

Effect of Bridge Type on Electronic Structure and Rectification in Molecular Junctions

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- 1- Other DFT-NEGF Computational Details for Two-Probe Systems
- 2- Cartesian coordinates for isolated molecular systems(without electric field)

Group (A)

A-D

S	-5.31771255	-0.08142815	-0.02014900
S	5.24814175	0.06714808	-0.02515273
C	3.47504222	0.00794162	-0.00282173
N	2.86793253	1.12421331	-0.42571549
C	1.53457559	1.10664903	-0.42471761
C	0.77558542	0.00335451	-0.00045403
C	1.53804178	-1.09677840	0.42192630
N	2.87340780	-1.11123417	0.42128113
H	1.04738733	2.00714833	-0.79491689
H	1.05460266	-1.99916133	0.79234800
C	-0.70285919	0.00104637	0.00043533
C	-1.43095730	1.14676357	0.36420929
C	-1.42895056	-1.14677811	-0.36410067
C	-2.82472087	1.15055439	0.36419595
H	-0.90461134	2.04479141	0.67730703
C	-2.82153557	-1.15249795	-0.36458174
H	-0.90035035	-2.04310562	-0.67800451
C	-3.53606434	-0.00128418	-0.00019909
H	-3.35327908	2.05283881	0.66073857
H	-3.35327138	-2.05302246	-0.66100537
H	5.40389901	-1.18417250	0.45323431
H	-5.53956937	1.19848546	0.34281517

A-π-D

S	6.50063800	-0.09250800	-0.00250400
S	-6.41985200	0.11964800	-0.00419800
C	-4.65109200	-0.00514200	-0.00034500
N	-4.17023400	-1.25402900	-0.01211200
C	-2.84311900	-1.37103100	-0.01060700
C	-1.95989700	-0.27578700	0.00231200
C	-2.60176300	0.97731600	0.01585400
N	-3.92630000	1.12423300	0.01429500
H	-2.45403900	-2.38924100	-0.02026000
H	-2.03053500	1.90320200	0.02939800
C	1.89272500	0.26222000	0.00055100
C	2.51068300	-1.00454300	0.01162900
C	2.73747000	1.38935300	-0.01036000
C	3.89466500	-1.13695600	0.01074300
H	1.90658200	-1.90722000	0.02145200
C	4.12423800	1.26816500	-0.01104700
H	2.29601000	2.38360800	-0.01867700
C	4.72081100	-0.00059500	-0.00063500

H	4.33240000	-2.13196500	0.01941300
H	4.74211400	2.16242100	-0.01960900
H	-6.43326200	1.46820200	0.01021400
H	6.59211700	-1.43818500	0.01126600
C	-0.51531900	-0.49053500	0.00180300
H	-0.22045200	-1.53933800	0.00164500
C	0.44275300	0.46308800	0.00009800
H	0.13928900	1.50953000	-0.00286800

A-σ-D

S	-6.40748700	0.00222462	-0.33009618
S	6.31634098	0.03570308	0.25278618
C	4.56614106	-0.00462654	-0.03662359
N	3.97001426	-1.19143434	-0.16566712
C	2.66669207	-1.15657326	-0.37216807
C	1.93076891	0.02488953	-0.45575007
C	2.68565105	1.19050617	-0.31480780
N	3.98647575	1.19437743	-0.10738164
H	2.18162964	-2.12480404	-0.48510284
H	2.21562049	2.17034953	-0.38070847
C	-1.85122745	0.02723933	0.47588081
C	-2.55114921	-1.18493065	0.37663635
C	-2.57737292	1.21819010	0.34176646
C	-3.92572154	-1.21065810	0.13810185
H	-2.01375604	-2.12579460	0.48110396
C	-3.95758464	1.20500281	0.12533631
H	-2.06353787	2.17403011	0.42623274
C	-4.64193748	-0.01174339	0.02165305
H	-4.44104807	-2.16227214	0.04063950
H	-4.50601769	2.13959132	0.05061297
H	6.45622136	-1.30572190	0.24642406
H	-6.80185073	-0.70842366	0.74996346
C	0.43568978	0.04146888	-0.65511109
H	0.12974029	-0.83179099	-1.24481909
C	-0.35214289	0.04622552	0.68287707
H	-0.06536796	0.93542178	1.25853521
H	-0.04437283	-0.82315245	1.27758341
H	0.14880530	0.92517985	-1.23891132

Group (B)

2A-2D

S	-9.60345305	0.08187671	-0.00864640
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C	-7.10966171	-1.19157726	0.17939410
C	-5.71788178	-1.18639956	0.17732918
C	-4.98923606	0.00076351	-0.00065028
C	-5.71714749	1.18943558	-0.17883705
C	-7.10764549	1.19498950	-0.18077933
C	-7.81992558	0.00164477	-0.00067745
H	-7.63910026	-2.12740188	0.33213928
H	-5.18967241	-2.12000323	0.34557036
H	-5.18772799	2.12219222	-0.34742372
H	-7.64072013	2.12874830	-0.33342583

C	-3.50726610	-0.00011133	-0.00053825
C	-2.77925122	-1.06607052	-0.55689752
C	-2.77853931	1.06524170	0.55610517
C	-1.38889477	-1.06797798	-0.55694224
H	-3.30999518	-1.88723445	-1.02855472
C	-1.38817863	1.06569086	0.55696783
H	-3.30874621	1.88711876	1.02707961
C	-0.66302970	-0.00150492	0.00023858
H	-0.85977272	-1.89032168	-1.02924575
H	-0.85853573	1.88760448	1.02943599
C	0.81287751	-0.00222310	0.00054440
C	1.57468719	1.16458014	-0.17147291
C	1.57354460	-1.16973987	0.17281246
H	1.08375443	2.12223275	-0.33626044
H	1.08170709	-2.12694434	0.33750037
C	3.52552630	-0.00355099	0.00091355
C	5.00036396	-0.00443364	0.00097933
C	5.74823655	-1.17735818	0.18081739
C	5.74827217	1.16718445	-0.17880085
H	5.24278474	-2.12771229	0.32722821
H	5.24290874	2.11763191	-0.32511340
C	7.67796812	-0.00518542	0.00074193
N	7.08269531	1.18160687	-0.18113016
N	7.08090045	-1.19054437	0.18260637
N	2.90565682	1.17805293	-0.16772123
N	2.90446777	-1.18449293	0.16941744
H	-9.82540094	-1.23724257	0.14686258
H	9.60954901	1.25672850	-0.19356168

2A- π -2D

S	10.78156480	-0.25066014	0.01476786
S	-10.61587364	0.27619609	0.04055787
N	-8.33428364	-1.12263966	-0.16725959
C	-7.00153016	-1.19826035	-0.17850285
C	-6.17386180	-0.07726015	-0.01195590
C	-6.84338802	1.14378498	0.16951252
N	-8.17303974	1.24293545	0.18425514
H	-6.56888537	-2.18376453	-0.32491364
H	-6.28199542	2.06349130	0.30623831
C	2.64295321	1.46988528	0.20991366
C	1.84240830	0.32285140	0.04468608
C	2.50711340	-0.90811273	-0.13292489
C	3.89444350	-0.98101386	-0.14381961
C	4.69382739	0.16826924	0.02292720
C	4.03306728	1.39639754	0.20036044
H	2.16266784	2.43467907	0.35960576
H	1.93615662	-1.82113299	-0.27574679
H	4.37082054	-1.94326543	-0.31135744
H	4.61311292	2.30118091	0.36064507
C	-2.67298998	0.86727096	0.12747007
N	-3.99869459	0.96118064	0.14143725
C	-1.98500030	-0.34938937	-0.05253110
C	-4.70246630	-0.17608104	-0.02663004
C	-2.82923613	-1.46326319	-0.21696008
N	-4.15778061	-1.39260587	-0.20639791
H	-2.40160863	-2.45549527	-0.36353456
C	6.17350466	0.08298039	0.01159380
C	6.84706432	-1.01028031	0.58611353

C	6.95830003	1.09268982	-0.57247263
C	8.23729588	-1.09256172	0.58124383
H	6.27760684	-1.79806415	1.07193589
C	8.34999142	1.01818762	-0.58590697
H	6.47529836	1.94039246	-1.05123524
C	9.00595436	-0.07716058	-0.00706765
H	8.92033485	1.81326294	-1.05954805
H	-10.85831312	-1.03629876	-0.15459546
H	11.06455382	0.92247322	-0.58768813
H	8.72529361	-1.94530991	1.04654910
H	-2.13351734	1.80225350	0.26595910
C	-8.85349903	0.10061698	0.01450618
C	0.38658461	0.46827544	0.06638813
H	0.04363871	1.49163521	0.21515239
C	-0.53525288	-0.51108558	-0.07616902
H	-0.20133493	-1.53715156	-0.22557039

2A-σ-2D

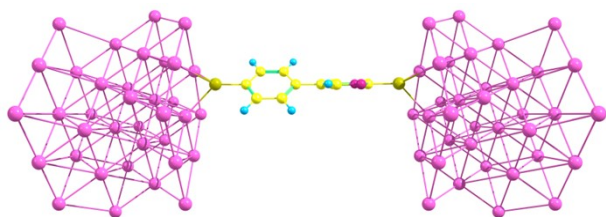
S	-10.70235744	-0.00669103	0.26876164
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N	8.17376720	1.15517803	-0.29833033
C	6.84563089	1.17014228	-0.16025340
C	6.10033284	0.02417938	0.15329266
C	6.84603248	-1.15391365	0.31522540
N	8.17249522	-1.19293802	0.18226380
H	6.35016509	2.12616843	-0.30283834
H	6.35054715	-2.08907671	0.55963635
C	-2.50938692	1.08010957	-0.72882430
C	-1.78920680	-0.11321611	-0.57521550
C	-2.51197179	-1.27817883	-0.28116685
C	-3.89948655	-1.25246826	-0.14069411
C	-4.62280622	-0.05636907	-0.29214482
C	-3.89705817	1.11019891	-0.59129076
H	-1.98011802	1.99839423	-0.97771736
H	-1.98282529	-2.22152435	-0.15709967
H	-4.42581612	-2.16992829	0.10965115
H	-4.42709337	2.04586544	-0.74955774
C	2.68347729	-1.05789073	0.72990892
N	4.01097054	-1.09940994	0.60509328
C	1.92880146	0.10949708	0.56220442
C	4.63016894	0.05540861	0.30226335
C	2.68458054	1.24907558	0.26113832
N	4.01210930	1.23754294	0.13029924
H	2.19899432	2.21618651	0.12698867
C	-6.10026865	-0.02711386	-0.14824725
C	-6.90301222	-1.07267685	-0.63784901
C	-6.75025346	1.04707825	0.48275888
C	-8.28962066	-1.04890209	-0.50578617
H	-6.43957890	-1.90816250	-1.15586853
C	-8.13719174	1.08006316	0.62216692
H	-6.16274273	1.86222724	0.89727338
C	-8.92311097	0.03037636	0.12761457
H	-8.60089161	1.92343290	1.12778874
C	-0.28043049	-0.13630238	-0.68872824
H	0.05215028	-1.10896593	-1.07320620
H	0.05252388	0.61687156	-1.41433830
C	0.42484146	0.13199175	0.66894151
H	0.09286090	-0.61989346	1.39581228
H	0.09423666	1.10473787	1.05417380

H	10.68457307	1.18246888	-0.57122751
H	-10.84036401	1.19465928	0.86631478
H	-8.88055321	-1.86845069	-0.90715748
H	2.19706111	-2.00025765	0.98368870

3- Cartesian coordinates for two-probe systems

Group (A)

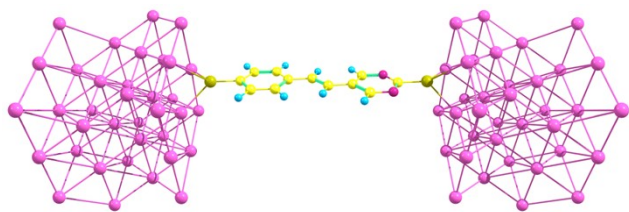
A-D



Au	0.000000e+00	0.000000e+00	1.214474e+00
Au	2.974599e+00	0.000000e+00	1.214474e+00
Au	5.949197e+00	0.000000e+00	1.214474e+00
Au	-1.487299e+00	2.576078e+00	1.214474e+00
Au	1.487299e+00	2.576078e+00	1.214474e+00
Au	4.461898e+00	2.576078e+00	1.214474e+00
Au	-2.974599e+00	5.152156e+00	1.214474e+00
Au	0.000000e+00	5.152156e+00	1.214474e+00
Au	2.974599e+00	5.152156e+00	1.214474e+00
Au	1.487299e+00	8.586927e-01	3.643224e+00
Au	4.461898e+00	8.586927e-01	3.643224e+00
Au	7.436497e+00	8.586927e-01	3.643224e+00
Au	0.000000e+00	3.434771e+00	3.643224e+00
Au	2.974599e+00	3.434771e+00	3.643224e+00
Au	5.949197e+00	3.434771e+00	3.643224e+00
Au	-1.487299e+00	6.010849e+00	3.643224e+00
Au	1.487299e+00	6.010849e+00	3.643224e+00
Au	4.461898e+00	6.010849e+00	3.643224e+00
Au	0.000000e+00	1.717385e+00	6.071974e+00
Au	2.974599e+00	1.717385e+00	6.071974e+00
Au	5.949197e+00	1.717385e+00	6.071974e+00
Au	-1.487299e+00	4.293463e+00	6.071974e+00
Au	1.487299e+00	4.293463e+00	6.071974e+00
Au	4.461898e+00	4.293463e+00	6.071974e+00
Au	-2.974599e+00	6.869542e+00	6.071974e+00
Au	0.000000e+00	6.869542e+00	6.071974e+00
Au	2.974599e+00	6.869542e+00	6.071974e+00
Au	2.992467e+00	5.162419e+00	8.455645e+00
Au	-2.992611e+00	5.163128e+00	8.458933e+00
Au	8.291337e-04	-2.529623e-02	8.465124e+00
Au	-1.614339e+00	2.501847e+00	8.465739e+00
Au	1.616585e+00	2.499402e+00	8.468695e+00
Au	-2.561015e-04	5.290861e+00	8.480394e+00
Au	4.462301e+00	2.583061e+00	8.484243e+00
Au	5.953688e+00	-7.124897e-03	8.486888e+00
Au	2.969515e+00	-8.697177e-03	8.493102e+00
S	7.201413e-03	3.404991e+00	1.021569e+01
C	1.709480e-02	3.394280e+00	1.198969e+01
H	-5.046958e-01	5.496811e+00	1.211973e+01
H	5.387488e-01	1.286754e+00	1.215768e+01

C	-2.711612e-01	4.585921e+00	1.269215e+01
C	3.044679e-01	2.210660e+00	1.270876e+01
C	-2.657802e-01	4.590589e+00	1.408949e+01
C	3.032930e-01	2.231025e+00	1.410715e+01
H	-5.197605e-01	5.514789e+00	1.462903e+01
H	5.588959e-01	1.317074e+00	1.466358e+01
C	2.133854e-02	3.417498e+00	1.482617e+01
C	2.437149e-02	3.431808e+00	1.630156e+01
H	9.563393e-01	5.391662e+00	1.654341e+01
H	-9.081985e-01	1.476671e+00	1.657612e+01
C	5.196119e-01	4.518062e+00	1.705981e+01
C	-4.729690e-01	2.359156e+00	1.707735e+01
N	5.188957e-01	4.552156e+00	1.839662e+01
N	-4.828263e-01	2.351821e+00	1.841308e+01
C	1.264259e-02	3.458994e+00	1.899244e+01
S	-9.135999e-03	3.463282e+00	2.078063e+01
Au	4.463286e+00	2.582653e+00	2.247789e+01
Au	2.967605e+00	-2.639690e-03	2.247899e+01
Au	5.957661e+00	-1.391459e-03	2.247984e+01
Au	-1.611294e+00	2.495365e+00	2.249353e+01
Au	7.376675e-03	5.309394e+00	2.249413e+01
Au	1.613231e+00	2.501613e+00	2.250264e+01
Au	2.601415e-03	-2.382568e-02	2.250848e+01
Au	2.997387e+00	5.161224e+00	2.250972e+01
Au	-2.990426e+00	5.160340e+00	2.251043e+01
Au	3.265987e-03	1.714092e+00	2.489095e+01
Au	2.977865e+00	1.714092e+00	2.489095e+01
Au	5.952463e+00	1.714092e+00	2.489095e+01
Au	-1.484033e+00	4.290170e+00	2.489095e+01
Au	1.490565e+00	4.290170e+00	2.489095e+01
Au	4.465164e+00	4.290170e+00	2.489095e+01
Au	-2.971333e+00	6.866248e+00	2.489095e+01
Au	3.265987e-03	6.866248e+00	2.489095e+01
Au	2.977865e+00	6.866248e+00	2.489095e+01
Au	1.490565e+00	8.553995e-01	2.731970e+01
Au	4.465164e+00	8.553995e-01	2.731970e+01
Au	7.439763e+00	8.553995e-01	2.731970e+01
Au	3.265987e-03	3.431478e+00	2.731970e+01
Au	2.977865e+00	3.431478e+00	2.731970e+01
Au	5.952463e+00	3.431478e+00	2.731970e+01
Au	-1.484033e+00	6.007556e+00	2.731970e+01
Au	1.490565e+00	6.007556e+00	2.731970e+01
Au	4.465164e+00	6.007556e+00	2.731970e+01
Au	3.265987e-03	-3.293200e-03	2.974845e+01
Au	2.977865e+00	-3.293200e-03	2.974845e+01
Au	5.952463e+00	-3.293200e-03	2.974845e+01
Au	-1.484033e+00	2.572785e+00	2.974845e+01
Au	1.490565e+00	2.572785e+00	2.974845e+01
Au	4.465164e+00	2.572785e+00	2.974845e+01
Au	-2.971333e+00	5.148863e+00	2.974845e+01
Au	3.265987e-03	5.148863e+00	2.974845e+01
Au	2.977865e+00	5.148863e+00	2.974845e+01

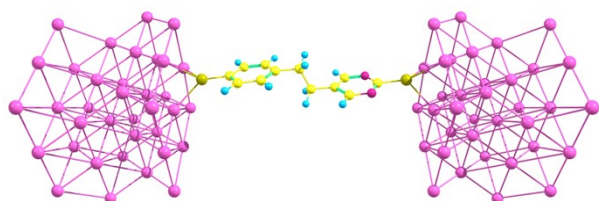
A- π -D



Au	0.000000e+00	0.000000e+00	1.214474e+00
Au	2.974599e+00	0.000000e+00	1.214474e+00
Au	5.949197e+00	0.000000e+00	1.214474e+00
Au	-1.487299e+00	2.576078e+00	1.214474e+00
Au	1.487299e+00	2.576078e+00	1.214474e+00
Au	4.461898e+00	2.576078e+00	1.214474e+00
Au	-2.974599e+00	5.152156e+00	1.214474e+00
Au	0.000000e+00	5.152156e+00	1.214474e+00
Au	2.974599e+00	5.152156e+00	1.214474e+00
Au	1.487299e+00	8.586927e-01	3.643224e+00
Au	4.461898e+00	8.586927e-01	3.643224e+00
Au	7.436497e+00	8.586927e-01	3.643224e+00
Au	0.000000e+00	3.434771e+00	3.643224e+00
Au	2.974599e+00	3.434771e+00	3.643224e+00
Au	5.949197e+00	3.434771e+00	3.643224e+00
Au	-1.487299e+00	6.010849e+00	3.643224e+00
Au	1.487299e+00	6.010849e+00	3.643224e+00
Au	4.461898e+00	6.010849e+00	3.643224e+00
Au	0.000000e+00	1.717385e+00	6.071974e+00
Au	2.974599e+00	1.717385e+00	6.071974e+00
Au	5.949197e+00	1.717385e+00	6.071974e+00
Au	-1.487299e+00	4.293463e+00	6.071974e+00
Au	1.487299e+00	4.293463e+00	6.071974e+00
Au	4.461898e+00	4.293463e+00	6.071974e+00
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Au	1.616926e+00	2.491589e+00	8.462717e+00
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Au	6.205233e-05	5.269508e+00	8.480419e+00
Au	4.461540e+00	2.570662e+00	8.488876e+00
Au	5.950778e+00	-2.254426e-02	8.493373e+00
Au	2.972923e+00	-2.229934e-02	8.493501e+00
S	-7.271934e-04	3.415566e+00	1.021140e+01
C	1.359053e-03	3.542771e+00	1.197355e+01
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H	1.789469e-02	1.392245e+00	1.228075e+01
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H	2.040806e-02	1.548219e+00	1.474719e+01
C	3.730101e-03	3.728859e+00	1.481233e+01
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H	2.853299e-03	4.939090e+00	1.659729e+01
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Au	2.974668e+00	1.722446e+00	2.720741e+01
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Au	4.461967e+00	4.298524e+00	2.720741e+01
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Au	6.925277e-05	6.874602e+00	2.720741e+01
Au	2.974668e+00	6.874602e+00	2.720741e+01
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Au	4.461967e+00	8.637534e-01	2.963616e+01
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Au	2.974668e+00	3.439831e+00	2.963616e+01
Au	5.949267e+00	3.439831e+00	2.963616e+01
Au	-1.487230e+00	6.015910e+00	2.963616e+01
Au	1.487369e+00	6.015910e+00	2.963616e+01
Au	4.461967e+00	6.015910e+00	2.963616e+01
Au	6.925277e-05	5.060698e-03	3.206491e+01
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Au	-1.487230e+00	2.581139e+00	3.206491e+01
Au	1.487369e+00	2.581139e+00	3.206491e+01
Au	4.461967e+00	2.581139e+00	3.206491e+01
Au	-2.974529e+00	5.157217e+00	3.206491e+01
Au	6.925277e-05	5.157217e+00	3.206491e+01
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A-σ-D



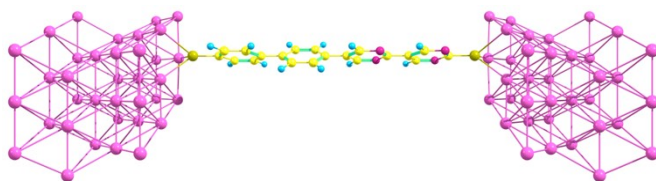
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Au	2.963933e+00	6.850258e+00	2.705540e+01
Au	1.476634e+00	8.394091e-01	2.948415e+01
Au	4.451232e+00	8.394091e-01	2.948415e+01
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Au	2.963933e+00	3.415487e+00	2.948415e+01
Au	5.938532e+00	3.415487e+00	2.948415e+01
Au	-1.497965e+00	5.991565e+00	2.948415e+01
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Au	4.451232e+00	5.991565e+00	2.948415e+01
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Au	5.938532e+00	-1.928363e-02	3.191290e+01
Au	-1.497965e+00	2.556794e+00	3.191290e+01
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Au	4.451232e+00	2.556794e+00	3.191290e+01
Au	-2.985264e+00	5.132873e+00	3.191290e+01
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Group (B)

2A-2D

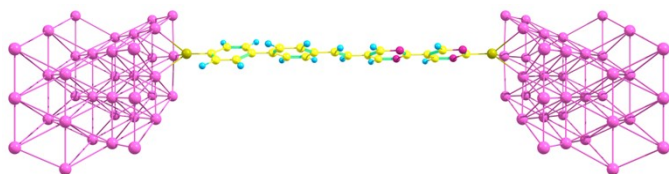


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Au	-1.487299e+00	2.576078e+00	1.214474e+00
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Au	4.461898e+00	2.576078e+00	1.214474e+00
Au	-2.974599e+00	5.152156e+00	1.214474e+00
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Au	2.974599e+00	5.152156e+00	1.214474e+00
Au	1.487299e+00	8.586927e-01	3.643224e+00
Au	4.461898e+00	8.586927e-01	3.643224e+00
Au	7.436497e+00	8.586927e-01	3.643224e+00
Au	0.000000e+00	3.434771e+00	3.643224e+00
Au	2.974599e+00	3.434771e+00	3.643224e+00
Au	5.949197e+00	3.434771e+00	3.643224e+00
Au	-1.487299e+00	6.010849e+00	3.643224e+00

Au 1.487299e+00 6.010849e+00 3.643224e+00
 Au 4.461898e+00 6.010849e+00 3.643224e+00
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 Au 4.461898e+00 4.293463e+00 6.071974e+00
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 Au 4.460030e+00 2.580904e+00 3.097610e+01

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Au	-1.617229e+00	2.487936e+00	3.099262e+01
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Au	-1.486153e+00	4.288201e+00	3.338975e+01
Au	1.488445e+00	4.288201e+00	3.338975e+01
Au	4.463044e+00	4.288201e+00	3.338975e+01
Au	-2.973453e+00	6.864279e+00	3.338975e+01
Au	1.146058e-03	6.864279e+00	3.338975e+01
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Au	4.463044e+00	8.534299e-01	3.581850e+01
Au	7.437643e+00	8.534299e-01	3.581850e+01
Au	1.146058e-03	3.429508e+00	3.581850e+01
Au	2.975745e+00	3.429508e+00	3.581850e+01
Au	5.950344e+00	3.429508e+00	3.581850e+01
Au	-1.486153e+00	6.005586e+00	3.581850e+01
Au	1.488445e+00	6.005586e+00	3.581850e+01
Au	4.463044e+00	6.005586e+00	3.581850e+01
Au	1.146058e-03	-5.262820e-03	3.824725e+01
Au	2.975745e+00	-5.262820e-03	3.824725e+01
Au	5.950344e+00	-5.262820e-03	3.824725e+01
Au	-1.486153e+00	2.570815e+00	3.824725e+01
Au	1.488445e+00	2.570815e+00	3.824725e+01
Au	4.463044e+00	2.570815e+00	3.824725e+01
Au	-2.973453e+00	5.146893e+00	3.824725e+01
Au	1.146058e-03	5.146893e+00	3.824725e+01
Au	2.975745e+00	5.146893e+00	3.824725e+01

2A- π -2D

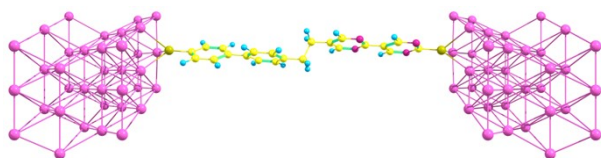


Au	0.000000e+00	0.000000e+00	1.214474e+00
Au	2.974599e+00	0.000000e+00	1.214474e+00
Au	5.949197e+00	0.000000e+00	1.214474e+00
Au	-1.487299e+00	2.576078e+00	1.214474e+00
Au	1.487299e+00	2.576078e+00	1.214474e+00
Au	4.461898e+00	2.576078e+00	1.214474e+00
Au	-2.974599e+00	5.152156e+00	1.214474e+00
Au	0.000000e+00	5.152156e+00	1.214474e+00
Au	2.974599e+00	5.152156e+00	1.214474e+00
Au	1.487299e+00	8.586927e-01	3.643224e+00
Au	4.461898e+00	8.586927e-01	3.643224e+00
Au	7.436497e+00	8.586927e-01	3.643224e+00
Au	0.000000e+00	3.434771e+00	3.643224e+00
Au	2.974599e+00	3.434771e+00	3.643224e+00
Au	5.949197e+00	3.434771e+00	3.643224e+00
Au	-1.487299e+00	6.010849e+00	3.643224e+00

Au 1.487299e+00 6.010849e+00 3.643224e+00
 Au 4.461898e+00 6.010849e+00 3.643224e+00
 Au 0.000000e+00 1.717385e+00 6.071974e+00
 Au 2.974599e+00 1.717385e+00 6.071974e+00
 Au 5.949197e+00 1.717385e+00 6.071974e+00
 Au -1.487299e+00 4.293463e+00 6.071974e+00
 Au 1.487299e+00 4.293463e+00 6.071974e+00
 Au 4.461898e+00 4.293463e+00 6.071974e+00
 Au -2.974599e+00 6.869542e+00 6.071974e+00
 Au 0.000000e+00 6.869542e+00 6.071974e+00
 Au 2.974599e+00 6.869542e+00 6.071974e+00
 Au 2.988329e+00 5.161348e+00 8.452176e+00
 Au -2.993868e+00 5.164165e+00 8.456586e+00
 Au 3.570093e-04 -2.154506e-02 8.461782e+00
 Au -1.612982e+00 2.506126e+00 8.467504e+00
 Au -3.115747e-03 5.319219e+00 8.469317e+00
 Au 1.604367e+00 2.507319e+00 8.480984e+00
 Au 4.456818e+00 2.582868e+00 8.484222e+00
 Au 5.957543e+00 4.702285e-03 8.485055e+00
 Au 2.961270e+00 7.220869e-03 8.496426e+00
 S -1.514134e-02 3.466350e+00 1.020475e+01
 C -2.802583e-02 3.410473e+00 1.197454e+01
 H 9.374946e-01 1.466318e+00 1.204995e+01
 H -9.924923e-01 5.347411e+00 1.219193e+01
 C 5.041869e-01 2.285566e+00 1.264471e+01
 C -5.717364e-01 4.479514e+00 1.272308e+01
 C 4.878556e-01 2.236302e+00 1.404149e+01
 C -5.766550e-01 4.418465e+00 1.412052e+01
 H 9.357532e-01 1.370438e+00 1.455396e+01
 H -1.030380e+00 5.243148e+00 1.469327e+01
 C -4.982924e-02 3.298516e+00 1.481076e+01
 C -5.910153e-02 3.233934e+00 1.629050e+01
 H -4.403891e-01 1.090763e+00 1.639084e+01
 H 3.227209e-01 5.359969e+00 1.658897e+01
 C -2.558886e-01 2.008241e+00 1.696943e+01
 C 1.325313e-01 4.395335e+00 1.708278e+01
 C -2.610722e-01 1.949356e+00 1.836427e+01
 C 1.276271e-01 4.334804e+00 1.847513e+01
 H -4.274624e-01 9.834542e-01 1.886683e+01
 H 2.931420e-01 5.259916e+00 1.904709e+01
 C -7.082811e-02 3.107592e+00 1.915767e+01
 C -8.832964e-02 2.979847e+00 2.061034e+01
 H -2.522306e-01 1.952869e+00 2.097999e+01
 H 2.374867e-01 5.010670e+00 2.116320e+01
 C 7.368698e-02 3.980222e+00 2.152429e+01
 C 5.321942e-02 3.835433e+00 2.297035e+01
 H -2.936169e-01 1.674984e+00 2.313029e+01
 H 3.943896e-01 5.955736e+00 2.335002e+01
 C -1.410347e-01 2.621189e+00 2.367856e+01
 C 2.357732e-01 4.962343e+00 2.380948e+01
 N -1.533936e-01 2.534202e+00 2.500547e+01
 N 2.300296e-01 4.912256e+00 2.513845e+01
 C 3.406573e-02 3.691175e+00 2.568513e+01
 C 2.412675e-02 3.617267e+00 2.715493e+01
 H -3.192477e-01 1.470436e+00 2.728699e+01
 H 3.700127e-01 5.742345e+00 2.746770e+01
 C -1.702273e-01 2.405216e+00 2.785549e+01
 C 2.106429e-01 4.766086e+00 2.795703e+01
 N -1.830717e-01 2.335032e+00 2.919069e+01
 N 2.024214e-01 4.729108e+00 2.929289e+01

C	2.722700e-03	3.509032e+00	2.982269e+01
S	-1.599572e-02	3.429291e+00	3.160623e+01
Au	3.022781e-03	5.290030e+00	3.329289e+01
Au	4.459410e+00	2.575258e+00	3.329956e+01
Au	2.972368e+00	-1.276043e-02	3.330299e+01
Au	5.951147e+00	-1.563482e-02	3.330331e+01
Au	1.615209e+00	2.490788e+00	3.332139e+01
Au	-1.621634e+00	2.482492e+00	3.332140e+01
Au	2.243443e-03	-2.935126e-02	3.333569e+01
Au	2.993601e+00	5.153022e+00	3.333683e+01
Au	-2.988392e+00	5.151954e+00	3.333797e+01
Au	4.560626e-04	1.703366e+00	3.571558e+01
Au	2.975055e+00	1.703366e+00	3.571558e+01
Au	5.949654e+00	1.703366e+00	3.571558e+01
Au	-1.486843e+00	4.279444e+00	3.571558e+01
Au	1.487755e+00	4.279444e+00	3.571558e+01
Au	4.462354e+00	4.279444e+00	3.571558e+01
Au	-2.974143e+00	6.855522e+00	3.571558e+01
Au	4.560626e-04	6.855522e+00	3.571558e+01
Au	2.975055e+00	6.855522e+00	3.571558e+01
Au	1.487755e+00	8.446729e-01	3.814433e+01
Au	4.462354e+00	8.446729e-01	3.814433e+01
Au	7.436953e+00	8.446729e-01	3.814433e+01
Au	4.560626e-04	3.420751e+00	3.814433e+01
Au	2.975055e+00	3.420751e+00	3.814433e+01
Au	5.949654e+00	3.420751e+00	3.814433e+01
Au	-1.486843e+00	5.996829e+00	3.814433e+01
Au	1.487755e+00	5.996829e+00	3.814433e+01
Au	4.462354e+00	5.996829e+00	3.814433e+01
Au	4.560626e-04	-1.401976e-02	4.057308e+01
Au	2.975055e+00	-1.401976e-02	4.057308e+01
Au	5.949654e+00	-1.401976e-02	4.057308e+01
Au	-1.486843e+00	2.562058e+00	4.057308e+01
Au	1.487755e+00	2.562058e+00	4.057308e+01
Au	4.462354e+00	2.562058e+00	4.057308e+01
Au	-2.974143e+00	5.138136e+00	4.057308e+01
Au	4.560626e-04	5.138136e+00	4.057308e+01
Au	2.975055e+00	5.138136e+00	4.057308e+01

2A-σ-2D



Au	0.000000e+00	0.000000e+00	1.214474e+00
Au	2.974599e+00	0.000000e+00	1.214474e+00
Au	5.949197e+00	0.000000e+00	1.214474e+00
Au	-1.487299e+00	2.576078e+00	1.214474e+00
Au	1.487299e+00	2.576078e+00	1.214474e+00
Au	4.461898e+00	2.576078e+00	1.214474e+00
Au	-2.974599e+00	5.152156e+00	1.214474e+00
Au	0.000000e+00	5.152156e+00	1.214474e+00
Au	2.974599e+00	5.152156e+00	1.214474e+00
Au	1.487299e+00	8.586927e-01	3.643224e+00
Au	4.461898e+00	8.586927e-01	3.643224e+00
Au	7.436497e+00	8.586927e-01	3.643224e+00
Au	0.000000e+00	3.434771e+00	3.643224e+00
Au	2.974599e+00	3.434771e+00	3.643224e+00

Au	5.949197e+00	3.434771e+00	3.643224e+00
Au	-1.487299e+00	6.010849e+00	3.643224e+00
Au	1.487299e+00	6.010849e+00	3.643224e+00
Au	4.461898e+00	6.010849e+00	3.643224e+00
Au	0.000000e+00	1.717385e+00	6.071974e+00
Au	2.974599e+00	1.717385e+00	6.071974e+00
Au	5.949197e+00	1.717385e+00	6.071974e+00
Au	-1.487299e+00	4.293463e+00	6.071974e+00
Au	1.487299e+00	4.293463e+00	6.071974e+00
Au	4.461898e+00	4.293463e+00	6.071974e+00
Au	-2.974599e+00	6.869542e+00	6.071974e+00
Au	0.000000e+00	6.869542e+00	6.071974e+00
Au	2.974599e+00	6.869542e+00	6.071974e+00
Au	2.995031e+00	5.163620e+00	8.454734e+00
Au	-2.993608e+00	5.163710e+00	8.459220e+00
Au	-1.615636e+00	2.500824e+00	8.462735e+00
Au	1.582159e-03	-2.212744e-02	8.464242e+00
Au	5.113407e-04	5.307784e+00	8.469036e+00
Au	1.601815e+00	2.508989e+00	8.479533e+00
Au	4.455864e+00	2.582898e+00	8.485401e+00
Au	5.955864e+00	-2.294300e-03	8.486147e+00
Au	2.962746e+00	1.798245e-03	8.494391e+00
S	-7.857378e-03	3.466243e+00	1.021467e+01
C	1.128835e-01	3.459535e+00	1.198568e+01
H	1.057495e+00	1.507205e+00	1.202995e+01
H	-8.144874e-01	5.411366e+00	1.223969e+01
C	6.800420e-01	2.343238e+00	1.263887e+01
C	-3.631681e-01	4.547776e+00	1.275101e+01
C	7.713742e-01	2.324155e+00	1.403261e+01
C	-2.611605e-01	4.512968e+00	1.414583e+01
H	1.246519e+00	1.466055e+00	1.453078e+01
H	-6.560833e-01	5.351449e+00	1.473877e+01
C	3.064462e-01	3.405408e+00	1.481581e+01
C	4.123223e-01	3.376449e+00	1.629430e+01
H	-2.718738e-02	1.253882e+00	1.647098e+01
H	8.966770e-01	5.487325e+00	1.649475e+01
C	2.272676e-01	2.175491e+00	1.701557e+01
C	7.082875e-01	4.545289e+00	1.703133e+01
C	3.323259e-01	2.146613e+00	1.841059e+01
C	8.106525e-01	4.512588e+00	1.842654e+01
H	1.822628e-01	1.194357e+00	1.894487e+01
H	1.060028e+00	5.436987e+00	1.897263e+01
C	6.284569e-01	3.313177e+00	1.914287e+01
C	6.997021e-01	3.288424e+00	2.065226e+01
H	-1.407795e+00	2.821917e+00	2.094385e+01
H	-1.040549e+00	4.562629e+00	2.095421e+01
H	1.064390e+00	2.300242e+00	2.100067e+01
H	1.431424e+00	4.041246e+00	2.101130e+01
C	-6.762771e-01	3.574500e+00	2.130314e+01
C	-6.142591e-01	3.551980e+00	2.280712e+01
H	-1.070345e+00	1.432296e+00	2.305095e+01
H	-1.537789e-01	5.668479e+00	2.307612e+01
C	-8.156992e-01	2.380600e+00	2.356296e+01
C	-3.148619e-01	4.693501e+00	2.357604e+01
N	-7.324988e-01	2.332666e+00	2.489415e+01
N	-2.220440e-01	4.686940e+00	2.490687e+01
C	-4.320364e-01	3.496489e+00	2.551172e+01
C	-3.288080e-01	3.469268e+00	2.698487e+01
H	1.472062e-01	5.577012e+00	2.720092e+01
H	-7.686347e-01	1.354352e+00	2.720465e+01

C	-2.064818e-02	4.625449e+00	2.773263e+01
C	-5.271651e-01	2.290862e+00	2.773630e+01
N	7.646865e-02	4.625764e+00	2.906465e+01
N	-4.385298e-01	2.254546e+00	2.906984e+01
C	-1.450805e-01	3.434076e+00	2.964959e+01
S	-1.967112e-02	3.428577e+00	3.143207e+01
Au	2.971643e+00	-8.585891e-03	3.313763e+01
Au	4.464966e+00	2.583166e+00	3.313783e+01
Au	5.955249e+00	-7.059626e-03	3.314040e+01
Au	2.693788e-03	5.298175e+00	3.314158e+01
Au	-1.613179e+00	2.493154e+00	3.315400e+01
Au	1.785701e-03	-2.726147e-02	3.316568e+01
Au	1.618915e+00	2.493460e+00	3.316581e+01
Au	2.993326e+00	5.158769e+00	3.316667e+01
Au	-2.993093e+00	5.160894e+00	3.316798e+01
Au	3.509477e-03	1.713625e+00	3.555220e+01
Au	2.978108e+00	1.713625e+00	3.555220e+01
Au	5.952707e+00	1.713625e+00	3.555220e+01
Au	-1.483790e+00	4.289704e+00	3.555220e+01
Au	1.490809e+00	4.289704e+00	3.555220e+01
Au	4.465408e+00	4.289704e+00	3.555220e+01
Au	-2.971089e+00	6.865782e+00	3.555220e+01
Au	3.509477e-03	6.865782e+00	3.555220e+01
Au	2.978108e+00	6.865782e+00	3.555220e+01
Au	1.490809e+00	8.549328e-01	3.798095e+01
Au	4.465408e+00	8.549328e-01	3.798095e+01
Au	7.440006e+00	8.549328e-01	3.798095e+01
Au	3.509477e-03	3.431011e+00	3.798095e+01
Au	2.978108e+00	3.431011e+00	3.798095e+01
Au	5.952707e+00	3.431011e+00	3.798095e+01
Au	-1.483790e+00	6.007089e+00	3.798095e+01
Au	1.490809e+00	6.007089e+00	3.798095e+01
Au	4.465408e+00	6.007089e+00	3.798095e+01
Au	3.509477e-03	-3.759895e-03	4.040970e+01
Au	2.978108e+00	-3.759895e-03	4.040970e+01
Au	5.952707e+00	-3.759895e-03	4.040970e+01
Au	-1.483790e+00	2.572318e+00	4.040970e+01
Au	1.490809e+00	2.572318e+00	4.040970e+01
Au	4.465408e+00	2.572318e+00	4.040970e+01
Au	-2.971089e+00	5.148396e+00	4.040970e+01
Au	3.509477e-03	5.148396e+00	4.040970e+01
Au	2.978108e+00	5.148396e+00	4.040970e+01