

Supporting information for :

Mechanistic elucidation of forming Ta₃N₅/LaTiO₂N heterojunction in improving photocatalytic activity

Linlin Wang^a, Chunyu Jin^a, Hao Dong^{*a}, Xin Zhou^{*b,c}

^a *School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, Liaoning, China*

^b *Interdisciplinary Research Center for Biology and Chemistry, Liaoning Normal University, Dalian 116029, P. R. China*

^c *College of Environment and Chemical Engineering, Dalian University, Dalian 116622, Liaoning, China*

* Corresponding authors.

E-mail addresses: hdong@lnnu.edu.cn (H. D.), xzhou@lnnu.edu.cn (X. Z.)

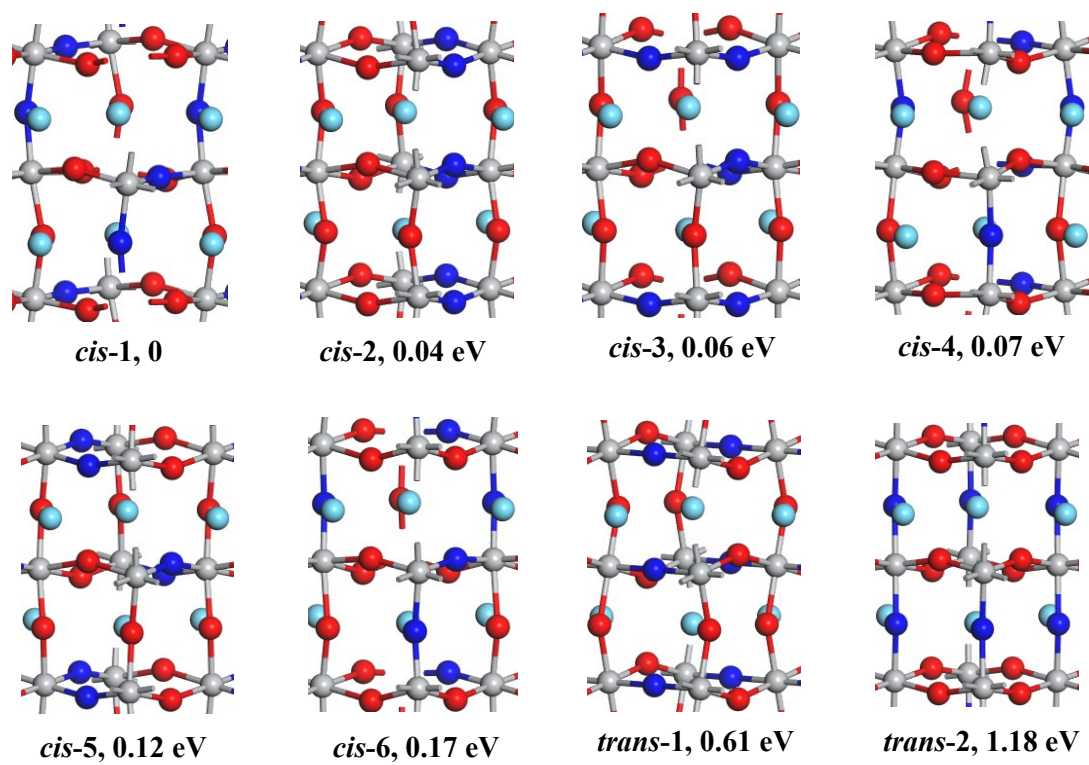


Fig. S1 Eight possible structures of bulk LaTiO_2N and the relative energies. Coloring scheme: light blue (La), grey (Ti), red (O) and blue (N).

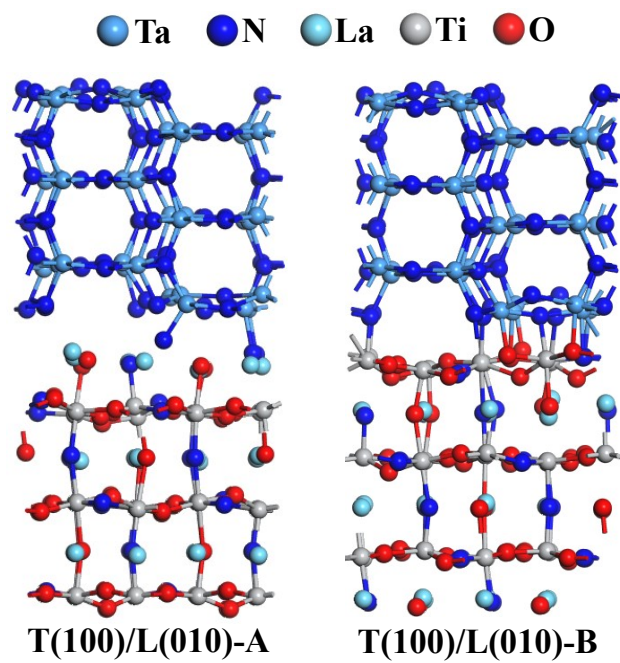


Fig. S2 The relaxed interfacial structures between $\text{Ta}_3\text{N}_5(100)$ and $\text{LaTiO}_2\text{N}(010)$ surfaces.

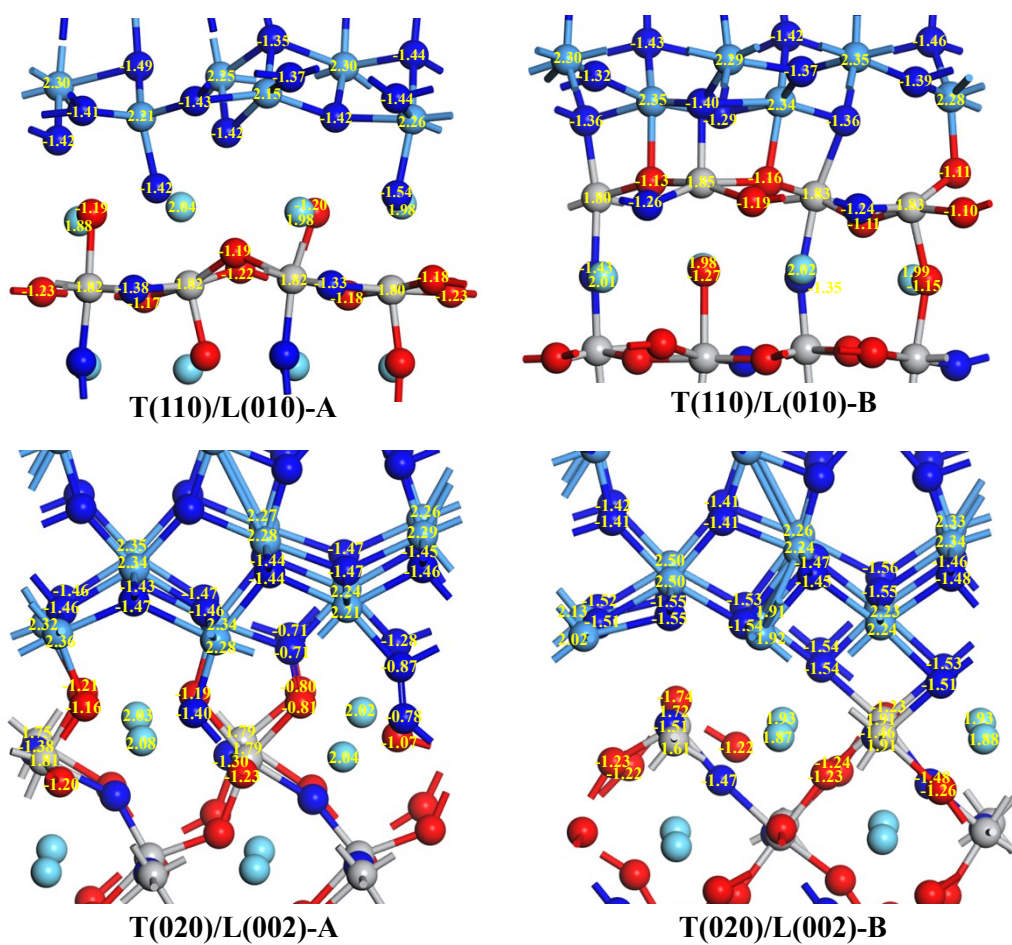


Fig. S3 The net charges of the atoms in the interfacial region of each heterojunction structure obtained by Bader charge calculations (in e).

The optimized structures of the studied heterojunction structures:

Ta₃N₅(110)/LaTiO₂N(010)-A

1.0000000000000000

10.7531003952000006 0.0000000000000000 0.0000000000000000

-0.0492210665000000 5.5469818259999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 50.9818992614999971

Ta N La O Ti

24 56 16 32 16

Direct

0.2234301963961775 0.1581400652531577 0.3718523278732159

0.2419860806572241 0.4683835692959452 0.4393271092304174

0.2279680406025472 0.6503817990002707 0.2291896405968798

0.2264201153780186 0.9065903713600362 0.2999827384242432

0.7304679008501409 0.3412528559931161 0.2067521091295081

0.7350676959022328 0.5864650238614449 0.2749014377929003

0.7362919847471127 0.8334471972798094 0.3433632189976593

0.7382203015100606 0.1057321273138601 0.4120691498509504

0.5224987252031993 0.2755808467421307 0.3608309402274639

0.5496872553645002 0.5091353865932393 0.4272633042932761

0.5342907082336292 0.7583320286442282 0.2239997002845257

0.5349519790444434 0.0101977927679903 0.2947407084020752

0.0386918893283650 0.2480464924633362 0.2094544539585913

0.0370825395332451 0.4831646293435762 0.2791538878754522

0.0395636527080397 0.7374284147041263 0.3491929616832541

0.0414023805391151 0.0193729766084076 0.4219772259309209

0.9247536359880831 0.2632545499041024 0.3672104186802543

0.9047695386654795 0.5202830727192238 0.4406256298287212

0.9244197505195613 0.7548779813517625 0.2242481004846855

0.9239255766428923 0.0108445915708215 0.2962259607205071

0.4173293707424259 0.2506398367350587 0.2096337361525322

0.4285886313042205 0.4810965835237584 0.2787481646715322

0.4179505693366729 0.7479315119874317 0.3469437483085304

0.4364180512813650 0.0130908740347121 0.4168364633953089

0.2296574584540967 0.3641361854963081 0.2028356752209136

0.2248135577431376 0.6611968640510003 0.2696520590773560

0.2285964437062656 0.9107368734265322 0.3408313384830769

0.2357879483465523 0.1857463364294698 0.4122381874992606

0.7173178865302265 0.3919453649448004 0.4392349162010021

0.7330451328057083 0.5551250786142518 0.2355466343195861

0.7353985398372564 0.8424190339310738 0.3031925104412429

0.7459772695897432 0.0721311393306141 0.3732191123862107

0.0984517118655761 0.1639795370264157 0.2902239100947519

0.0998299965833334 0.4206488788991245 0.3613927609477963

0.0985138543175682	0.7047607698375321	0.4371245241961260
0.0391036992581373	0.2568194150026355	0.4507339915127212
0.0958921696999104	0.8917513305846994	0.2179513267801118
0.0503665713011531	0.4348078272375831	0.2398007794208298
0.0572458842073785	0.7122535515744510	0.3093024243777550
0.0582000009993752	0.9658862173854289	0.3806361928049180
0.5985029275386904	0.3317653586257587	0.2849129909450001
0.5958084250421760	0.5841147169361330	0.3511182656247555
0.6056176844459263	0.8545282431343104	0.4202157866512868
0.5558037306060141	0.4882026648253785	0.1960100998201110
0.5582414184104427	0.7769942654017835	0.2647034199898162
0.5589944853202982	0.0233663436522057	0.3342604958303929
0.6014658975690256	0.0597934905371139	0.2131800188727718
0.5626016381595420	0.2967982332794015	0.3987139377099855
0.3636343874875553	0.1649823386786538	0.2900870085949627
0.3569082077157996	0.4241673279062352	0.3579896222546062
0.3740981196011871	0.7127203708878241	0.4320497026014448
0.4516051782735027	0.2496355402731095	0.4466708887221981
0.3633895781172558	0.8938635092338978	0.2185225374183501
0.4053561021655752	0.4387336986386355	0.2400319805191605
0.4000854943710560	0.7203575644264589	0.3076346057283486
0.4012629639302932	0.9768544445632725	0.3774580073240083
0.8629179285365390	0.3295321990332731	0.2857009957373197
0.8644514740325294	0.5766385100453325	0.3541081413268339
0.8656051367127230	0.8720214242132762	0.4310408936388243
0.9032791806255500	0.4858543900139349	0.1953845224623808
0.9088769567141312	0.7752046612892731	0.2651241628972135
0.9126151700928541	0.0281364829356689	0.3358771276996190
0.8578009072027026	0.0582848087264138	0.2140382424350590
0.9081986438837036	0.3031183564391517	0.4065741644939520
0.2805610146998133	0.4457226761870051	0.4760738411507575
0.8674747565382923	0.5388848350645549	0.4798766259073431
0.3528617822524494	0.4572544343654630	0.6460981595286944
0.8501965973184509	0.4553686464850347	0.6463487483759180
0.0960894118661321	0.9564123501449143	0.5676960092962009
0.5926186556012284	0.9732729824144604	0.5642161642425571
0.0987394894344044	0.9527318297955678	0.7253224288179927
0.5989909437097309	0.9553247245146230	0.7253992105305157
0.4662167607085292	0.1946905750540114	0.6059907137874005
0.9679133829618470	0.2037161872884433	0.6057832493314582
0.4927411433477967	0.2313494073385110	0.7630568288007760
0.9927561588657375	0.2313947730900756	0.7627527954334224
0.2241768433117784	0.7145823344490920	0.5295011130253533
0.7067500707672173	0.6916997137580622	0.5269603817213009

0.2237557847685752	0.6936070941154985	0.6859396178369445
0.7234923552152670	0.6944979384093715	0.6859722503796566
0.0910530827740776	0.5145076754002644	0.4933608588402479
0.6301473388351319	0.4552903541702122	0.4882376988026936
0.1139107207520550	0.4851447573731603	0.6485681691244781
0.6138898095180105	0.4855795405248612	0.6481753314932710
0.3584208576963557	0.0025477184875605	0.5679239130321748
0.8602378679756230	0.0103346749789310	0.5667675281788059
0.3645976840815729	0.9762349455705898	0.7295803509810810
0.8643769863754728	0.9774097018455792	0.7293893077278131
0.1084578924497840	0.5056012088149952	0.5679808727372553
0.6179801301311563	0.5045123199648974	0.5678715253554727
0.1229551197893868	0.4774997826282403	0.7281064132413195
0.6229798299159475	0.4784590394943369	0.7281538293942647
0.3399356600833805	0.0104481370858920	0.4841784638231443
0.8795031078539285	0.0042498141259920	0.4825674094681930
0.3639079160985049	0.9908402377529396	0.6466370492201267
0.8599829920469787	0.9916570200950905	0.6461926209793615
0.3997607172224540	0.5265477909946902	0.5628739625045057
0.8754722154797913	0.5387805332537796	0.5663845506403420
0.3929746648394181	0.5216542689613830	0.7256251738147454
0.8930762478114678	0.5243969775883656	0.7256084384231237
0.1213279597076521	0.9797323668621932	0.4913408848993083
0.6671184659412952	0.0349690303219050	0.4872112470918188
0.1412645569229570	0.0348716309059429	0.6455076018482127
0.6357711732516241	0.0279605389616757	0.6451984557826937
0.4716551637507694	0.7492002377993908	0.5105256929739572
0.9556443648020514	0.8077417112943002	0.5245464160915516
0.4743382701497835	0.7807004798693539	0.6795450861519953
0.9747380295566153	0.7817488993640425	0.6787663663119502
0.2226664724611911	0.2909592802373408	0.5994222499162009
0.7197742409954212	0.2893271200445177	0.6010720483290144
0.2437815067350570	0.2349182896925809	0.7596010726125979
0.7439407296140913	0.2360910207706538	0.7595893162232175
0.2507732112482451	0.2254046614179930	0.5318481264784355
0.7489920265517505	0.2244365313900366	0.5304492597393151
0.2722221323297206	0.1903914632649345	0.6914546690952061
0.7717485755727914	0.1905395594873718	0.6913563709157220
0.2712388370001207	0.7907530351198734	0.6047815995615463
0.7686719229268545	0.7975785601159259	0.6049458896940764
0.2446697159993161	0.7312894141257247	0.7607529282679911
0.7448392925549937	0.7320228254504547	0.7607555479201631
0.5202619675654138	0.6912584373129452	0.6100445525015382
0.0173256220549629	0.6978238435043178	0.6122478882617822

0.9939964537373741	0.7314838449522282	0.7709032254273612
0.4939768025680330	0.7314157576666639	0.7705145293323266
0.4851530952954141	0.2465505522025029	0.5167782276071899
-0.0000057226013640	0.2935595861217828	0.5291946896468117
0.0232632138339739	0.2910679109802428	0.6854595970796050
0.5232736762682252	0.2909483676524518	0.6851595462667582
0.1085512359196378	0.0026219136869459	0.6055946873975798
0.6085541392911546	0.0013529300666609	0.6043521577237811
0.1122142682104472	0.9804732930968632	0.7632329474529610
0.6126747507588458	0.9812571359995588	0.7632546209361055
0.3603686778211707	0.5107533114815371	0.5264699366736095
0.8542962857210424	0.5198842268692631	0.5286700642108951
0.3638159170110565	0.4928931090445258	0.6854454444082267
0.8634345453070777	0.4937753629585372	0.6851765622227491
0.1138990202569115	0.9957545300679048	0.5295578670373026
0.6113860167076890	0.9800152345744774	0.5248061108522352
0.1191258032636769	0.9794371110731475	0.6884744346371642
0.6191202479016241	0.9799192661100549	0.6885230352179369
0.3682005361959714	0.4859521891869888	0.6096607637791105
0.8668085297778586	0.4897627760577453	0.6096764754301469
0.3780415977083383	0.4793792692922370	0.7638062103730340
0.8782945239761808	0.4804325524377850	0.7637172768146271

Ta₃N₅(110)/LaTiO₂N(010)-B

1.0000000000000000

10.7531003952000006	0.0000000000000000	0.0000000000000000
-0.0492210665000000	5.5469818259999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	50.6230010985999996

Ta	N	La	O	Ti
24	56	16	32	16

Direct

0.2294435769723071	0.0254613295113706	0.3746856460906181
0.2421983200776925	0.2706023286871885	0.4438994676561804
0.2305054216726554	0.5227040554447446	0.2347081336653056
0.2315500845606542	0.7759885888629275	0.3057067586114990
0.7318766246924686	0.2137295770161266	0.2117683862011161
0.7353134260449059	0.4570630288000873	0.2804622725282376
0.7321931392672241	0.7060273691613170	0.3502098928129714
0.7276574833462587	0.9444935271285290	0.4225378108357231
0.5384659481931977	0.1293025328499635	0.3716944683826974
0.5470502341092678	0.3605313683223050	0.4442480370763705
0.5366481216332338	0.6294447778038483	0.2294596830024744
0.5398206638798282	0.8749935953384594	0.3014698179291708

0.0411852451945038	0.1211865948575642	0.2146023421936099
0.0383606122688982	0.3499898212301955	0.2846602192492771
0.0358438112818089	0.5912326730690712	0.3540673947627759
0.0423852430828191	0.8551946355103479	0.4231866221308440
0.9178208793596345	0.1214131884348192	0.3727302161190928
0.9508984726399292	0.3809851637688291	0.4421310585125506
0.9261752450837113	0.6283228901496413	0.2293601510100331
0.9246554173357170	0.8796564714715334	0.3015996576874885
0.4200911445205412	0.1222468236449933	0.2149500025839630
0.4322141520412096	0.3462071905823600	0.2847335279874221
0.4265866011857481	0.5977519150221842	0.3537352387658205
0.4275694741555825	0.8566822146495001	0.4234498841098629
0.2314985512347900	0.2368667254833643	0.2080733599565960
0.2278520558022046	0.5296940194056367	0.2754345921112696
0.2332405150729720	0.7656916279234404	0.3461610899417853
0.2315473996071591	0.0210500562150588	0.4140161468512907
0.6989326305705056	0.1686071272143966	0.4536873585768588
0.7331650467592002	0.4273584921931270	0.2407069268923290
0.7326611888055645	0.7090914959514604	0.3092415132485852
0.7359236495363678	0.9464011530469766	0.3806331356637777
0.0997874289623698	0.0341090947719446	0.2963506341131605
0.0976820168972577	0.2800096255476393	0.3659066875856831
0.1084873183628504	0.5270662361638155	0.4311849590455770
0.0839667965159193	0.0745364279125570	0.4531983557432902
0.0978991969771792	0.7652302043412457	0.2234503919326898
0.0519425184206157	0.3087861846710263	0.2451463627184461
0.0553891054124202	0.5859183410461024	0.3144539899909447
0.0527038002666669	0.8351548868895707	0.3835522832687124
0.6009913957799283	0.1983864405149447	0.2909745316403430
0.6002473540264008	0.4437869385025253	0.3595880625289671
0.5982117499519785	0.6856816772598940	0.4293883081102039
0.5573114048854395	0.3601910771695033	0.2009088003252229
0.5598450128028004	0.6465006865360230	0.2703944545454843
0.5607512489155471	0.8917109810050073	0.3415277681815045
0.6032689763985970	0.9320696730436331	0.2185815662582741
0.5619717001412139	0.1499553378381668	0.4109968346599516
0.3661125777783742	0.0309721430460876	0.2961954872034244
0.3662434370082568	0.2776013203497699	0.3654733085520488
0.3620653456842849	0.5804830740063937	0.4453273409034813
0.4043419485962951	0.1109718812825469	0.4496638692106410
0.3655464942727605	0.7652722001846713	0.2238682956093771
0.4081660799074326	0.3095502685929417	0.2455546897843585
0.4062999987257168	0.5844243683414108	0.3138935770355871
0.4074102880345710	0.8261576528239720	0.3840938154973065

0.8647867545573580	0.1991180021053692	0.2908248836802966
0.8631569822317934	0.4432262962484153	0.3605584313257179
0.8694297740717883	0.6897572353549104	0.4348200873383470
0.9053238205865282	0.3591278890611299	0.2004136866779098
0.9071863709010139	0.6481962492456487	0.2704575586714096
0.9035512597071857	0.8987124219388690	0.3415127739263663
0.8597837538424933	0.9308853860060031	0.2188221948708885
0.9046210601683325	0.1365976945808342	0.4139948131359455
0.3494247037385393	0.5945359912720588	0.6129434272636470
0.8488873461403619	0.5870748240079293	0.6133965417168407
0.3401108230176798	0.5807424801513911	0.7743933058159458
0.8402740520990867	0.5800324957842751	0.7743793672018454
0.1047360006270500	0.1586171544541463	0.5318052652347626
0.5918111855151700	0.0969096022469970	0.5327118881820405
0.0979605978444732	0.0693922479060057	0.6934747952375619
0.5966611623766961	0.0668323690524049	0.6934935762242912
0.4585210682041110	0.2899497183840247	0.5751252218456538
0.9612277897335750	0.2869194192408989	0.5775323957553437
0.4600194473486710	0.2644488621628160	0.7368252194057037
0.9598183575156056	0.2642474007729815	0.7366927044154987
0.2324708692078614	0.8356419125693638	0.4967252167560940
0.7331645253187613	0.8274108249324106	0.4989233623622224
0.2080502074508596	0.7754794904285270	0.6556045643942817
0.7073351277888609	0.7789931405512079	0.6546923861597540
0.1072847267618478	0.5805014026830578	0.6124754993946880
0.6089564577154747	0.5678860227052378	0.6115197414333708
0.1137298580242291	0.5189585768088238	0.7715191432766015
0.6134565999980252	0.5185370626552324	0.7715478870693269
0.3614503831488740	0.1020630625505781	0.5279530696708319
0.8603683450710631	0.0945710955282338	0.5340307290681139
0.3586930335677994	0.0624896639343123	0.6921694765139772
0.8593260003174090	0.0619936168867291	0.6923132987333894
0.1243645881513558	0.6091647403625216	0.5327470113803532
0.5958720344417037	0.5907089050787022	0.5292914654969568
0.1057048057579926	0.5653751884106349	0.6919706713517285
0.6056963330330919	0.5670324942188902	0.6919154126170045
0.3581360543576881	0.0752267645277949	0.6109974891801023
0.8563683785885804	0.0741695559992723	0.6122680950537339
0.3535306245960240	0.0380796436433344	0.7710113917152075
0.8536685474246479	0.0385322917248233	0.7709875086213478
0.3661411224284721	0.5404400253633291	0.5299210104158795
0.8942095646330198	0.5565642053788757	0.5346854751757729
0.3784833845177704	0.5938754062542935	0.6939132151023630
0.8779318828443839	0.5949396089563959	0.6937729072818560

0.1303325564780994	0.0736513391057235	0.6134688881864270
0.6237475877007685	0.1012573353894640	0.6137193871717140
0.1360404584621106	0.1018571352758546	0.7770438627968470
0.6365427183420344	0.1021926368992895	0.7771172232690463
0.4820297598131307	0.8646168410029957	0.4950396875145947
0.9818607102599701	0.8502214278268581	0.5010419192955793
0.4549375890685160	0.8946349973777923	0.6509012296194179
0.9570432630947222	0.8884625303684646	0.6511298120233061
0.2064714941012956	0.4047343315972974	0.5738473366523410
0.7086851112794164	0.3995052761766976	0.5702366138673589
0.2066085771589217	0.3818512540122363	0.7311496521574405
0.7065985409640947	0.3815138770407163	0.7310572726697842
0.2397942714842151	0.3349292915019268	0.4844828615543788
0.7423525521435678	0.3369558056775528	0.5051053107105854
0.2643716278545453	0.2770226760208324	0.6555192808943908
0.7631189021659028	0.2786430970897849	0.6564384537526246
0.2648980545719204	0.8959931284303526	0.5668267046306267
0.7650819801929756	0.8966135594694753	0.5715243343669992
0.2685905983018622	0.8884656425736688	0.7322726993256459
0.7685895826140725	0.8882521815523461	0.7322756246729278
0.5128625892581624	0.7839795613561242	0.5747565342505225
0.0159492005247560	0.7942616898876987	0.5736163422477583
0.0197390695502846	0.7632468013746894	0.7375395925122722
0.5198488709455522	0.7633495214854926	0.7376968725378498
0.5158480751050973	0.3926436795714180	0.4845500188757262
0.9618956142758249	0.3713641061000112	0.4804654553846177
0.0145206123191555	0.3863680216919411	0.6515822805760262
0.5146689851467385	0.3931982908194016	0.6519659989531501
0.1101337613913344	0.1053927984397357	0.5691173115260793
0.6052328045552744	0.0927829953891448	0.5690064780485009
0.1059814908020313	0.0678032203441548	0.7305506270642902
0.6057072521474668	0.0678402232532372	0.7305416641056816
0.3601059985606796	0.6279723604500135	0.4852934538133689
0.8572374586114212	0.5998858997170691	0.4981144291930383
0.3568234941897138	0.5833365914027172	0.6507368901091082
0.8555691799832498	0.5819024004340219	0.6512464984809981
0.1102452937203806	0.0676570388780096	0.4919800032073878
0.6286322360089571	0.0822848000978714	0.4916890008646430
0.1154460727079141	0.0628295675644051	0.6530310119395015
0.6128445890974586	0.0641945260091027	0.6530658282550740
0.3654236467046094	0.5743497973147877	0.5737335383389257
0.8655895239484968	0.5723436617771709	0.5744455710262423
0.3641179082855620	0.5555338197335884	0.7365003540725508
0.8639009400210075	0.5554068227964362	0.7365765887414021

Ta₃N₅(020)/LaTiO₂N(002)-A

1.0000000000000000

10.7483997344999995 0.0000000000000000 0.0000000000000000

-0.0335853658000000 7.9026285805000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 40.5632019043000014

Ta N La O Ti

24 56 16 32 16

Direct

0.7519132517722832 0.0027927792581674 0.2795488630093180

0.7518038222171527 0.5002139258360739 0.2797039539427486

0.2481431163218036 0.0026584850786457 0.4346340819350946

0.2480969975101803 0.5077533209311802 0.4322601836727289

0.7539079828098788 0.2563941526868376 0.4126255622553964

0.7513989462641101 0.7494007922398156 0.4130013407689162

0.2487960235535494 0.2511693938393301 0.3100969990261644

0.2487965310046796 0.7524045338659467 0.3100421082365537

0.0379890589402963 0.0013780955677336 0.2758715645337114

0.0381368220300644 0.5009196905044014 0.2761727166437615

0.9399436054735805 0.0078899647703506 0.4492676886089895

0.9646733369061224 0.5102992879733159 0.4517942654454815

0.5632387386438639 0.0026174468219276 0.4543322691194765

0.5616641787045257 0.4991946531057933 0.4514284104197530

0.4660481828563843 0.0018731528853394 0.2774643298403211

0.4659661899335644 0.5016990455760768 0.2777396461092478

0.0645757623522894 0.2517041239767810 0.3938133131995197

0.0637528145045879 0.7533048910785163 0.3927665296606644

0.9303755214464778 0.2505341977983732 0.3292054586125217

0.9266561149869686 0.7515953460069860 0.3286427592355385

0.5621566551167489 0.2517684006993278 0.3312293843978334

0.5623536187067103 0.7528183401584636 0.3311407676319767

0.4400408451513690 0.2503197704390302 0.3964277425148690

0.4398892772508524 0.7558950498690958 0.3961986116957429

0.7570130397379646 0.0041275468095933 0.4288616253059750

0.7479789619899437 0.5024139902789844 0.4264009190946480

0.2516910325653566 0.0015672011834529 0.2952023490030784

0.2515856413011190 0.5016027061405385 0.2957863869470914

0.7544949958267626 0.2515669879473399 0.3017677479162900

0.7544696485986550 0.7515186784906540 0.3022634082911724

0.2489232651712895 0.2525132845008912 0.4158827196534830

0.2509813408610060 0.7555041604475573 0.4146094238787479

0.6093744817974592 0.0022702262742019 0.2506399483882664

0.6092252669610321 0.5011811797528457 0.2508802361028660

0.3804481632459158	-0.0072117885091560	0.4713401377667637
0.3823324685069230	0.4928572574946973	0.4696649279100363
0.1237233126455929	0.0068586836531684	0.4730927993441585
0.1297603916037943	0.5506155632524956	0.4681144924055413
0.8926807963676220	0.0016103873709862	0.2498657162255107
0.8928152628410954	0.5008969246780123	0.2501589112307952
0.6220108062270908	0.2510244946466982	0.3753064672578090
0.6217583037301841	0.7578064665670734	0.3754335890559136
0.3867639534917470	0.2501204813839972	0.3506757304220707
0.3869951122761784	0.7533495954232078	0.3505438385707076
0.1166459241254428	0.2480059334177750	0.3484598961491493
0.1187611056505498	0.7561664373103524	0.3483870672806427
0.8795442138620516	0.2488668006386089	0.3739015593393410
0.8811004197276221	0.7531244004422647	0.3741780710928649
0.5703593137536070	0.0021303825098870	0.3173198372239815
0.5698658826443677	0.5021645398863689	0.3176786699742673
0.4319864806277907	0.0032929102193862	0.4120136288261418
0.4368831447468451	0.5040263690166414	0.4108077877217482
0.0665097972862714	0.0005728946513982	0.4099636732933268
0.0684945840498448	0.5020543204300358	0.4060870573659791
0.9369272892753961	0.0013875280982227	0.3161337468505319
0.9379025668229147	0.5012100886943546	0.3166063857660731
0.5843120630075680	0.2498026763905291	0.4406446949334993
0.5867883103678853	0.7529687553840929	0.4421385126293157
0.4252503370887863	0.2516703318630273	0.2842566065891656
0.4259449404305008	0.7518028007554577	0.2842843850794848
0.0808368847805293	0.2512885751496022	0.2817941569762939
0.0795555671753331	0.7513814654693680	0.2822852973230389
0.9290851114823353	0.2585747814722169	0.4391389449105924
0.9215240963736157	0.7505257595582887	0.4411077171205037
0.2263983194642677	0.2461966255793709	0.6039971706532190
0.2111979884640068	0.2426604783775094	0.7613187676107430
0.7280998627831697	0.2424604035992106	0.6065725704415278
0.7126930178787843	0.2426903708836421	0.7608244742638972
0.5311326370579736	0.7401003627113537	0.5411818629182931
0.4709382124832211	0.7461542282161052	0.6803953064882479
0.9936552604703239	0.7389282919345682	0.5369004075191731
0.9752421110111844	0.7461865129507249	0.6804555124615195
0.1158813466761631	0.0190596412081919	0.5062679430530740
0.1189932033703805	0.0063769042993408	0.6491434163432440
0.6169876348863582	0.0041531425772337	0.5004541961797800
0.6189211472058908	0.0043393077053871	0.6499444805652916
0.3326475965996843	0.5233885739477852	0.5659342077143242
0.3235006269371909	0.4961580398204369	0.7149124635788783

0.8050006210884159	0.5237374088354061	0.5621214883493845
0.8237276787422312	0.4971946796709140	0.7142666229201921
0.2615328148508077	0.2301307041432602	0.5339420962379101
0.2284960362716135	0.2476024733077580	0.6701532019934148
0.7414234458887634	0.2482321731668029	0.5222940684143963
0.7280382028576329	0.2468280111744593	0.6700271489040709
-0.0431915215620957	0.7495915827629296	0.5999332615899126
0.4610555855714027	0.7472708484786662	0.6026192141144875
0.4442635324245615	0.7460735083514486	0.7398378078776527
0.9472371874208440	0.7460443947224404	0.7395754812906199
0.2135348686217416	0.7160697728178136	0.5144860565124301
0.2175039148069717	0.7424798734967917	0.6696348708752583
0.7500948663316087	0.7436469979093295	0.5160777318639027
0.7187611877849370	0.7418310884500542	0.6700413882321195
-0.0270458854049301	0.2445798149609671	0.6052303483555190
-0.0506904755175072	0.2460973184876436	0.7405151653140764
0.4754991468787232	0.2414627446960228	0.6051715630308420
0.4501683183299358	0.2463366168713407	0.7412315719208036
0.2153095969486012	0.7432553234547864	0.6124447939294529
0.2099731611802342	0.7473382407252096	0.7613827083161609
0.7130646219289933	0.7404883752472496	0.6136737650393299
0.7143628649533946	0.7478801875832141	0.7614262156181825
-0.0619044097160181	0.2361138366753396	0.5476114513339525
-0.0372799979019061	0.2428906337305836	0.6816705780407911
0.5014544880165973	0.2446813171506117	0.5437360804199303
0.4621596242542317	0.2430383961084088	0.6827582703528241
0.3602493099691224	0.4795429833999355	0.5038125740917339
0.3601089929171202	0.4909906381412481	0.6394095659941574
0.8802383844112950	0.4791538358569835	0.4956694421383533
0.8622478556806392	0.4946852972716436	0.6386667543550684
0.0674231913165572	-0.0039304848486336	0.5804491421074216
0.0640988520774685	0.9978995651147718	0.7230461991682942
0.5638665936844849	0.9941994678137647	0.5832309370475108
0.5637049692047081	0.9961430463719023	0.7236916529424995
0.0540021374026536	0.4990563016389985	0.5859947862894864
0.0634645518292811	0.4949945300357989	0.7241229720116982
0.5584828207371980	0.4934683757220981	0.5863522772578540
0.5631020602214694	0.4972527513826405	0.7247882602583946
0.3332545545682647	-0.0308395663285407	0.5679593815637871
0.3202048191923342	-0.0064856831131355	0.7148003776123283
0.8119379363986952	0.9462620194476645	0.5642412398299705
0.8199900007202603	-0.0071082779499126	0.7138403841412941
0.3576775079299416	-0.0220095053374591	0.5055059985387395
0.3620827373223552	0.0002288411247893	0.6391359333816589

0.8775498713197608	0.0080395337348740	0.4954810012448602
0.8649943556323276	-0.0076052070578170	0.6374719934709633
0.1297099001163966	0.4387897301819246	0.5252710149755044
0.1193123813468102	0.4822264484126318	0.6534598968411873
0.6126695335214131	0.4882534658305946	0.4985034409726068
0.6177784866340091	0.4820288795308942	0.6545060863096953
-0.0138618041678598	0.9915823242974475	0.5361121374563874
-0.0227918429024553	0.9901889545850611	0.6747889826671032
0.4992402048845832	0.9738738615617782	0.5367540448755976
0.4781298258171946	0.9911972683802723	0.6755571439755776
0.2249842680946148	0.4939203623659533	0.6018902333801711
0.2089650005163950	0.4913012893106646	0.7493096409195406
0.7245973928858824	0.4927333948816310	0.6014500659536495
0.7106245983527179	0.4924470199045846	0.7490836047582737
-0.0254223581204280	0.4970160301869008	0.5383705444835694
0.9645735643560372	0.5035016687554513	0.6780363720475673
0.4882619591088679	0.5065551586830029	0.5395920559945447
0.4639746211956540	0.5033959892261540	0.6787691984271939
0.2205128313692998	0.0014317365305535	0.6051882052589187
0.2061659478176951	0.0018959941386905	0.7498776070293272
0.7210402998161330	0.0010744489882845	0.6039954725722951
0.7080333929987942	0.0009471349230735	0.7495998392832446

Ta₃N₅(020)/LaTiO₂N(002)-B

1.0000000000000000

10.7483997344999995	0.0000000000000000	0.0000000000000000
---------------------	--------------------	--------------------

-0.0335853658000000	7.9026285805000001	0.0000000000000000
---------------------	--------------------	--------------------

0.0000000000000000	0.0000000000000000	40.9926986693999993
--------------------	--------------------	---------------------

Ta	N	La	O	Ti
----	---	----	---	----

24	56	16	32	16
----	----	----	----	----

Direct

0.7329337990973721	0.0034704515570121	0.5643159549382207
0.7289175042614594	0.5021019850536173	0.5643553417078903
0.2161822072587603	0.0031317711835044	0.7204567346924102
0.2162138224739104	0.5032614929587624	0.7204172422748855
0.7184037850584415	0.2529130539530079	0.6917072739429138
0.7183131305685195	0.7530558084071980	0.6917587692921848
0.2299967713194924	0.2535386094585009	0.5869422403148280
0.2292467366944071	0.7532050230033631	0.5869849656507686
0.0225285952417171	0.0034755429787181	0.5574769040810043
0.0197423935239350	0.5027894822577597	0.5582523956540006
0.9304701741555655	0.0033381960828070	0.7225538228911367
0.9305532363951773	0.5034409098890041	0.7224598671133290

0.4997626628752316	0.0028298313623304	0.7233575095474422
0.4997172948414175	0.5029378425301980	0.7233314375774146
0.4453231651151952	0.0024179156399068	0.5581648169989594
0.4431170064659561	0.5032129155960969	0.5578407636735367
0.0500158361752707	0.2533802629710487	0.6714220596462610
0.0498821275622770	0.7537080006829403	0.6712431202039759
0.9017967840154667	0.2523358156867219	0.6099050339774406
0.9006943939742821	0.7536743230958016	0.6097881440656816
0.5368993789150827	0.2535999831891992	0.6061829120800808
0.5378519482648357	0.7525849381765259	0.6062657697553325
0.4132579256064500	0.2528860402525459	0.6702144327378406
0.4128031789895378	0.7530048828368433	0.6701404183344465
0.2364097351997675	0.2480736744334715	0.3477200275920758
0.2276743677427997	0.2465430169989843	0.4962742060939557
0.7412141784856411	0.2458450132272798	0.3433799495095726
0.7221160177529525	0.2500921793631072	0.4889652622313551
0.4994980933967805	0.7473549469787657	0.2745227138060120
0.4794857708880390	0.7496183445452479	0.4177911453623850
0.0042070135966016	0.7497883507995717	0.2736125138637175
0.9778629549134858	0.7504946223849482	0.4206609484980216
0.0608869926809914	0.8368697988946284	0.2525412066261422
0.1009408668164766	0.0011561785510611	0.3830301077295160
0.5561652510659981	0.8343727162721849	0.2529001067231783
0.5994175145196132	0.0173211894328787	0.3822710090933855
0.3530884085940293	0.5234869822774759	0.3130479199379861
0.3490264644378123	0.5075427714555549	0.4564243585944409
0.8542175885287870	0.5392088393330576	0.3142314942339962
0.8493613320082539	0.4919125966126395	0.4541766596153474
0.7178137375207599	0.0031391665956539	0.7069613300259090
0.7178850199096197	0.5030849570905390	0.7068663807031428
0.2288217568956445	0.0028537075577590	0.5704488797481925
0.2287608436811993	0.5033456208078471	0.5712344688991069
0.7319835295334296	0.2527853391579570	0.5797071690011003
0.7321647361418204	0.7533204598724574	0.5797052391167314
0.2140992698566516	0.2531654078385154	0.6984019538584862
0.2139676961362595	0.7532356968779997	0.6983096066389821
0.5858044919348960	0.9989699737441914	0.5270773914551509
0.5898446261545407	0.5051305129439178	0.5278137211952936
0.3564664803944502	0.0029074551677740	0.7496987663359402
0.3564273184878767	0.5030100320445251	0.7496728153373662
0.0736291975397325	0.0034061260150407	0.7491304893717919
0.0736108534604553	0.5035916528288951	0.7490635203289275
0.8768488715622778	0.0066225941967486	0.5273771023836425
0.8826711786068837	0.4997841045297282	0.5266460955268749

0.5858953690926122	0.2531626816808347	0.6523929371198802
0.5858950638752044	0.7534410565326263	0.6524868008576955
0.3546479625986752	0.2522960917397513	0.6254846886692970
0.3545227123285344	0.7530796091649609	0.6254752254991804
0.0907458378742505	0.2527342865289575	0.6256673488011943
0.0904827246727004	0.7545781248439174	0.6253751680165810
0.8460714057081069	0.2521139612298061	0.6527391554661344
0.8463330838480257	0.7533740039343554	0.6527321136466419
0.5705176230873499	0.0032658752598103	0.5961014150985310
0.5721756264005420	0.5030626137484898	0.5962188402766363
0.3948441923703762	0.0028355600340537	0.6836895901423802
0.3947610964484516	0.5029424615312199	0.6836645196286417
0.0341435027740287	0.0031992280741850	0.6829105877300873
0.0341497464538971	0.5034572146867250	0.6827848362463318
0.9025045230191103	0.0030230810963536	0.5949664176073365
0.9029304377783044	0.5031357662651647	0.5954935163609945
0.5408109939523233	0.2530297863126555	0.7172172309402419
0.5410348127353701	0.7529982014187269	0.7172995332511651
0.4059682097289054	0.2525046611211416	0.5600920375394394
0.4069386167166936	0.7529196563102286	0.5606679720948684
0.0554885267481102	0.2534457793090488	0.5606206478711487
0.0548471001811351	0.7530556987758503	0.5595058644962071
0.8932856711644194	0.2532839385049245	0.7160113194884763
0.8932441968624022	0.7532995815729642	0.7159833131495263
0.2494997127009574	0.2596234715225731	0.2828965554000860
0.2418990924998075	0.2611978150791751	0.4194622459726586
0.7532271603314621	0.2646230963076708	0.2804292434902709
0.7355869190770089	0.2495205524490020	0.4240613478962986
0.9892977899839333	0.7395844758010293	0.3553038969240976
0.4952346254465402	0.7503180478176946	0.3526301876749778
0.4957738423129999	0.7508475213790432	0.4880757158744820
0.9698104854510000	0.7568393055223834	0.4871939434819406
0.2672185547229438	0.7147733606526065	0.2667414295534613
0.2385729188813269	0.7548021868106172	0.4190736987901099
0.7608213923691789	0.7265419558520806	0.2718656589174194
0.7370559441370310	0.7466010743287768	0.4230474288264228
0.9931098066980634	0.2464751084882917	0.3535602108836049
0.9786533679794800	0.2543717034043488	0.4872153051967397
0.4972212837853134	0.2589074873172146	0.3523311315951427
0.4883968133107732	0.2570906259348932	0.4890126308926126
0.2625489867915468	0.7479353230043466	0.3620868308177183
0.2411384683254983	0.7524746578946528	0.5015058913433837
0.7527187856078484	0.7442283956760751	0.3651721210369567
0.7417026206341408	0.7528492187925918	0.4909907586940608

0.0079224687389975	0.2414614620025522	0.2932376947263906
0.0172130271029608	0.2495677564721210	0.4288946570362138
0.5184822793588939	0.2394072303715430	0.2915836856959209
0.4936060983291305	0.2472438608136951	0.4305889372205173
0.3800991805483484	0.4618011097252505	0.2485302677927097
0.3827872640873248	0.4622517574438513	0.3846437826607507
0.8812645337138828	0.4676838405342374	0.2500484463653335
0.8869251277584443	0.4615172547903699	0.3842486374599808
0.1505115480763323	0.9581313075611748	0.3113713967492590
0.1274706609692629	0.9721515622888710	0.4565590910993240
0.6484197875152333	0.9403273714578628	0.3123189574671790
0.6279325532302928	0.9758405527306017	0.4528261892586314
0.0917452704570888	0.5210040713963389	0.3278663288737766
0.0899861418323368	0.5211939660348227	0.4674221364706400
0.5941246598714698	0.5242335914188259	0.3262806906126619
0.6001476473589251	0.5258800430476467	0.4594705401988159
0.4058464190055902	0.9907623367096117	0.3283921229929042
0.3845237702378754	0.9940134352988428	0.4676835649009275
0.9044209830923945	0.9710659244355249	0.3278314546032977
0.8769254687394484	0.0091856131936549	0.4602553627189388
0.3409431544742626	0.0153328324681512	0.2611678923709007
0.3425112052720204	0.0279689424834390	0.3959263406256482
0.8420403470120734	0.0144168317773247	0.2609772129046650
0.8494972976642512	0.0426515148669991	0.3927273417773371
0.1459108852664123	0.4793374909088370	0.2592517331346440
0.1415759038860578	0.5014561123795814	0.3969997473926400
0.6466377103568238	0.4877199266901561	0.2579443536155760
0.6340758273046315	0.4713820548767694	0.3937947240821250
0.9871833092611980	0.0020647410251464	0.2851877011259902
0.9910214551502901	0.9978625129461705	0.4191752678233490
0.4862427422736949	0.0024005976540575	0.2848954529812693
0.4970880166326562	0.9987164071968451	0.4187363211988478
0.2484999667083080	0.5014224826541026	0.3489731753815925
0.2403341256790249	0.5035802797651331	0.4906977611361372
0.7477861685890491	0.4984574051476696	0.3491368539606907
0.7365728417167653	0.4941296418500297	0.4937159664418139
0.9954658054175489	0.4863425844896158	0.2815399293267810
0.9820888671744009	0.5052556511275236	0.4232200335366196
0.4964150135042454	0.4812409156701346	0.2797228197872869
0.4899557230789084	0.5097382684874292	0.4215888626808340
0.2386080752849777	0.0056211187592616	0.3505756852942242
0.2374674202339024	0.0031437658768476	0.4913287583619390
0.7397666322364960	0.0069359170823370	0.3503542302845342
0.7357329910370316	0.0103245447435119	0.4943080860196956

