Z-Scheme versus Type-II Junction in g-C_3N_4/TiO_2 and g-C_3N_4/$SrTiO_3$/TiO_2 Heterostructures

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Supporting Information

S1 g-C_3N_4 monolayers

Table S1: Fractional atomic coordinates of flat g-C_3N_4 monolayer model. The lattice parameters are reported in the main text and in the first row. Atoms are reported as following: 6C, 8N.

a = 7.070 Å	*b* = 7.070 Å	*c* = 50.5 Å
0.2656957587196013	0.1552328928416662	0.0518100000000032
0.2547521743718770	0.4711845154726760	0.0518100000000032
0.2546972977521333	0.8283249433141634	0.0518100000000032
0.6119361026251114	0.8283426094879971	0.0518100000000032
0.9278222557374131	0.8173534124708075	0.0518100000000032
0.9278491034334427	0.1552442308870621	0.0518100000000032
0.0404621999017804	0.0426162149216987	0.0518100000000032
0.0390426973193146	0.3706589692826556	0.0518100000000032
0.0389942839224328	0.7131163231469421	0.0518100000000032
0.3699031732912905	0.0440329561522854	0.0518100000000032
0.3737948528803666	0.7092859818447893	0.0518100000000032
0.7124436692709079	0.0440439275373339	0.0518100000000032
0.3699294161485489	0.3706502703252353	0.0518100000000032
0.7124070146257565	0.7131227523146955	0.0518100000000032

Table S2: Fractional atomic coordinates of corrugated g-C_3N_4 monolayer model. The lattice parameters are reported in the main text and in the first row. Atoms are reported as following: 6C, 8N.

a = 6.877 Å	*b* = 6.877 Å	*c* = 30.24 Å
0.0920052282792464	0.5821613430081070	0.9852614808628016
0.7419661029064573	0.9054368764828559	0.0073051086664166
0.0967760836520577	0.9032239163479429	0.0000000000000000
0.4281346095150259	0.5718653904849740	0.0000000000000000
0.4178386569918931	0.9079947717207535	0.0147385191371983
0.0945631235171441	0.2580338970935422	0.9926948913335836
0.6387202636645082	0.0187217702526972	0.0187817732364113
0.0045933105434918	0.7130996865831856	0.9772338638679401

0.3143188690873339	0.3529918137281671	0.9961030709836985
0.9751196539014917	0.0248803460985086	0.0000000000000000
0.3121173685054067	0.6878826314945861	0.0000000000000000
0.9812782297473027	0.3612797363354919	0.9812182267635888
0.2869003134168143	0.9954066894565085	0.0227661361320597
0.6470081862718329	0.6856811309126659	0.0038969290163015

Table S3: Fractional atomic coordinates of corrugated (1-x2) g-C_3N_4 monolayer model. The lattice parameters are reported in the main text and in the first row. Atoms are reported as following: 12C, 16N.

a = 6.832 Å	*b* = 13.332 Å	*c* = 50.72 Å
0.4806167042707388	0.5900912303493672	0.5380132992256884
0.4883088576284274	0.7587411559280794	0.5323515464021634
0.4879443281784559	0.9378873369446178	0.5287367861995053
0.8480999136977778	0.9441633837643479	0.5211850378613249
0.1719545843016396	0.9407498850101957	0.5200513260000180
0.1709850434389356	0.6136781622452031	0.5513077547496497
0.4802801462992045	0.0900235099899123	0.5448134049846944
0.4883597466798803	0.2588377252002755	0.5504612158524850
0.4884824677703165	0.4381398629535614	0.5540690602683175
0.8485881537939951	0.4443853635654890	0.5616073578853236
0.1725204455562933	0.4410500436414476	0.5627383177078966
0.1706939315919714	0.1135590705716203	0.5314941960488678
0.2748395511161535	0.5477488481268930	0.5503204579434421
0.2947516842101593	0.7257646643995269	0.5443900904352927
0.3011262989589077	0.8958677950156430	0.5151393806000344
0.5732628508676336	0.5239990491651331	0.5378042454099351
0.6105725584737934	0.8783950803230186	0.5253166111229652
0.9542915312529263	0.5607983401529095	0.5582597138872617
0.5783797043516554	0.6942165903394556	0.5272971382239638
0.9516601012059243	0.8877320789007275	0.5146039671380619
0.2744545902977342	0.0475977772648567	0.5324848572107304
0.2947352609900991	0.2257643561015900	0.5384069743289799
0.3018000064775659	0.3962798712399267	0.5676567054003584
0.5728618946023266	0.0239057027342709	0.5450196615879876
0.6110008280834621	0.3786260655927006	0.5574773285907191
0.9538693362434029	0.0606135832272963	0.5245520317527773
0.5782093209350450	0.1942882040252117	0.5555456543324941
0.9522410927982827	0.3880290153367461	0.5681638272252937

S2 TiO_2 (001) and (101) surface models

Table S4: Fractional atomic coordinates of TiO_2 (001) surface model. Atoms are reported as following: 10Ti, 20O.

a = 3.690 Å	*b* = 3.822 Å	*c* = 50.560 Å
0.8750000161199480	0.3749999516401630	0.4991784707273216
0.8750000161199480	0.8750000161199480	0.4530788614238114

0.3749999516401630	0.8750000161199480	0.4033957318183706
0.3749999516401630	0.3749999516401630	0.3564873814444304
0.8750000161199480	0.3749999516401630	0.3069263126826495
0.8750000161199480	0.8750000161199480	0.2600040893173475
0.3749999516401630	0.8750000161199480	0.2104430205555737
0.3749999516401630	0.3749999516401630	0.1635346721816265
0.8750000161199480	0.3749999516401630	0.1138515425762000
0.8750000161199480	0.8750000161199480	0.0677519332726756
0.3749999516401630	0.3749999516401630	0.5099565758960302
0.8750000161199480	0.8750000161199480	0.4915558751084002
0.8750000161199480	0.3749999516401630	0.4611858220560811
0.3749999516401630	0.8750000161199480	0.4434952992350481
0.8750000161199480	0.8750000161199480	0.4128378815612019
0.3749999516401630	0.3749999516401630	0.3953148292413720
0.3749999516401630	0.8750000161199480	0.3645554398079763
0.8750000161199480	0.3749999516401630	0.3470622886703517
0.3749999516401630	0.3749999516401630	0.3163495084999802
0.8750000161199480	0.8750000161199480	0.2988354837143187
0.8750000161199480	0.3749999516401630	0.2680949202856855
0.3749999516401630	0.8750000161199480	0.2505808955000169
0.8750000161199480	0.8750000161199480	0.2198681153296455
0.3749999516401630	0.3749999516401630	0.2023749641920208
0.3749999516401630	0.8750000161199480	0.1716155747586324
0.8750000161199480	0.3749999516401630	0.1540925224388023
0.3749999516401630	0.3749999516401630	0.1234351047649491
0.8750000161199480	0.8750000161199480	0.1057445819439162
0.8750000161199480	0.3749999516401630	0.0753745288916040
0.3749999516401630	0.8750000161199480	0.0569738281039740

Table S5: Fractional atomic coordinates of (2x1) TiO_2 (101) surface model. Atoms are reported as following: 48Ti, 96O.

a = 7.288 Å	*b* = 10.295 Å	*c* = 65 Å
0.150164	0.44091	0.699625
0.400164	0.940861	0.698508
0.150164	0.710855	0.689565
0.400164	0.210904	0.690682
0.150164	0.571608	0.645396
0.400164	0.071658	0.646512
0.150164	0.848975	0.632665
0.400164	0.349025	0.633781
0.150164	0.703447	0.590549
0.400164	0.203497	0.591666
0.150164	0.982756	0.576949
0.400164	0.482805	0.578066
0.150164	0.83539	0.535245
0.400164	0.33544	0.536362
0.401172	0.607734	0.522291
0.159596	0.969308	0.480591
0.408985	0.469941	0.480378

0.159751	0.243003	0.466235
0.408819	0.739221	0.466356
0.168271	0.092616	0.425453
0.414488	0.601698	0.423372
0.168297	0.362691	0.410485
0.42038	0.873655	0.410722
0.650164	0.44091	0.699625
0.900164	0.940861	0.698508
0.650164	0.710855	0.689565
0.900164	0.210904	0.690682
0.650164	0.571608	0.645396
0.900164	0.071658	0.646512
0.650164	0.848975	0.632665
0.900164	0.349025	0.633781
0.650164	0.703447	0.590549
0.900164	0.203497	0.591666
0.650164	0.982756	0.576949
0.900164	0.482805	0.578066
0.650164	0.83539	0.535245
0.900164	0.33544	0.536362
0.651239	0.110626	0.521878
0.901213	0.607643	0.522552
0.657303	0.968849	0.479911
0.90849	0.466846	0.480598
0.658065	0.239884	0.467108
0.908712	0.740437	0.468018
0.671528	0.099538	0.423177
0.9232	0.593544	0.425059
0.662967	0.367138	0.413225
0.920197	0.862052	0.414852
0.151171	0.112078	0.521724
0.150164	0.59858	0.71234
0.400164	0.098629	0.713457
0.150164	0.89061	0.70171
0.400164	0.390659	0.702827
0.400164	0.751334	0.690184
0.150164	0.251383	0.691301
0.150164	0.531558	0.675526
0.400164	0.031509	0.674409
0.150164	0.74387	0.657765
0.400164	0.24392	0.658882
0.150164	0.030922	0.642587
0.400164	0.530971	0.643704
0.400164	0.887337	0.634478
0.150164	0.387387	0.635594
0.150164	0.672168	0.620708
0.400164	0.172218	0.621825
0.150164	0.879792	0.602138
0.400164	0.379841	0.603254
0.150164	0.164288	0.589592
0.400164	0.664238	0.588475

0.400164	0.021424	0.579067
0.150164	0.521473	0.580183
0.150164	0.805377	0.565461
0.400164	0.305427	0.566577
0.150164	0.012769	0.546728
0.400164	0.512818	0.547845
0.150164	0.296771	0.53424
0.400164	0.796721	0.533123
0.401134	0.157735	0.523473
0.151159	0.653952	0.523983
0.154244	0.939499	0.510666
0.402939	0.438135	0.511362
0.153721	0.144869	0.491349
0.404774	0.642861	0.491433
0.158846	0.422097	0.479329
0.408002	0.924378	0.478701
0.409043	0.288688	0.467621
0.159589	0.786776	0.467909
0.165785	0.06847	0.455835
0.413957	0.568157	0.455439
0.169057	0.272943	0.435666
0.41598	0.773587	0.435279
0.171616	0.538863	0.42459
0.423019	0.046688	0.423803
0.417789	0.417472	0.40746
0.16455	0.921946	0.409789
0.162128	0.1846	0.401503
0.396477	0.703352	0.399543
0.650164	0.59858	0.71234
0.900164	0.098629	0.713457
0.650164	0.89061	0.70171
0.900164	0.390659	0.702827
0.900164	0.751334	0.690184
0.650164	0.251383	0.691301
0.650164	0.531558	0.675526
0.900164	0.031509	0.674409
0.650164	0.74387	0.657765
0.900164	0.24392	0.658882
0.650164	0.030922	0.642587
0.900164	0.530971	0.643704
0.900164	0.887337	0.634478
0.650164	0.387387	0.635594
0.650164	0.672168	0.620708
0.900164	0.172218	0.621825
0.650164	0.879792	0.602138
0.900164	0.379841	0.603254
0.650164	0.164288	0.589592
0.900164	0.664238	0.588475
0.900164	0.021424	0.579067
0.650164	0.521473	0.580183
0.650164	0.805377	0.565461

0.900164	0.305427	0.566577
0.650164	0.012769	0.546728
0.900164	0.512818	0.547845
0.650164	0.296771	0.53424
0.900164	0.796721	0.533123
0.900981	0.157437	0.523615
0.650951	0.653784	0.523965
0.65309	0.939382	0.510662
0.904374	0.437099	0.511474
0.656401	0.14443	0.491503
0.905413	0.641427	0.492105
0.65828	0.422196	0.479659
0.908747	0.923192	0.478951
0.908594	0.28942	0.466988
0.65747	0.786924	0.46842
0.661027	0.06963	0.455578
0.912468	0.566654	0.45614
0.654378	0.275692	0.436437
0.905124	0.774056	0.438331
0.663885	0.555154	0.423185
0.915608	0.049699	0.425455
0.91469	0.419043	0.41014
0.677595	0.914542	0.409482
0.679438	0.207793	0.400643
0.955945	0.703395	0.403567

Table S6: Fractional atomic coordinates of $SrTiO_3$ (001) surface model. Atoms are reported as following: 5Sr, 6Ti, 17O.

a = Å	*b* = Å	*c* = 50.560 Å
0.4939000321069564	0.4939000321069564	0.4139023974687427
0.4949703079089783	0.4949703079089783	0.3332221972284379
0.4956336094199208	0.4956336094199208	0.2543059999999997
0.4949703079089783	0.4949703079089783	0.1753898027715610
0.4939000321069564	0.4939000321069564	0.0947116025312516
0.9874575053701030	0.9874575053701029	0.4485223552270958
-0.0080763105316143	-0.0080763105316143	0.3715813878415665
-0.0054374208500386	-0.0054374208500386	0.2934760294830372
-0.0054374208500386	-0.0054374208500386	0.2151379705169638
-0.0080763105316143	-0.0080763105316143	0.1370306121584329
0.9874575053701029	0.9874575053701029	0.0600896447729034
0.5094576313139828	0.0098294192074742	0.4504070383793144
0.0098294192074742	0.5094576313139828	0.4504070383793144
0.0034735512469244	0.0034735512469244	0.4113925951147268
0.5037294332863256	0.0060805224113316	0.3719422707768223
0.0060805224113316	0.5037294332863256	0.3719422707768223
0.0019929915622828	0.0019929915622828	0.3327862079924270
0.5015345301683160	0.0027054653287902	0.2935548403225508

0.0027054653287902	0.5015345301683160	0.2935548403225508
0.0012301438037725	0.0012301438037725	0.2543059999999997
0.5015345301683160	0.0027054653287902	0.2150591596774506
0.0027054653287902	0.5015345301683160	0.2150591596774506
0.0019929915622828	0.0019929915622828	0.1758257920075724
0.5037294332863256	0.0060805224113316	0.1366697292231771
0.0060805224113316	0.5037294332863256	0.1366697292231771
0.0034735512469244	0.0034735512469244	0.0972214048852676
0.5094576313139828	0.0098294192074742	0.0582049616206845
0.0098294192074742	0.5094576313139828	0.0582049616206845

S3 g-C_3N_4/TiO_2 interface model

Table S7: Fractional atomic coordinates of g-C_3N_4/TiO_2 interface model. Atoms are reported as following: 12C, 16N, 60Ti, 120O.

a = 7.381 Å	b = 13.635 Å	c = 50 Å
0.4716069733467858	0.5927709002647824	0.5331162577545469
0.4857293317917050	0.7614589322650582	0.5291559612853788
0.4848532684790638	0.9400501719665532	0.5271013430044122
0.8533508506318110	0.9414950281760610	0.5239033721537925
0.1602689396680320	0.9314112585086204	0.5232646725945107
0.1732501659888645	0.6096127432311675	0.5455822887828561
0.4848828103571890	0.0982664323342906	0.5408837790389481
0.4924556355277834	0.2650309306016049	0.5463393067478624
0.4813475620809990	0.4414744382310802	0.5499147511712974
0.8536582689456389	0.4441064448579282	0.5549163721064271
0.1624295648908216	0.4354209438933425	0.5562145303085888
0.1752347641697664	0.1093041006141360	0.5316604926510398
0.2681369646230627	0.5446960244717811	0.5443698831891225
0.3022170053293790	0.7233269790414195	0.5419725158279425
0.2789925269434534	0.8852202422371658	0.5175180768930500
0.5709333980739988	0.5349474130010692	0.5345245447745888
0.6120868836519988	0.8825814612084105	0.5245811146764982
0.9636152142081300	0.5578836070492980	0.5503635166415018
0.5612234389047414	0.6963143380045947	0.5214210680571028
0.9445360347261308	0.8792757369746900	0.5208632564823601
0.2712262886733198	0.0446419779323751	0.5330487344222006
0.2962102726532641	0.2224043299729053	0.5364318424850629
0.2858609754070913	0.3911029720405587	0.5615286327440822
0.5838057150059428	0.0399018029725138	0.5397857111860608
0.6126887075090850	0.3844299739017281	0.5530450930445596
0.9656805985064266	0.0568542796696025	0.5259242618656782
0.5873135022086269	0.2064444939263456	0.5494346387142748
0.9504048581810322	0.3861685048729263	0.5612484921388099
0.2968320326132374	0.4042627652256353	0.4630177219949291
0.1546032854707453	0.7405098500982740	0.4631032197959553
0.4645909442803931	0.0725464252920681	0.4617194321665629
0.7984725097020796	0.4055978249643828	0.4625062647426353
0.6534417169621671	0.7370758929742180	0.4640920756173191

0.9609903082583047	0.0719102617514907	0.4629060082918368
0.1378002976285122	0.2382626737946760	0.4164253334952960
0.4718999609977249	0.5725684756364627	0.4167810110330587
0.3028998025586241	0.9039970091720128	0.4160565371966728
0.6391611301327021	0.2394494483227559	0.4160133502116557
0.9724906368811143	0.5729758692881355	0.4165342612499722
0.8023547214764291	0.9032714512467769	0.4169334978311796
0.2195959050231500	0.5705916635072185	0.3664314381950977
0.3856457293068724	0.2376138306425114	0.3662183675158487
0.7192831191427138	0.5707016183475047	0.3664245744312947
0.5534961899593729	0.9037909722268803	0.3664126405468620
0.8862167173589038	0.2374922187229712	0.3661786407887951
0.0520083009389106	0.9038802310666048	0.3663813200828693
0.2195460687776124	0.0702405520752741	0.3189511516244560
0.5526856543078420	0.4039038698146732	0.3188952021963423
0.3850795433678908	0.7371684348734378	0.3189517244170583
0.7194986311871512	0.0701452997669648	0.3189578346828827
0.0528493504144534	0.4039859762857288	0.3188791762354293
0.8850859506633395	0.7372415121870922	0.3189569586345351
0.3024370165634044	0.4038689886871727	0.2688502857414886
0.1353001199334141	0.7374557202686373	0.2689053196556110
0.4697852333940681	0.0706012675319955	0.2688793282102769
0.8024309566971335	0.4038853279239745	0.2688652770754643
0.6352454332709980	0.7373941691748639	0.2689034904197035
0.9697357412038107	0.0705781066633446	0.2688731880384897
0.1354758898308946	0.2375688204086963	0.2215076639206212
0.4677388923306295	0.5708713193370063	0.2215387071400601
0.3021977337605788	0.9039816971970055	0.2214976075800302
0.6353914833473676	0.2375021820938646	0.2215119766974191
0.9676166199140520	0.5707721805056949	0.2215469012866722
0.8022925559281160	0.9040784507657958	0.2215062113796279
0.2181602394089102	0.5710792830759416	0.1715271240012046
0.3855809965259570	0.2377932529689506	0.1714967172131431
0.7181714520394077	0.5710931145786251	0.1715204465041268
0.5519144794028238	0.9041628968576230	0.1715166582678544
0.8855653004506114	0.2377878753093801	0.1715016644332763
0.0518809269542239	0.9041607408175980	0.1715170794071427
0.2158306219984138	0.0712679153633642	0.1243206363486786
0.5502840883405731	0.4045583186040473	0.1242764602638112
0.3838361387119470	0.7379691304856644	0.1242651218520181
0.7158646320484272	0.0713034131684745	0.1243219415490781
0.0503127527823838	0.4045971178436580	0.1242784247067687
0.8838219111727863	0.7379328484758961	0.1242607123133826
0.3011224978906691	0.4042920493633319	0.0743406940775588
0.1351095690994767	0.7379108460818751	0.0743310385530613
0.4675768917145010	0.0711872803223904	0.0743176680458909
0.8011241509753660	0.4042763006863912	0.0743409251761614
0.6350953070181324	0.7379102340427236	0.0743391142517959
0.9675896155912855	0.0712052189516600	0.0743082410151837
0.1316794581886871	0.2380794579644680	0.0280103428151959
0.4640553387065058	0.5713312159914711	0.0281080774272029

0.2987455054668644	0.9045308217512075	0.0280287653288338
0.6316964059478929	0.2380878379259194	0.0280134444632634
0.9640522570855098	0.5713350963757984	0.0281083991411025
0.7986895326120984	0.9044818388861813	0.0280254047045910
0.2340325497841240	0.0727318906193803	0.4743915824884793
0.5646854464563652	0.4033269746100860	0.4742981029616131
0.3882991186480773	0.7384354652780277	0.4739232927651055
0.7247167335436093	0.0708032052957850	0.4735732925556388
0.0659037388843531	0.4051825612041694	0.4751253569134385
0.8921597696587118	0.7367556734157427	0.4724698746255079
0.1466296701253838	0.2377714127421030	0.4554456759870742
0.4769513174213855	0.5708946908894905	0.4557988930731185
0.3115533332445858	0.9060674554678606	0.4546166330953306
0.6511575026103655	0.2390083276742966	0.4548545449456048
0.9797730115949822	0.5716767951587778	0.4552664366245925
0.8111351659972220	0.9050240949848422	0.4560016823801923
0.2954823242366972	0.4048441228014542	0.4247762100452786
0.1428503738225687	0.7385863504179164	0.4243908525949805
0.4619377934958074	0.0724611809710482	0.4235886344736182
0.7967066975974995	0.4055934981652757	0.4242083050174527
0.6393405794024254	0.7380277316477275	0.4253430386477665
0.9624938533506405	0.0712378381758448	0.4247395369731153
0.2214572966912886	0.5719884295209030	0.4068648243271339
0.3871871482447852	0.2398738534986679	0.4067562773139176
0.7212580603287696	0.5727500486623323	0.4069612053896635
0.5547022691681324	0.9051346900071379	0.4068528803898613
0.8875929873020358	0.2390446039607602	0.4066958290876612
0.0516614285520262	0.9037760285444633	0.4068729970965903
0.1348081761226707	0.2364283981015589	0.3758407189280146
0.4694857888711337	0.5704884341281219	0.3760690877273393
0.3023658402450259	0.9035160112488492	0.3756627217725475
0.6358872244174479	0.2374843812706150	0.3756394143689021
0.9692115736332267	0.5704127972366588	0.3758742715787357
0.8023221148588846	0.9034280285491083	0.3760986764783584
0.2192820121848219	0.0705560518670380	0.3581743589397657
0.5516920578042970	0.4039606856891568	0.3581447995304698
0.3862958898613817	0.7372113434811617	0.3581963656305799
0.7195360309036469	0.0705191550551544	0.3581581562464675
0.0530858854046020	0.4039946715086257	0.3581271887488933
0.8856122149641512	0.7372924439791815	0.3581888379161507
0.2191382052377933	0.5706086767605720	0.3271371733189645
0.3857533685988341	0.2372587464060603	0.3270527792320861
0.7190779121205356	0.5705943319179330	0.3271546103078503
0.5531534686052663	0.9037975649398868	0.3271279222269725
0.8861123685230833	0.2372730284366029	0.3270283705418838
0.0517666290403258	0.9038617572950265	0.3271172054516169
0.3025895580587969	0.4039088540669005	0.3093756399111455
0.1355303270104859	0.7374267024422692	0.3094419203729986
0.4693834853312049	0.0702414220116736	0.3094362801784905
0.8024354189723326	0.4037796221313351	0.3094032610727731
0.6351626420309799	0.7370349237311686	0.3094188357587717

0.9697734794651560	0.0706143980243348	0.3094042829395009
0.2198304921132189	0.0707018478883046	0.2783677844398286
0.5525845490595224	0.4040481127229729	0.2783404402291615
0.3855770381672454	0.7375065035964747	0.2783816000215921
0.7197742780399796	0.0706681549424901	0.2783730838969247
0.0525669600076475	0.4040194224004375	0.2783328981561931
0.8855731132419453	0.7374983475713939	0.2783905454184895
0.1361431909870708	0.2373636054051912	0.2607118076052672
0.4689377084424471	0.5707303961744177	0.2607130556221817
0.3026475654104835	0.9040584331646239	0.2607139413710983
0.6361077558807546	0.2373499760148818	0.2607169838545887
0.9688916060431869	0.5707169925769988	0.2607373117530886
0.8027092493935029	0.9040615964923882	0.2607166938163926
0.3015801122246429	0.4040632927648450	0.2296331464059181
0.1349550256232101	0.7374107218103156	0.2296659960100555
0.4687917178379238	0.0707160808705778	0.2296510803291476
0.8015175614904964	0.4040285979804056	0.2296527323098548
0.6350003966721506	0.7374466066995059	0.2296608925399151
0.9688188811108958	0.0707546168011624	0.2296375353989843
0.2178175444825095	0.5707008458192699	0.2120257646575940
0.3852825807732994	0.2374695842875317	0.2119891664994941
0.7178285191835204	0.5707014913449108	0.2120241620482779
0.5519197234754817	0.9038907394580918	0.2120055518667255
0.8852286881163309	0.2374766867210683	0.2119915202941259
0.0519059875883704	0.9038992442792817	0.2120013636216481
0.1355313613836651	0.2378625739930557	0.1809492557946858
0.4682539864758540	0.5711239453255560	0.1809735215442055
0.3021461673743340	0.9043485923618994	0.1809488664671299
0.6355392545469540	0.2378840006846613	0.1809343867442997
0.9682734383350557	0.5711555108342686	0.1809877946529916
0.8021691527867586	0.9043839667045570	0.1809518939297574
0.2184953390243125	0.0710759924260698	0.1634739620276228
0.5520130477328963	0.4044603538370573	0.1634452081266127
0.3851328629531265	0.7376931840328660	0.1634645635036741
0.7185036488547502	0.0710770586211181	0.1634758091832616
0.0520245311071304	0.4044708619227292	0.1634484308097550
0.8851577046994852	0.7376904331918882	0.1634656801735619
0.2165768460979685	0.5711317825919388	0.1323018935915621
0.3829509747784263	0.2377792152124404	0.1322932351256952
0.7166195214871144	0.5711234880688388	0.1323003483400068
0.5495809868368202	0.9043554664682710	0.1323257453329792
0.8829241331941304	0.2377977475910094	0.1322989937443595
0.0495972230565725	0.9043435142350810	0.1323257503524207
0.2997231639314065	0.4042067025265070	0.1148357540807947
0.1333564295139089	0.7376188734040723	0.1148377249020067
0.4657707868253301	0.0708156912465160	0.1148491452202263
0.7997410859159868	0.4042275661004496	0.1148354583610488
0.6333484646985509	0.7376034554631152	0.1148440761132022
0.9657667312595469	0.0708144743207231	0.1148492876684857
0.2160900419199122	0.0714546408225419	0.0838648984205911
0.5496118086703525	0.4046284957026223	0.0838484497359086

0.3834097889406786	0.7381701710160132	0.0838478891587482
0.7161193445279815	0.0714753357732389	0.0838694137553974
0.0496189933210272	0.4046263756100563	0.0838491174174339
0.8834204270667162	0.7381683833146778	0.0838408904312334
0.1237937082934597	0.2379230490963158	0.0663341415023192
0.4569287276190824	0.5712031713490898	0.0664191587605076
0.2906791392446386	0.9045835139410221	0.0663474172473916
0.6238064802927336	0.2379340876314928	0.0663420945005914
0.9569564135503561	0.5712086473100408	0.0664165807398477
0.7906615581316950	0.9045689706662049	0.0663386722974567
0.3187612767085072	0.4046022201567117	0.0355474675344732
0.1524595492767315	0.7379031402760555	0.0355630393243648
0.4858715844227051	0.0712694580989288	0.0355443697872657
0.8187885911414253	0.4046111696463330	0.0355496741458824
0.6524160897870218	0.7378760082462462	0.0355650402671350
0.9858602684463221	0.0712551863162464	0.0355373188080227
0.2340580848838234	0.5713381698641763	0.0164298216983656
0.4012797151889987	0.2378993827858729	0.0163615087979044
0.7340461573582325	0.5713376237958996	0.0164313444386541
0.5681707508812588	0.9045707160231280	0.0163800463110292
0.9012664200780153	0.2378913146114705	0.0163615428511671
0.0681843179861148	0.9045666414177554	0.0163781064324507

S4 g-C_3N_4/$SrTiO_3$/TiO_2 interface model

Table S8: Fractional atomic coordinates of g-C_3N_4/$SrTiO_3$/TiO_2 interface model. Atoms are reported as following: 12C, 16N, 30Sr, 96Ti, 222O.

a = 7.662 Å	*b* = 13.817 Å	*c* = 60 Å
0.4332327412116360	0.1788737786499328	0.2065889993573469
0.4537340410992992	0.3478591510897265	0.2068054474811027
0.4429149627483095	0.5233750893217402	0.2089854964046337
0.8260402861788151	0.5255981772748928	0.2120605387392422
0.1208007711210070	0.5117463543220940	0.2093486835121789
0.1418615785229775	0.1899197800582240	0.1953108218881198
0.4565630675864522	0.6903250234080406	0.2050919900464160
0.4619252206690924	0.8539658521477647	0.2011053071590053
0.4344838631792377	0.0223077106839901	0.1950873899912001
0.8222382857849654	0.0235764177413120	0.1906481259500760
0.1186420389256634	0.0112343600243831	0.1899250306531812
0.1507424024205820	0.6957451235171470	0.2115171608692216
0.2300319320612671	0.1254058229210749	0.1978198782173327
0.2737990864198335	0.3036236593225417	0.1957673630367562
0.2276809866987719	0.4606802859848893	0.2106980730767842
0.5298672253607788	0.1224489692410048	0.2062382435871416
0.5769954677475843	0.4690073559041155	0.2097663422981269
0.9348589936356583	0.1376864023660837	0.1923390671860262
0.5251669175067679	0.2867240913223751	0.2148594784308498
0.9078661243833891	0.4637326306940183	0.2079881814949427
0.2408525558704916	0.6319196232747010	0.2080797250314085

0.2663203912624659	0.8080828687838603	0.2086212249316667
0.2363396726052903	0.9651089970432752	0.1867805596599965
0.5562091999042718	0.6352464442671180	0.2057381834384991
0.5728954430582948	0.9664728590529778	0.1934642166007321
0.9455837744762235	0.6398603827058049	0.2179093515722262
0.5616401082060449	0.8009318548655463	0.2010379937446125
0.9093902617612559	0.9620020728272013	0.1864341823926379
0.2445242704931122	0.2237491214165641	0.5635830395165639
0.7449002105137654	0.2240389928188558	0.5628793606020923
0.0838222737578418	0.5632693235794562	0.5615625335490786
0.5838716519301231	0.5632679507363652	0.5622021563648496
0.4045750806647510	0.8842172891207112	0.5634773535674882
0.9053975791382745	0.8850612750892148	0.5645104809676365
0.2389998509383827	0.2138791488053575	0.4955198632518794
0.7381672694619037	0.2144139164646442	0.4966005657716338
0.0679284433608168	0.5453501654442121	0.4943384467149874
0.5665474488617890	0.5452847307739208	0.4927308491112850
0.4007836846730941	0.8781324211250736	0.4951631501792710
0.9018663169717670	0.8798135187129769	0.4935186685172418
0.2252119661106331	0.2006170803323889	0.4282922292191601
0.7255656312787798	0.2004367549607463	0.4266589862872367
0.0537371323673437	0.5311080040780858	0.4240643432666455
0.5560185559255647	0.5319925891207078	0.4260694656840207
0.3930505385251420	0.8690066765143604	0.4246383730290797
0.8911893854019634	0.8665670572351581	0.4268895815023852
0.2132257931010604	0.1870884124693840	0.3581019792845190
0.7108355356147079	0.1881062471923174	0.3600075370210276
0.0403556230456880	0.5168755252363633	0.3575119028984559
0.5396837660081149	0.5162913018606151	0.3558039903958880
0.3782270306079876	0.8540779958327189	0.3589371344352250
0.8819681833747683	0.8564100572561554	0.3568012619558373
0.1971357405501565	0.1738454611119971	0.2908092932250545
0.6969019286239906	0.1732758759864075	0.2886810638088051
0.0214863381592982	0.5020873709770981	0.2870450938554686
0.5278695338166444	0.5001801324688011	0.2888468525656936
0.3681939442758278	0.8473409558462003	0.2883724261955387
0.8751579294506657	0.8423309137484178	0.2921970416536609
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000261020148	0.0000000000000000	0.9999999983335073
0.3333399273606119	0.3333886854941710	0.0003535114467397
0.8333399534626338	0.3333886854941710	0.0003535097802470
0.1666798286192090	0.6667773709883420	0.0007070228933088
0.6666798547212309	0.6667773709883420	0.0007070212268161
0.1716647966328324	0.1612558211742225	0.9618721906314107
0.6716648227348543	0.1612558211742225	0.9618721889649251
0.0050046978914295	0.4946445066683935	0.9622257037446431
0.5050047239934514	0.4946445066683935	0.9622257020781575
0.3383446252520486	0.8280331921625645	0.9625792151913899
0.8383446513540633	0.8280331921625645	0.9625792135248972
0.4132132902690913	0.1565432194327769	0.9221083831671706
0.9132133163711060	0.1565432194327769	0.9221083815006779

0.2465531915276884	0.4899319049269479	0.9224618962804030
0.7465532176297032	0.4899319049269479	0.9224618946139103
0.0798930927862855	0.8233205904211189	0.9228154093936354
0.5798931188883003	0.8233205904211189	0.9228154077271427
0.0720608129004988	0.3142323664316179	0.8823058869197201
0.5720459291096919	0.3142350063854490	0.8823095089979721
0.4067149401741035	0.6476642826377889	0.8824730832017251
0.9067201359013366	0.6476630194264577	0.8824712198876064
0.2378228852184330	0.9797465004261812	0.8822529746267892
0.7378270341023883	0.9797537873628935	0.8822508620276595
0.3129515938318439	0.3018780612486506	0.8409954826411079
0.8129057263220393	0.3018567598232414	0.8409987179386325
0.1457167306339006	0.6350237997550483	0.8410781246326523
0.6457059956134896	0.6350189322501737	0.8410771593380448
0.4784559951325779	0.9682739635314641	0.8409567805867881
0.9784400971533685	0.9682735115896188	0.8409561428918092
0.1363612449500358	0.1246654112110880	0.8008285458503975
0.6363631093607719	0.1246763010993088	0.8008266236241814
0.4695852772991628	0.4581179420231125	0.8008017985268193
0.9695943760871636	0.4581309129878425	0.8008016888786170
0.3018862268469698	0.7912219074909067	0.8007985950435862
0.8019259958490275	0.7912279649804469	0.8007987156831792
0.3770254245583031	0.1123084631422780	0.7595023019712527
0.8770320357410557	0.1123201219460705	0.7595088939210540
0.2098719346740077	0.4460310666563474	0.7595228936259367
0.7098170959510024	0.4460079131838335	0.7595172361182057
0.0434404139196271	0.7791853064896755	0.7595075103665230
0.5434152214640506	0.7791774015724124	0.7595041307464306
0.0322215623197064	0.2690924502132713	0.7194974190530167
0.5323771047833605	0.2690710822807776	0.7194984075396271
0.3657296649163400	0.6024596595570385	0.7193654390127758
0.8657397443122725	0.6024561623814729	0.7193608218628691
0.1987998573289873	0.9356014576299249	0.7193523282406724
0.6988473876608964	0.9356689965186091	0.7193616161363460
0.2759161216352248	0.2565909895113268	0.6783422672409101
0.7759986265332478	0.2566727101372500	0.6782893310579377
0.1104836766970509	0.5907655114739746	0.6781069156607245
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0.5157308891071500	0.0029356639505305	0.2562618041695994

S5 Lattice strain calculation

The g-C_3N_4/TiO_2 and g-C_3N_4/$SrTiO_3$/TiO_2 interfaces are made by a g-C_3N_4 monolayers supported on the oxide semiconductors, having a thickness (~2nm) sufficient to obtain converged electronic properties. Therefore, it is a reasonable approximation to release the strain on g-C_3N_4, by fixing the lattice parameters, a, b and γ to those of the semiconductors. 2D unit cell, is defined by 3 variables, two lattice vectors, and the angle between the two. Therefore, it is important to mention that the calculation of lattice strain should include not only the lattice parameters a, and b, but also the lattice angle γ. Namely, the applied strain on g-C_3N_4 can be calculated as follows:

$$\epsilon_a(\%) = \frac{\left(a_{oxide} - a_{g-C_3N_4}\right)}{a_{oxide}} * 100 \qquad (Eq.S1)$$

$$\epsilon_b(\%) = \frac{\left(b_{oxide} - b_{g-C_3N_4}\right)}{b_{oxide}} * 100 \qquad (Eq.S2)$$

$$\epsilon_\gamma(\%) = \frac{\left(\gamma_{oxide} - \gamma_{g-C_3N_4}\right)}{\gamma_{oxide}} * 100 \qquad (Eq.S3)$$

Where $\epsilon_a(\%)$, $\epsilon_b(\%)$,and $\epsilon_\gamma(\%)$ are the applied strains on a, b, and γ lattice parameters. The working lattice vectors, *i.e.* those imposed in the simulation box of the interface will be those of the oxide.