

Electronic Supplementary Information (ESI)

This file contains the lattice vectors and cartesian coordinates (in Bohr) for the following systems (all fully converged);

21.79° Twisted bi-layer
13.17° Twisted bi-layer
13.17° Twisted bi-layer + TCNQ molecule (AC)
13.17° Twisted bi-layer + TCNQ molecule (AB)
9.43° Twisted bi-layer
6.01° Twisted bi-layer

POSITIONS AND LATTICE VECTORS IN BOHR#####

21.79° Twisted Angle :

Lattice Vectors (Cartesian, Bohr):

```
-1.696152242    20.567087540    0.000000000
-18.660441678    8.814237699    0.000000000
0.000000000    0.000000000    46.145716919
```

28 # Number of atoms

#Cartesian Coordinates: chemical_specie_label, atomic_number, coordinates

1	51	-2.982866464	9.575866420	-2.745189850
1	51	-3.402283927	5.007077511	0.268880567
1	51	-7.529839693	3.240279552	-2.895345097
1	51	-8.202213809	-1.175147424	0.298982370
1	51	4.706925578	8.746293714	-2.903678126
1	51	4.300377663	4.312649998	0.301237927
1	51	0.256208386	2.390390789	-2.863634582
1	51	-0.247279354	-1.942235953	0.462234647
1	51	-4.384691011	-3.866156429	-2.589193210
1	51	-4.884526654	-8.392126935	0.477414805
1	51	8.010436323	1.745765942	-2.825122919
1	51	7.506664913	-2.818965836	0.176936405
1	51	3.256914163	-4.666697128	-2.768837155
1	51	2.865381586	-9.172868937	0.341971554
1	51	-9.879714517	12.668642517	7.101388693
1	51	-8.549362745	8.456627074	10.362877271
1	51	-11.662175719	5.107106589	7.318626138
1	51	-10.434208061	0.727426097	10.394655006
1	51	-2.194751487	14.779331264	6.904669616
1	51	-0.966083303	10.565099521	10.194797897
1	51	-4.201515473	7.285173062	7.218611622
1	51	-2.913993158	2.983527178	10.370222326
1	51	-6.075431761	-0.171868034	7.186424308
1	51	-4.853733147	-4.688657010	10.060093892
1	51	3.434542979	9.291331610	7.169561809
1	51	4.532382826	4.982928345	10.377426033
1	51	1.382672721	1.878472616	7.139305762
1	51	2.468560290	-2.551929579	10.194331867

13.17°

-3.902803402	33.783108929	0.000000000
-31.209351507	13.514751566	0.000000000
0.000000000	0.000000000	48.234830549

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1	51	-7.776608065	15.821560133	-2.298708920
1	51	-7.744610332	10.989698066	0.306352164
1	51	-11.625671911	9.028734235	-3.047757333
1	51	-11.756788367	4.485585976	0.021901497
1	51	-15.542956045	2.140984199	-3.195616528
1	51	-15.821421800	-2.140206651	0.231913757
1	51	-0.135805673	15.796076081	-2.857314097
1	51	-0.043881628	11.225322370	0.196296081
1	51	-3.878887273	8.948065246	-2.991920996
1	51	-3.840026770	4.485862437	0.192440233
1	51	-7.749334246	2.103302217	-2.852806352
1	51	-7.848953822	-2.071436532	0.728753042
1	51	-11.650578968	-4.752804855	-2.201127460
1	51	-11.986323214	-9.039340663	1.247970540
1	51	7.784396643	15.695587960	-3.005470632
1	51	7.542941924	11.355030172	0.352104145
1	51	3.859471068	9.034134229	-2.968581489
1	51	3.907057089	4.566388107	0.206438527
1	51	0.063134018	2.292182932	-2.972210520
1	51	0.212814578	-2.046845951	0.368189512
1	51	-3.942593531	-4.514401691	-2.238910268
1	51	-3.780191415	-8.749695222	1.273875498
1	51	-7.791075133	-11.249658056	-1.536870095
1	51	-7.622671152	-16.002935853	1.224723121
1	51	11.740050438	8.972651118	-2.270206987
1	51	11.584736553	4.375418081	0.711066506
1	51	7.912432046	2.372101829	-2.854655526
1	51	7.872581703	-2.280170353	0.039113891
1	51	3.840012832	-4.447298286	-2.982531318
1	51	4.105925395	-8.864516733	0.259741296
1	51	-0.235152783	-11.176111125	-2.179742718
1	51	0.182571832	-15.832632813	0.713036037
1	51	15.802763540	2.425616652	-2.229251190
1	51	15.635680429	-2.495076052	0.201709529
1	51	11.770476506	-4.395948823	-3.204062038
1	51	11.715043776	-8.998733151	-0.201989246
1	51	7.672921101	-11.244644436	-3.171661623
1	51	7.807898654	-15.695803903	0.047074431
1	51	-15.233450789	19.391868877	6.244027208
1	51	-13.924872413	15.302299420	9.698973855
1	51	-17.382586122	11.812788274	7.246740638
1	51	-16.147528187	7.704433521	10.675753761
1	51	-19.460990226	4.495627315	7.687053726
1	51	-18.335110792	0.021872652	10.674010386
1	51	-7.180759964	20.972808122	6.249981482
1	51	-6.371550098	16.828708833	9.782562049
1	51	-9.596646029	13.561271683	6.788278841
1	51	-8.563637615	9.502313217	10.350681718

1	51	-11.927973626	6.293264264	7.450369400
1	51	-10.753806004	1.874652084	10.481024385
1	51	-14.161268127	-0.953878155	7.241918802
1	51	-12.869551978	-5.698637219	9.681004273
1	51	0.482019414	22.877526597	7.256951144
1	51	1.246737740	18.530988053	10.516265463
1	51	-1.763606939	15.390331751	7.165467600
1	51	-0.929092367	11.104609738	10.470924403
1	51	-4.221006301	8.088326184	7.290738314
1	51	-3.243645293	3.720004071	10.456047599
1	51	-6.525140410	0.871763746	7.123622806
1	51	-5.463901945	-3.849232540	9.722434417
1	51	-8.679340217	-6.619737645	6.218646387
1	51	-7.766694556	-11.261064049	9.023521690
1	51	5.638365616	17.335122044	7.457468823
1	51	6.743694521	12.814939047	10.346349599
1	51	3.333964141	9.772527407	7.290804697
1	51	4.302640371	5.400855972	10.455271781
1	51	1.013876587	2.386640194	7.271230683
1	51	1.958359568	-2.092599374	10.316917680
1	51	-1.015998956	-5.025933180	6.742113820
1	51	-0.372947037	-9.626216710	9.684001106
1	51	10.766645801	11.694782718	6.767254789
1	51	11.973338544	7.262852068	9.756869858
1	51	8.424314098	3.996288800	7.133775710
1	51	9.659050900	-0.183140173	10.476258863
1	51	6.427382532	-3.402175105	7.429786342
1	51	7.310195412	-7.752006351	10.669438605

13.17° + TCNQ (AC)

-3.931264675	33.866073422	0.000000000
-31.282425990	13.565905513	0.000000000
0.000000000	0.000000000	54.412840971

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1	51	-7.284482645	16.091466047	-1.739546578
1	51	-7.122308020	11.365658257	1.062083848
1	51	-11.021449816	9.477934533	-2.342729705
1	51	-11.200849893	4.587698382	0.145142684
1	51	-15.045344097	2.641116876	-3.274029857
1	51	-15.112505108	-1.914495718	-0.192248969
1	51	0.330856590	16.191617023	-2.301075868
1	51	0.683417668	11.550120170	0.630289858
1	51	-3.328089509	9.323009200	-2.359392877
1	51	-3.294742407	4.526664034	0.308937637
1	51	-7.198597817	2.556947578	-3.023543302
1	51	-7.357271042	-1.999365832	0.028686568
1	51	-11.176192606	-4.349546665	-3.161201136
1	51	-11.430902087	-8.615974591	0.299817147
1	51	8.191760570	16.093844590	-3.120584071
1	51	8.289022155	11.653584049	0.134355508
1	51	4.326099493	9.298641569	-2.823699669
1	51	4.383916299	4.740981016	0.254828947

1	51	0.579898772	2.468151849	-2.981810509
1	51	0.621380597	-2.018725152	0.165267730
1	51	-3.336254373	-4.385363993	-2.839043428
1	51	-3.446138257	-8.586208320	0.720101052
1	51	-7.288106223	-11.192358104	-2.227422313
1	51	-7.527274124	-15.583152826	1.082286368
1	51	12.181471628	9.249074846	-2.893839593
1	51	12.019740745	4.869874378	0.422488819
1	51	8.314448770	2.598590394	-2.921191389
1	51	8.365793560	-1.937025074	0.158797496
1	51	4.514887108	-4.119204391	-3.086130722
1	51	4.646420980	-8.487407768	0.234159051
1	51	0.456743074	-10.956705681	-2.310183415
1	51	0.642799114	-15.288010596	1.096503666
1	51	16.125068524	2.510724376	-2.358984592
1	51	16.086393941	-2.086015019	0.623643632
1	51	12.385121302	-4.089102315	-2.922315245
1	51	12.334769465	-8.761821280	-0.056014911
1	51	8.291819505	-10.917817834	-3.075244001
1	51	8.520277093	-15.311096222	0.218817838
1	51	-15.771138841	18.664392670	6.610614511
1	51	-14.643533644	14.273782884	9.681689355
1	51	-18.166646946	10.962874757	7.084690271
1	51	-16.963210203	6.748398288	10.394170094
1	51	-20.118609331	3.604925571	7.185198076
1	51	-19.287200413	-0.839591098	10.315362229
1	51	-8.029022473	20.585601557	5.894148086
1	51	-7.010814643	16.009310145	8.764218387
1	51	-10.648289906	12.778690429	6.219062251
1	51	-9.267561561	8.736461212	9.704608210
1	51	-12.763682862	5.312875592	7.168316427
1	51	-11.469931510	1.105285282	10.454961068
1	51	-14.772503562	-2.081027860	7.430912636
1	51	-13.719529194	-6.587679101	10.404303923
1	51	-0.157459935	22.199052857	6.241851660
1	51	0.452301168	17.588768883	9.168192465
1	51	-2.612377483	14.430580153	5.859450465
1	51	-1.630029590	10.198174625	9.227456551
1	51	-5.136824429	7.024403458	6.486223105
1	51	-3.869728958	2.952723573	9.939658351
1	51	-7.301516601	-0.264102890	7.134634260
1	51	-6.075690303	-4.610160340	10.303252248
1	51	-9.438595697	-7.528843458	7.106065668
1	51	-8.164313713	-12.294365572	9.508853617
1	51	5.246957738	16.261730267	6.844340309
1	51	5.956495867	11.916090361	10.133177324
1	51	3.010287105	8.839338540	6.637002704
1	51	3.700733298	4.579898336	10.013383255
1	51	0.444752056	1.503402119	6.849321359
1	51	1.389674362	-2.747322047	10.241977785
1	51	-1.871864704	-5.621178451	6.880935036
1	51	-0.700848625	-10.488078071	9.165712388

1	51	10.394735838	10.766976560	7.069462685
1	51	11.391422348	6.274269577	10.042569083
1	51	8.049837918	3.128560027	7.008979297
1	51	8.943877948	-1.156996945	10.322663071
1	51	5.672639492	-4.188596376	7.135685761
1	51	6.605991107	-8.787629893	10.013446563
2	6	-1.679693489	20.579237109	16.142148804
2	6	-4.259578979	21.392472179	16.012138645
2	6	-6.184649317	19.486060138	16.015276356
2	6	-5.567431716	16.936307862	15.962972910
2	6	-2.981080750	16.123228719	15.909952162
2	6	-1.059577718	18.029062668	16.089718379
2	6	-2.337371306	13.492664470	15.600137996
2	6	-4.897587050	24.031968202	15.732321965
2	6	0.217316723	12.691270515	15.349712686
2	6	-3.002942852	25.905549968	15.373014689
2	6	-4.226106863	11.608634554	15.251638663
2	6	-7.437022658	24.815084112	15.329453231
3	7	-5.810117556	10.054781546	14.907337210
3	7	-1.412715715	27.437194294	14.952862366
4	1	-7.078486852	15.498493452	15.932022841
4	1	-0.168319558	22.014749315	16.234311462
3	7	2.356367222	12.050970528	15.106168516
3	7	-9.550564606	25.435579440	14.884004651
4	1	-8.187157157	20.071128688	16.004318591
4	1	0.940901075	17.441898970	16.164537461

13.17 + TCNQ (AB - FINAL)

-3.881548768 33.856616057 0.000000000
-31.196898511 13.525981887 0.000000000
0.000000000 0.000000000 54.412840971

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1	51	-8.136577325	15.263999664	-2.815384012
1	51	-7.964248634	10.682991437	0.232258330
1	51	-11.851189583	8.413213699	-2.903300063
1	51	-11.890882318	3.900827293	0.224588581
1	51	-15.588530362	1.486052871	-3.058815626
1	51	-16.014552961	-2.736491047	0.446211954
1	51	-0.295811478	15.142933533	-3.445532101
1	51	-0.335841524	10.881364515	0.028653626
1	51	-4.165126058	8.435020768	-3.029003729
1	51	-4.005854798	4.092416483	0.331704534
1	51	-7.849115880	1.711161962	-2.766190302
1	51	-7.805754770	-2.564630767	0.684191365
1	51	-11.794380428	-5.121971383	-2.083072393
1	51	-11.826152108	-9.428716765	1.356679163
1	51	7.709241044	14.925552797	-2.751728394
1	51	7.327700283	10.718384313	0.772751699
1	51	3.724893935	8.331615255	-2.642553318
1	51	3.654112613	3.930319510	0.622493644
1	51	-0.099037501	1.739726018	-2.742184157
1	51	0.007507237	-2.829088770	0.293282431

1	51	-4.118216087	-5.025684180	-2.571311725
1	51	-3.780910473	-9.525392766	0.557647159
1	51	-8.103538577	-11.760662837	-1.981660831
1	51	-7.800698324	-16.473746186	0.828929684
1	51	11.651492497	8.467650095	-1.745216187
1	51	11.682429356	3.769281179	1.097515853
1	51	7.810996258	1.813851835	-2.287716124
1	51	7.697269723	-3.089643245	0.191164882
1	51	3.747334576	-4.943288329	-3.147263505
1	51	3.875134319	-9.677616913	-0.352242171
1	51	-0.372414268	-11.791083753	-3.125028510
1	51	-0.059932343	-16.361117879	-0.080950763
1	51	15.523525005	1.721662989	-2.268376199
1	51	15.440508196	-3.094260362	0.371807410
1	51	11.641591498	-4.998583331	-3.119718627
1	51	11.433112004	-9.740546994	-0.359374941
1	51	7.636198117	-11.890954882	-3.708435754
1	51	7.421757747	-16.262482832	-0.382234510
1	51	-15.097291392	20.329454618	6.263921188
1	51	-14.362163784	16.201223642	9.897250006
1	51	-17.568222763	13.143863665	6.659006588
1	51	-16.495996367	8.573844415	9.495312275
1	51	-20.096728019	5.779935456	6.451355841
1	51	-18.760241301	1.336430421	9.365253943
1	51	-7.456651767	22.169183888	7.450461165
1	51	-6.688172608	17.861575314	10.768248176
1	51	-9.716355320	14.872469609	7.300615193
1	51	-8.990581379	10.305838188	10.216482992
1	51	-12.002391809	7.591508721	6.482512949
1	51	-11.275667026	3.164607925	9.635085054
1	51	-14.374201157	0.151351151	6.257090582
1	51	-13.469021756	-4.450290820	9.128228193
1	51	-0.208411379	24.124986053	7.465310012
1	51	1.150438791	19.700994160	10.444412376
1	51	-2.426254033	16.742747822	7.490275343
1	51	-1.176938681	12.135899697	10.182654983
1	51	-4.623579042	9.167718024	7.083928182
1	51	-3.706683932	4.750761357	10.206905618
1	51	-6.788556263	1.635823887	6.902325140
1	51	-6.074474035	-2.742753068	10.167700889
1	51	-8.847302049	-5.843863540	6.561575267
1	51	-8.386327523	-10.313700415	9.713025908
1	51	4.971001599	18.526210445	6.664471521
1	51	6.491005658	14.002897418	9.371533310
1	51	2.799680400	11.029356025	6.546475488
1	51	3.985433385	6.636313571	9.591256514
1	51	0.492077708	3.280992882	7.016679276
1	51	1.667857900	-0.847104437	10.450573572
1	51	-1.531174930	-4.115385775	7.408500987
1	51	-0.579424678	-8.419428874	10.695358082
1	51	10.598373133	12.952510216	5.814040100
1	51	11.529287428	8.441959281	8.810473368

1	51	8.016136073	5.178948442	6.150044717
1	51	9.267196324	1.116007707	9.683669054
1	51	5.786690111	-2.267573685	7.125608348
1	51	7.233657347	-6.559919024	10.213522122
2	6	16.834883076	-6.809351662	16.313504075
2	6	14.314816761	-5.814643844	16.223482623
2	6	12.262861525	-7.586074727	16.266305099
2	6	12.700567177	-10.172093001	16.174755703
2	6	15.223867202	-11.162120815	16.045303108
2	6	17.274605558	-9.395496157	16.236145845
2	6	15.680741608	-13.814303696	15.623115672
2	6	13.860405906	-3.135977161	15.968383760
2	6	18.163207581	-14.759227399	15.207755612
2	6	15.873038205	-1.404536929	15.571483122
2	6	13.656598714	-15.542838834	15.221229950
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