0.0893842823330457 0.2329451996676838  
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0.2630378437777814 0.5057670944048872 0.2627721397307889

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0.2328167662155936 0.4762800582717247 0.0428771827866862  
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