Supporting Information

Impact of molecular packing on electronic polarization in organic crystals: The case of pentacene *vs.* TIPS-pentacene

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I. Electrostatic Potential Plots

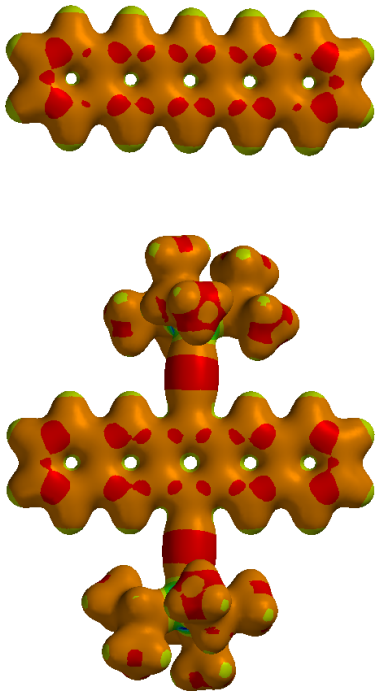

Figure S1. Electrostatic potential surface of pentacene (top) and TIPS-pentacene (bottom). The electron attraction/repulsion of the acene backbones are similar in both molecules. The surfaces are created with an isovalue of 0.03 e/Å^3.

II. Interaction Energies of Additional Dimers

TIPS-pentacene has two symmetry-nonequivalent stacking partners, one with larger backbone overlap (considered in the main manuscript) and a second with smaller overlap. SAPT(0) results for this second partner are provided below along with a pentacene brickwork configuration assuming the same geometry.

Table S1. Dimer interaction energies of the second TIPS-pentacene dimer set (*i.e.* smaller backbone overlap), and corresponding pentacene brickwork configuration, as determined with SAPT(0)/jun-cc-pvdz and AMOEBA force field calculations. All units in kcal/mol.

	SAPT	AMOEBA
Pentacene brickwork	-10.70	-6.70
TIPS-Pentacene	-14.65	-5.52

Table S2. SAPT(0) energy components of the second TIPS-pentacene dimer set (*i.e.*, smaller backbone overlap), and corresponding pentacene brickwork configuration, as determined at the SAPT(0)/jun-cc-pvdz level. All units in kcal/mol.

	Electrostatic	Dispersion	Induction	Exchange
Pentacene brickwork	-5.16	-16.06	-1.20	11.73
TIPS-Pentacene	-5.90	-20.94	-1.37	13.55

III. Distributed Multipole Analysis (DMA) Electrostatic Interactions

Table S3. DMA electrostatic energies (HF/6-311G**) for a pentacene herringbone dimer (charge through 32-pole interactions). Here, A/B refer to the specific molecules in interaction; q denotes the 0-rank charge, μ the 1-rank dipole, Θ the 2-rank quadrupole, Ω the 3-rank octupole, Φ the 4-rank 16-pole, and Λ the 5-rank 32-pole. Rank refers to the total rank of the electrostatic interactions (*i.e.*, a dipole – quadrupole interaction is rank 1 plus rank 2 for a total rank 3) and E_{elect} is the sum electrostatic interaction energy for the given rank (*e.g.*, E_{elect} for rank 2 is the sum of μA+ μB, ΘA+ qB, qA+ ΘB). The second-rank quadrupole interactions are the largest contributor. All values in kcal/mol.

	qA	μA	ΘA	ΩA	ΦA	ΛA
qB	0.1143	0.0770	0.0440	0.0038	-0.0049	-0.0037
μB	-0.2814	-0.5053	-0.2452	-0.2329	0.0559	
ΘB	-0.0072	-0.1846	-0.0514	-0.0471		
ΩB	-0.0208	0.0170	0.0062			
ΦB	0.0178	-0.0083				
ΛB	-0.0087					

Rank	E_{elect}
0	0.1143
1	-0.2044
2	-0.4684
3	-0.4471
4	-0.2543
5	-0.0058

Table S4. DMA electrostatic energies (HF/6-311G**) of a pentacene brickwork dimer (charge through 32-pole interactions). See Table S3 for notations. The second-rank quadrupole interactions are the largest contributor. All values in kcal/mol.

	qA	μA	ΘA	ΩA	ΦA	ΛA
qB	-0.0731	0.0812	0.0342	0.0216	0.0008	-0.0040
μB	0.0812	0.6819	0.2820	0.0651	-0.0192	
ΘB	0.0342	0.2820	0.1031	-0.0060		
ΩB	0.0217	0.0651	-0.0060			
ΦB	0.0008	-0.0192				
ΛB	-0.0040					

Rank	E_{elect}
0	-0.0731
1	0.1624
2	0.7504
3	0.6073
4	0.2348
5	-0.0584

Table S5. DMA electrostatic energies (HF/6-311G**) for a TIPS-pentacene brickwork dimer (charge through 32-pole interactions). See Table S3 for notations. The second-rank quadrupole interactions are the largest contributor. All values in kcal/mol.

	qA	μA	ΘA	ΩA	ΦA	ΛA
qB	-0.3121	0.2002	0.2479	0.0779	-0.0146	-0.0129
μB	0.2001	0.1864	-0.0882	0.0121	-0.0125	
ΘB	0.2479	-0.0885	0.2567	0.0015		
ΩB	0.0780	0.0120	0.0016			
ΦB	-0.0146	-0.0125				
ΛB	-0.0129					

Rank	E_{elect}
0	-0.3121
1	0.4003
2	0.6822
3	-0.0207
4	0.2515
5	-0.0477

Table S6. DMA electrostatic energies (HF/6-311G**) for a lesser overlap pentacene brickwork dimer (charge through 32-pole interactions). See Table S3 for notations. The first-rank quadrupole interactions are the largest contributor. All values in kcal/mol.

	qA	μA	ΘA	ΩA	ΦA	ΛA
qB	-0.0720	-0.1994	-0.0574	0.0138	-0.0017	-0.0018
μB	-0.2004	0.4491	0.1277	-0.0086	0.0077	
ΘB	-0.0557	0.1273	0.0427	-0.0336		
ΩB	0.0133	-0.0088	-0.0334			
ΦB	-0.0014	0.0073				
ΛB	-0.0019					

Rank	E_{elect}
0	-0.0720
1	-0.3998
2	0.3360
3	0.2820
4	0.0222
5	-0.0556

Table S7. DMA electrostatic energies (HF/6-311G**) for a lesser overlap TIPS-pentacene brickwork dimer (charge through 32-pole interactions). See Table S3 for notations. The first-rank quadrupole interactions are the largest contributor. All values in kcal/mol.

	qA	μA	ΘA	ΩA	ΦA	ΛA
qB	-0.1127	-0.2172	-0.0732	0.0108	0.0028	-0.1127
μB	-0.2241	0.3961	0.0346	-0.0233	0.0057	
ΘB	-0.0626	0.0270	0.0862	-0.0504		
ΩB	0.0075	-0.0210	-0.0489			
ΦB	0.0045	0.0044				
ΛB	-0.0021					

Rank	E_{elect}
0	-0.1127
1	-0.4413
2	0.2604
3	0.0798
4	0.0491
5	-0.0929

IV. Extrapolated Polarization Energies

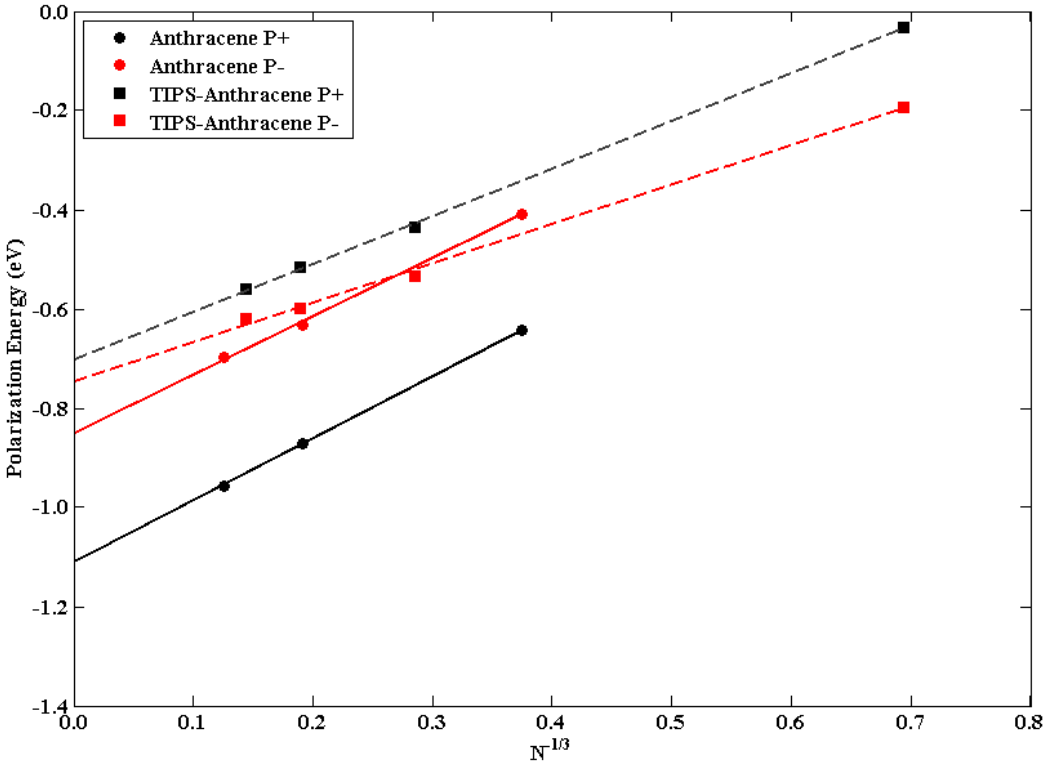

Figure S2. Polarization energy vs. $N^{-1/3}$, where N is the number of molecules in the cluster, for TIPS-anthracene and anthracene[1] clusters with radii ranging from 10 to 40 Å.

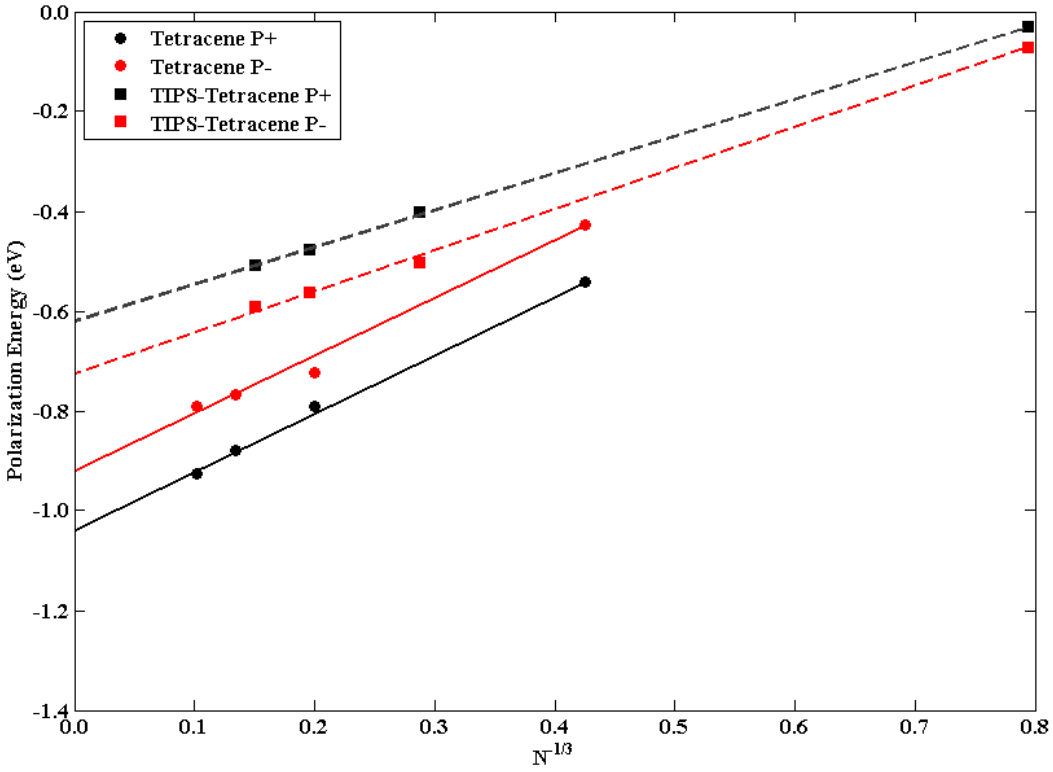

Figure S3. Polarization energy plotted vs. $N^{-1/3}$, where N is the number of molecules in the cluster, for TIPS-tetracene and tetracene[1] clusters with radii ranging from 10 to 40 Å.

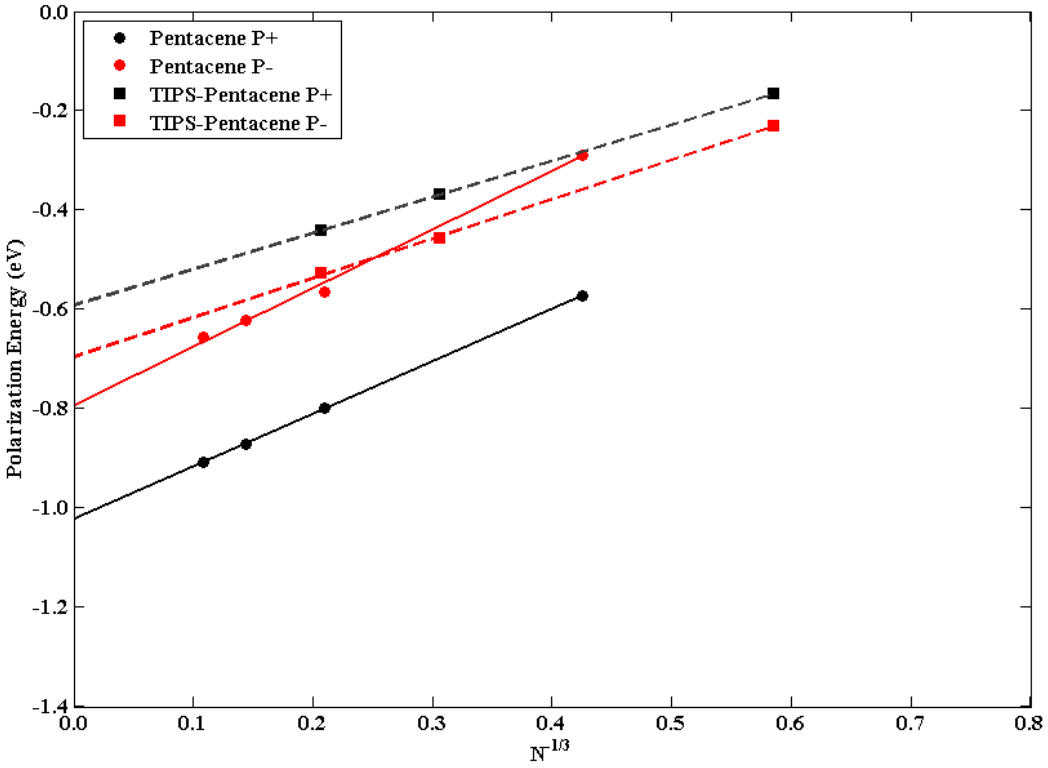

Figure S4. Polarization energy plotted vs. $N^{-1/3}$, where N is the number of molecules in the cluster, for TIPS-pentacene and pentacene[1] clusters with radii ranging from 10 to 30 Å.

V. Coordinates for Monomer and Dimer Structures

The monomer and dimer structures used in this work are given below along with single-point total energies. Monomer energies have been calculated at the B97d/6-31+g(d,p) level, and dimer energies have been calculated at the B97d/6-31+g(d,p) level with counterpoise correction. Pentacene and TIPS-pentacene geometries were taken from the crystal structure files, reported in the Methodology section, without further modification. The brickwork pentacene geometry is that of TIPS-pentacene where the TIPS groups have been replaced by hydrogen atoms.

Pentacene Monomer

Total Energy = -846.0973615 Hartrees

36

C	-1.189823	-0.464424	-0.584114
C	-1.018173	-0.574160	0.797712
C	-2.004460	-1.139299	1.634792
C	-1.827275	-1.248338	3.003075
C	-2.824304	-1.828717	3.849929
C	-2.625189	-1.932369	5.178703
C	-1.423462	-1.456290	5.777196
C	-0.443968	-0.904948	5.012571
C	-0.607971	-0.777299	3.599474
C	0.371536	-0.214842	2.793805
C	-0.209036	0.093474	-1.403045
H	-2.051187	-0.769494	-0.970265
H	-2.848721	-1.449413	1.203408
H	-3.665057	-2.137417	3.441300
H	-3.324255	-2.358163	5.761560
H	-1.311720	-1.541714	6.770915
H	0.392382	-0.554276	5.441861
H	1.250952	0.118849	3.205365
C	0.209036	-0.093474	1.403045
C	1.189823	0.464424	0.584114
C	1.018173	0.574160	-0.797712
C	2.004460	1.139299	-1.634792
C	1.827275	1.248338	-3.003075
C	2.824304	1.828717	-3.849929
C	2.625189	1.932369	-5.178703
C	1.423462	1.456290	-5.777196
C	0.443968	0.904948	-5.012571
C	0.607971	0.777299	-3.599474
C	-0.371536	0.214842	-2.793805
H	-1.250952	-0.118849	-3.205365
H	-0.392382	0.554276	-5.441861
H	1.311720	1.541714	-6.770915
H	3.324255	2.358163	-5.761560
H	3.665057	2.137417	-3.441300
H	2.848721	1.449413	-1.203408
H	2.051187	0.769494	0.970265

Brickwork Pentacene Monomer

Total Energy = -845.9836571 Hartrees

36

C	-3.969240	-0.486845	1.319840
C	-4.955030	0.344053	0.736361
C	-6.130430	0.699295	1.419620
C	-7.117805	1.480810	0.847846
C	-8.315286	1.834420	1.542320
C	-9.265260	2.591430	0.952404
C	-9.098190	3.046050	-0.383106
C	-7.987711	2.740990	-1.081870
C	-6.947209	1.944800	-0.504980
C	-5.788420	1.620350	-1.186420
C	-2.791360	-0.828060	0.615311
H	-4.117477	-0.863175	2.310446
H	-6.251990	0.390578	2.308860
H	-8.446208	1.531850	2.434200
H	-10.050250	2.822660	1.434790
H	-9.778060	3.571350	-0.788310
H	-7.894137	3.058960	-1.972430
H	-5.673100	1.942910	-2.073020
C	-4.773640	0.828060	-0.615311
C	-3.595760	0.486845	-1.319840
C	-2.609970	-0.344053	-0.736361
C	-1.434570	-0.699295	-1.419620
C	-0.447200	-1.480810	-0.847846
C	0.750290	-1.834420	-1.542320
C	1.700250	-2.591430	-0.952404
C	1.533190	-3.046050	0.383106
C	0.422710	-2.740990	1.081870
C	-0.617790	-1.944800	0.504980
C	-1.776580	-1.620350	1.186420
H	-1.891900	-1.942910	2.073020
H	0.329140	-3.058960	1.972430
H	2.213060	-3.571350	0.788310
H	2.485300	-2.822660	-1.434790
H	0.881210	-1.531850	-2.434200
H	-1.313010	-0.390578	-2.308860
H	-3.447523	0.863175	-2.310446

TIPS-Pentacene Monomer

Total Energy = -2286.3431381 Hartrees

100

Si	2.714699	-2.280379	5.324393
C	3.595757	-0.486845	1.319843
C	2.609971	0.344053	0.736361
C	1.434572	0.699295	1.419618
H	1.313012	0.390578	2.308859
C	0.447195	1.480809	0.847846
C	-0.750286	1.834425	1.542318
H	-0.881208	1.531850	2.434197
C	-1.700255	2.591431	0.952404
H	-2.485252	2.822662	1.434791
C	-1.533194	3.046047	-0.383106
H	-2.213057	3.571348	-0.788310
C	-0.422711	2.740988	-1.081865
H	-0.329137	3.058957	-1.972425
C	0.617791	1.944800	-0.504980
C	1.776576	1.620353	-1.186424
H	1.891903	1.942913	-2.073025
C	4.773639	-0.828060	0.615311
C	3.371240	-1.018324	2.634738
C	3.143056	-1.498730	3.716603
C	3.010307	-4.133902	5.162938
H	2.775385	-4.553431	6.039315
C	2.116453	-4.774966	4.085856
H	2.264693	-4.324765	3.227455
H	1.176293	-4.682983	4.345602
H	2.339753	-5.725520	3.999273
C	4.484880	-4.443702	4.883236
H	4.603901	-5.412710	4.792531
H	5.034278	-4.115868	5.625370
H	4.760641	-4.002194	4.053696
C	3.880699	-1.558541	6.605975
H	4.804532	-1.747773	6.271850
C	3.792399	-2.218354	7.983374
H	4.530352	-1.900690	8.544427
H	3.852630	-3.191153	7.884753
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C	0.388018	-2.656414	6.849065
H	0.779435	-3.554737	6.882049
H	-0.587679	-2.726871	6.796291
H	0.636142	-2.163500	7.658815
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H	0.865788	-0.165198	4.686983
H	0.664549	-0.034031	6.270201
H	-0.536787	-0.556923	5.351605
C	2.791361	0.828060	-0.615311
C	3.969243	0.486845	-1.319843
C	4.955029	-0.344053	-0.736361
C	6.130428	-0.699295	-1.419618
H	6.251988	-0.390578	-2.308859
C	7.117805	-1.480809	-0.847846
C	8.315286	-1.834425	-1.542318
H	8.446208	-1.531850	-2.434197
C	9.265255	-2.591431	-0.952404
H	10.050252	-2.822662	-1.434791
C	9.098194	-3.046047	0.383106
H	9.778057	-3.571348	0.788310
C	7.987711	-2.740988	1.081865
H	7.894137	-3.058957	1.972425

C	6.947209	-1.944800	0.504980
C	5.788424	-1.620353	1.186424
H	5.673097	-1.942913	2.073025
C	4.193760	1.018324	-2.634738
C	4.421944	1.498730	-3.716603
Si	4.850301	2.280379	-5.324393
C	4.554693	4.133902	-5.162938
H	4.789615	4.553431	-6.039315
C	5.448547	4.774966	-4.085856
H	5.300307	4.324765	-3.227455
H	6.388707	4.682983	-4.345602
H	5.225247	5.725520	-3.999273
C	3.080120	4.443702	-4.883236
H	2.961099	5.412710	-4.792531
H	2.530722	4.115868	-5.625370
H	2.804359	4.002194	-4.053696
C	3.684301	1.558541	-6.605975
H	2.760468	1.747773	-6.271850
C	3.772601	2.218354	-7.983374
H	3.034648	1.900690	-8.544427
H	3.712370	3.191153	-7.884753
H	4.626264	1.984330	-8.402597
C	3.778214	0.037562	-6.732467
H	4.655026	-0.206126	-7.096443
H	3.666096	-0.371234	-5.849659
H	3.074168	-0.284427	-7.332276
C	6.663803	1.932486	-5.648788
H	7.115820	2.412745	-4.896430
C	7.176982	2.656414	-6.849065
H	6.785565	3.554737	-6.882049
H	8.152679	2.726871	-6.796291
H	6.928858	2.163500	-7.658815
C	7.129476	0.559408	-5.475294
H	6.699212	0.165198	-4.686983
H	6.900451	0.034031	-6.270201
H	8.101787	0.556923	-5.351605

Pentacene Dimer

Total Energy = -1692.1923423 Hartrees

72

C	-0.181948	1.196078	0.221695
C	-1.162325	1.196571	1.218904
C	-0.993112	0.524627	2.442276
C	-1.963018	0.538257	3.423849
C	-1.790657	-0.123930	4.676539
C	-2.752240	-0.078466	5.621256
C	-3.965710	0.636025	5.396210
C	-4.177234	1.277133	4.230635
C	-3.188588	1.263380	3.195453
C	-3.377868	1.925090	1.997071
C	-0.354612	1.875565	-0.985343
H	0.671632	0.701306	0.374145
H	-0.130419	0.035704	2.577136
H	-0.949182	-0.616144	4.840157
H	-2.661615	-0.512284	6.487514
H	-4.637680	0.629708	6.131518
H	-5.024583	1.756005	4.048589
H	-4.208104	2.442487	1.837222
C	-2.393311	1.924311	0.985343
C	-2.565974	2.603797	-0.221695
C	-1.585597	2.603304	-1.218904
C	-1.754810	3.275248	-2.442276
C	-0.784904	3.261619	-3.423849
C	-0.957265	3.923805	-4.676539
C	0.004317	3.878342	-5.621256
C	1.217788	3.163850	-5.396210
C	1.429311	2.522742	-4.230635
C	0.440665	2.536495	-3.195453
C	0.629945	1.874785	-1.997071
H	1.460182	1.357389	-1.837222
H	2.276660	2.043871	-4.048589
H	1.889757	3.170167	-6.131518
H	-0.086307	4.312160	-6.487514
H	-1.798740	4.416019	-4.840157
H	-2.617504	3.764172	-2.577136
H	-3.419554	3.098570	-0.374145
C	0.184139	-2.364362	-0.584114
C	0.355789	-2.474098	0.797712
C	-0.630498	-3.039237	1.634792
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C	-1.450342	-3.728655	3.849929
C	-1.251227	-3.832307	5.178703
C	-0.049500	-3.356228	5.777196
C	0.929994	-2.804886	5.012571
C	0.765991	-2.677237	3.599474
C	1.745498	-2.114780	2.793805
C	1.164926	-1.806464	-1.403045
H	-0.677225	-2.669432	-0.970265
H	-1.474759	-3.349351	1.203408
H	-2.291095	-4.037355	3.441300
H	-1.950293	-4.258101	5.761560
H	0.062242	-3.441652	6.770915
H	1.766344	-2.454214	5.441861
H	2.624914	-1.781089	3.205365
C	1.582998	-1.993412	1.403045
C	2.563785	-1.435514	0.584114
C	2.392135	-1.325778	-0.797712
C	3.378422	-0.760639	-1.634792
C	3.201237	-0.651600	-3.003075
C	4.198266	-0.071221	-3.849929
C	3.999151	0.032431	-5.178703
C	2.797424	-0.443648	-5.777196
C	1.817930	-0.994990	-5.012571
C	1.981933	-1.122639	-3.599474

C	1.002426	-1.685096	-2.793805
H	0.123010	-2.018787	-3.205365
H	0.981580	-1.345662	-5.441861
H	2.685682	-0.358224	-6.770915
H	4.698217	0.458225	-5.761560
H	5.039019	0.237479	-3.441300
H	4.222683	-0.450525	-1.203408
H	3.425149	-1.130444	0.970265

Brickwork Pentacene Dimer

Total Energy = -1691.9849786 Hartrees

72

C	-3.969240	-0.486845	1.319840
C	-4.955030	0.344053	0.736361
C	-6.130430	0.699295	1.419620
C	-7.117805	1.480810	0.847846
C	-8.315286	1.834420	1.542320
C	-9.265260	2.591430	0.952404
C	-9.098190	3.046050	-0.383106
C	-7.987711	2.740990	-1.081870
C	-6.947209	1.944800	-0.504980
C	-5.788420	1.620350	-1.186420
C	-2.791360	-0.828060	0.615311
H	-4.117477	-0.863175	2.310446
H	-6.251990	0.390578	2.308860
H	-8.446208	1.531850	2.434200
H	-10.050250	2.822660	1.434790
H	-9.778060	3.571350	-0.788310
H	-7.894137	3.058960	-1.972430
H	-5.673100	1.942910	-2.073020
C	-4.773640	0.828060	-0.615311
C	-3.595760	0.486845	-1.319840
C	-2.609970	-0.344053	-0.736361
C	-1.434570	-0.699295	-1.419620
C	-0.447200	-1.480810	-0.847846
C	0.750290	-1.834420	-1.542320
C	1.700250	-2.591430	-0.952404
C	1.533190	-3.046050	0.383106
C	0.422710	-2.740990	1.081870
C	-0.617790	-1.944800	0.504980
C	-1.776580	-1.620350	1.186420
H	-1.891900	-1.942910	2.073020
H	0.329140	-3.058960	1.972430
H	2.213060	-3.571350	0.788310
H	2.485300	-2.822660	-1.434790
H	0.881210	-1.531850	-2.434200
H	-1.313010	-0.390578	-2.308860
H	-3.447523	0.863175	-2.310446
C	3.595800	-0.486845	1.319840
C	2.610000	0.344053	0.736361
C	1.434570	0.699295	1.419620
C	0.447200	1.480810	0.847846
C	-0.750290	1.834420	1.542320
C	-1.700250	2.591430	0.952404
C	-1.533190	3.046050	-0.383106
C	-0.422710	2.740990	-1.081870
C	0.617790	1.944800	-0.504980
C	1.776580	1.620350	-1.186420
C	4.773600	-0.828060	0.615311
H	3.447587	-0.863155	2.310458
H	1.313010	0.390578	2.308860
H	-0.881210	1.531850	2.434200
H	-2.485250	2.822660	1.434790
H	-2.213060	3.571350	-0.788310
H	-0.329140	3.058960	-1.972430
H	1.891900	1.942910	-2.073020
C	2.791400	0.828060	-0.615311
C	3.969200	0.486845	-1.319840
C	4.955000	-0.344053	-0.736361
C	6.130400	-0.699295	-1.419620
C	7.117800	-1.480810	-0.847846
C	8.315300	-1.834420	-1.542320
C	9.265300	-2.591430	-0.952404
C	9.098200	-3.046050	0.383106
C	7.987700	-2.740990	1.081870
C	6.947200	-1.944800	0.504980

C	5.788400	-1.620350	1.186420
H	5.673100	-1.942910	2.073020
H	7.894100	-3.058960	1.972430
H	9.778100	-3.571350	0.788310
H	10.050300	-2.822660	-1.434790
H	8.446200	-1.531850	-2.434200
H	6.252000	-0.390578	-2.308860
H	4.117413	0.863155	-2.310458

TIPS-Pentacene Dimer

Total Energy = -4572.7055938 Hartrees

200

Si	-4.850300	-2.280380	5.324390
C	-3.969240	-0.486845	1.319840
C	-4.955030	0.344053	0.736361
C	-6.130430	0.699295	1.419620
H	-6.251990	0.390578	2.308860
C	-7.117805	1.480810	0.847846
C	-8.315286	1.834420	1.542320
H	-8.446208	1.531850	2.434200
C	-9.265260	2.591430	0.952404
H	-10.050250	2.822660	1.434790
C	-9.098190	3.046050	-0.383106
H	-9.778060	3.571350	-0.788310
C	-7.987711	2.740990	-1.081870
H	-7.894137	3.058960	-1.972430
C	-6.947209	1.944800	-0.504980
C	-5.788420	1.620350	-1.186420
H	-5.673100	1.942910	-2.073020
C	-2.791360	-0.828060	0.615311
C	-4.193760	-1.018320	2.634740
C	-4.421940	-1.498730	3.716600
C	-4.554690	-4.133900	5.162940
H	-4.789620	-4.553430	6.039320
C	-5.448550	-4.774970	4.085860
H	-5.300310	-4.324770	3.227450
H	-6.388710	-4.682980	4.345600
H	-5.225250	-5.725520	3.999270
C	-3.080120	-4.443700	4.883240
H	-2.961100	-5.412710	4.792530
H	-2.530720	-4.115870	5.625370
H	-2.804360	-4.002190	4.053700
C	-3.684300	-1.558540	6.605970
H	-2.760470	-1.747770	6.271850
C	-3.772600	-2.218350	7.983370
H	-3.034650	-1.900690	8.544430
H	-3.712370	-3.191150	7.884750
H	-4.626260	-1.984330	8.402600
C	-3.778210	-0.037562	6.732470
H	-4.655030	0.206126	7.096440
H	-3.666100	0.371234	5.849660
H	-3.074170	0.284427	7.332280
C	-6.663803	-1.932490	5.648790
H	-7.115820	-2.412750	4.896430
C	-7.176982	-2.656410	6.849070
H	-6.785565	-3.554740	6.882050
H	-8.152679	-2.726870	6.796290
H	-6.928858	-2.163500	7.658810
C	-7.129476	-0.559408	5.475290
H	-6.699212	-0.165198	4.686980
H	-6.900451	-0.034031	6.270200
H	-8.101787	-0.556923	5.351610
C	-4.773640	0.828060	-0.615311
C	-3.595760	0.486845	-1.319840
C	-2.609970	-0.344053	-0.736361
C	-1.434570	-0.699295	-1.419620
H	-1.313010	-0.390578	-2.308860
C	-0.447200	-1.480810	-0.847846
C	0.750290	-1.834420	-1.542320
H	0.881210	-1.531850	-2.434200
C	1.700250	-2.591430	-0.952404
H	2.485300	-2.822660	-1.434790
C	1.533190	-3.046050	0.383106
H	2.213060	-3.571350	0.788310
C	0.422710	-2.740990	1.081870
H	0.329140	-3.058960	1.972430

C	-0.617790	-1.944800	0.504980
C	-1.776580	-1.620350	1.186420
H	-1.891900	-1.942910	2.073020
C	-3.371240	1.018320	-2.634740
C	-3.143060	1.498730	-3.716600
Si	-2.714700	2.280380	-5.324390
C	-3.010310	4.133900	-5.162940
H	-2.775380	4.553430	-6.039320
C	-2.116450	4.774970	-4.085860
H	-2.264690	4.324770	-3.227450
H	-1.176290	4.682980	-4.345600
H	-2.339750	5.725520	-3.999270
C	-4.484880	4.443700	-4.883240
H	-4.603900	5.412710	-4.792530
H	-5.034280	4.115870	-5.625370
H	-4.760640	4.002190	-4.053700
C	-3.880700	1.558540	-6.605970
H	-4.804530	1.747770	-6.271850
C	-3.792400	2.218350	-7.983370
H	-4.530350	1.900690	-8.544430
H	-3.852630	3.191150	-7.884750
H	-2.938740	1.984330	-8.402600
C	-3.786790	0.037562	-6.732470
H	-2.909970	-0.206126	-7.096440
H	-3.898900	-0.371234	-5.849660
H	-4.490830	-0.284427	-7.332280
C	-0.901200	1.932490	-5.648790
H	-0.449180	2.412750	-4.896430
C	-0.388020	2.656410	-6.849070
H	-0.779430	3.554740	-6.882050
H	0.587680	2.726870	-6.796290
H	-0.636140	2.163500	-7.658810
C	-0.435520	0.559408	-5.475290
H	-0.865790	0.165198	-4.686980
H	-0.664550	0.034031	-6.270200
H	0.536790	0.556923	-5.351610
Si	2.714700	-2.280380	5.324390
C	3.595800	-0.486845	1.319840
C	2.610000	0.344053	0.736361
C	1.434570	0.699295	1.419620
H	1.313010	0.390578	2.308860
C	0.447200	1.480810	0.847846
C	-0.750290	1.834420	1.542320
H	-0.881210	1.531850	2.434200
C	-1.700250	2.591430	0.952404
H	-2.485250	2.822660	1.434790
C	-1.533190	3.046050	-0.383106
H	-2.213060	3.571350	-0.788310
C	-0.422710	2.740990	-1.081870
H	-0.329140	3.058960	-1.972430
C	0.617790	1.944800	-0.504980
C	1.776580	1.620350	-1.186420
H	1.891900	1.942910	-2.073020
C	4.773600	-0.828060	0.615311
C	3.371200	-1.018320	2.634740
C	3.143100	-1.498730	3.716600
C	3.010300	-4.133900	5.162940
H	2.775400	-4.553430	6.039320
C	2.116450	-4.774970	4.085860
H	2.264690	-4.324770	3.227450
H	1.176290	-4.682980	4.345600
H	2.339750	-5.725520	3.999270
C	4.484900	-4.443700	4.883240
H	4.603900	-5.412710	4.792530
H	5.034300	-4.115870	5.625370
H	4.760600	-4.002190	4.053700
C	3.880700	-1.558540	6.605970
H	4.804500	-1.747770	6.271850
C	3.792400	-2.218350	7.983370
H	4.530400	-1.900690	8.544430

H	3.852600	-3.191150	7.884750
H	2.938700	-1.984330	8.402600
C	3.786800	-0.037562	6.732470
H	2.910000	0.206126	7.096440
H	3.898900	0.371234	5.849660
H	4.490800	0.284427	7.332280
C	0.901200	-1.932490	5.648790
H	0.449180	-2.412750	4.896430
C	0.388020	-2.656410	6.849070
H	0.779440	-3.554740	6.882050
H	-0.587680	-2.726870	6.796290
H	0.636140	-2.163500	7.658810
C	0.435520	-0.559408	5.475290
H	0.865790	-0.165198	4.686980
H	0.664550	-0.034031	6.270200
H	-0.536790	-0.556923	5.351610
C	2.791400	0.828060	-0.615311
C	3.969200	0.486845	-1.319840
C	4.955000	-0.344053	-0.736361
C	6.130400	-0.699295	-1.419620
H	6.252000	-0.390578	-2.308860
C	7.117800	-1.480810	-0.847846
C	8.315300	-1.834420	-1.542320
H	8.446200	-1.531850	-2.434200
C	9.265300	-2.591430	-0.952404
H	10.050300	-2.822660	-1.434790
C	9.098200	-3.046050	0.383106
H	9.778100	-3.571350	0.788310
C	7.987700	-2.740990	1.081870
H	7.894100	-3.058960	1.972430
C	6.947200	-1.944800	0.504980
C	5.788400	-1.620350	1.186420
H	5.673100	-1.942910	2.073020
C	4.193800	1.018320	-2.634740
C	4.421900	1.498730	-3.716600
Si	4.850300	2.280380	-5.324390
C	4.554700	4.133900	-5.162940
H	4.789600	4.553430	-6.039320
C	5.448500	4.774970	-4.085860
H	5.300300	4.324770	-3.227450
H	6.388700	4.682980	-4.345600
H	5.225200	5.725520	-3.999270
C	3.080100	4.443700	-4.883240
H	2.961100	5.412710	-4.792530
H	2.530700	4.115870	-5.625370
H	2.804400	4.002190	-4.053700
C	3.684300	1.558540	-6.605970
H	2.760500	1.747770	-6.271850
C	3.772600	2.218350	-7.983370
H	3.034600	1.900690	-8.544430
H	3.712400	3.191150	-7.884750
H	4.626300	1.984330	-8.402600
C	3.778200	0.037562	-6.732470
H	4.655000	-0.206126	-7.096440
H	3.666100	-0.371234	-5.849660
H	3.074200	-0.284427	-7.332280
C	6.663800	1.932490	-5.648790
H	7.115800	2.412750	-4.896430
C	7.177000	2.656410	-6.849070
H	6.785600	3.554740	-6.882050
H	8.152700	2.726870	-6.796290
H	6.928900	2.163500	-7.658810
C	7.129500	0.559408	-5.475290
H	6.699200	0.165198	-4.686980
H	6.900500	0.034031	-6.270200
H	8.101800	0.556923	-5.351610

References.

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