Supplement to the paper:

Physical origins of interactions in dimers of polycyclic aromatic hydrocarbons.

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Due to requirements of the journal, the supplementary data are presented in the PDF format. Machine readable ASCII files with these results can be requested by contacting the authors.

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I. MONOMER COORDINATES

A. Naphthalene

TABLE I: Coordinates of the naphthalene monomer. Monomer A is kept fixed. For the slipped-parallel orientation of the dimer, the monomer B is translated by vector $\frac{1}{2}\overrightarrow{C_6C_1}$. For the 'graphite' orientation, the monomer B is translated by $\frac{1}{2}\overrightarrow{C_4C_1}$

# x	y	z	label
# units in bohr			
-1.3386198285	-4.5991818499	0.0000000000	C1
-2.6501863720	-2.3524851534	0.0000000000	C2
-1.3552252350	0.0000000000	0.0000000000	C3
1.3552252350	0.0000000000	0.0000000000	C4
2.6501863720	-2.3524851534	0.0000000000	C5
1.3386198285	-4.5991818499	0.0000000000	C6
-2.6501863720	2.3524851534	0.0000000000	C7
2.6501863720	2.3524851534	0.0000000000	C8
1.3386198285	4.5991818499	0.0000000000	C9
-1.3386198285	4.5991818499	0.0000000000	C10
-4.7057547059	2.3479907627	0.0000000000	H1
-2.3549276534	-6.3838786304	0.0000000000	H2
-4.7057547059	-2.3479907627	0.0000000000	H3
4.7057547059	-2.3479907627	0.0000000000	H4
2.3549276534	-6.3838786304	0.0000000000	H5
4.7057547059	2.3479907627	0.0000000000	H6
2.3549276534	6.3838786304	0.0000000000	H7
-2.3549276534	6.3838786304	0.0000000000	H8

B. Anthracene

TABLE II: Coordinates of the anthracene monomer. Monomer A is kept fixed. For the slipped-parallel orientation of the dimer, the monomer B is translated by vector $\frac{1}{2}\overrightarrow{C_2C_1}$. For the 'graphite' orientation, the monomer B is translated by $\frac{1}{2}\overrightarrow{C_2C_1} + \frac{1}{2}\overrightarrow{C_6C_5}$

# x	y	z	label
# units in bohr			
1.36539694660984945	2.31298303604885325	0.00000000000000000	C1
-1.36539694660984945	2.31298303604885325	0.00000000000000000	C2
1.36539694660984945	-2.31298303604885325	0.00000000000000000	C3
-1.36539694660984945	-2.31298303604885325	0.00000000000000000	C4
-2.65252711195072566	0.00000000000000000	0.00000000000000000	C5
2.65252711195072566	0.00000000000000000	0.00000000000000000	C6
2.65926776455198688	4.68538472635659353	0.00000000000000000	C7
-2.65926776455198688	4.68538472635659353	0.00000000000000000	C8
2.65926776455198688	-4.68538472635659353	0.00000000000000000	C9
-2.65926776455198688	-4.68538472635659353	0.00000000000000000	C10
1.34761840450929915	-6.91759898392759531	0.00000000000000000	C11
-1.34761840450929915	-6.91759898392759531	0.00000000000000000	C12
1.34761840450929915	6.91759898392759531	0.00000000000000000	C13
-1.34761840450929915	6.91759898392759531	0.00000000000000000	C14
4.71449784493664037	-4.67888217922989380	0.00000000000000000	H1
2.35428299752924586	-8.70750775606379257	0.00000000000000000	H2
-2.35428299752924586	-8.70750775606379257	0.00000000000000000	H3
-4.71449784493664037	-4.67888217922989380	0.00000000000000000	H4
4.71449784493664037	4.67888217922989380	0.00000000000000000	H5
2.35428299752924586	8.70750775606379257	0.00000000000000000	H6
-2.35428299752924586	8.70750775606379257	0.00000000000000000	H7
-4.71449784493664037	4.67888217922989380	0.00000000000000000	H8
-4.70918393545675684	0.00000000000000000	0.00000000000000000	H9
4.70918393545675684	0.00000000000000000	0.00000000000000000	H10

C. Pyrene

TABLE III: Coordinates of the pyrene monomer. Monomer A is kept fixed. For the 'S' orientation of the dimer, the monomer B is translated by vector $\frac{1}{2}\overrightarrow{C_4C_3}$ For the 'L' orientation of the dimer, the monomer B is translated by vector $\frac{1}{2}\overrightarrow{C_16C_1}$ For the 'graphite' orientation, the monomer B is translated by $\frac{1}{2}\overrightarrow{C_8C_4}$

# x	y	z	label
# units in bohr			
-1.347940	0.000000	0.000000	'C1'
1.347940	0.000000	0.000000	'C2'
2.700586	2.336246	0.000000	'C3'
2.700586	-2.336246	0.000000	'C4'
-2.700586	-2.336246	0.000000	'C5'
-2.700586	2.336246	0.000000	'C6'
1.286507	4.656025	0.000000	'C7'
5.353553	2.287714	0.000000	'C8'
1.286507	-4.656025	0.000000	'C9'
5.353553	-2.287714	0.000000	'C10'
-1.286507	-4.656025	0.000000	'C11'
-5.353553	-2.287714	0.000000	'C12'
-1.286507	4.656025	0.000000	'C13'
-5.353553	2.287714	0.000000	'C14'
6.659291	0.000000	0.000000	'C15'
-6.659291	0.000000	0.000000	'C16'
2.325426	6.429069	0.000000	'H1'
6.386941	4.063820	0.000000	'H2'
2.325426	-6.429069	0.000000	'H3'
6.386941	-4.063820	0.000000	'H4'
-2.325426	-6.429069	0.000000	'H5'
-6.386941	-4.063820	0.000000	'H6'
-2.325426	6.429069	0.000000	'H7'
-6.386941	4.063820	0.000000	'H8'
8.712841	0.000000	0.000000	'H9'
-8.712841	0.000000	0.000000	'H10'

II. SAPT(DFT) RESULTS

A. Naphthalene dimer

TABLE IV: SAPT(DFT) results for the naphthalene dimer in aug-cc-pVDZ and aug-cc-pVTZ MC^{+}BS basis sets. R—distance between the rings (in Å) for all configurations except for the T-shape where R corresponds to the distance between centers of mass, 'elst'—$E^{(1)}_{\rm elst}$(KS), 'exch'—$E^{(1)}_{\rm exch}$(KS), 'ind'—$E^{(2)}_{\rm ind}$(CKS), 'ex-ind'—$\tilde{E}^{(2)}_{\rm exch-ind}$(CKS), 'disp'—$E^{(2)}_{\rm disp}$(CKS), 'ex-disp'—$\tilde{E}^{(2)}_{\rm exch-disp}$(CKS), $E_{\rm int}$—total interaction energy. Energies in kcal/mol

R	elst	exch	ind	ex-ind	disp	ex-disp	$E_{\rm int}$
Crossed configuration							
aug-cc-pVDZ basis set							
3.00	-17.4853	48.0299	-21.3363	20.7087	-31.3463	5.1016	3.6723
3.20	-9.1261	27.2645	-11.3458	10.8494	-22.9291	3.1552	-2.1319
3.40	-4.4977	15.3943	-6.0489	5.6019	-16.8702	1.9161	-4.5044
3.50	-3.0430	11.5508	-4.4226	3.9992	-14.5160	1.4856	-4.9459
3.60	-1.9723	8.6555	-3.2370	2.8397	-12.5158	1.1478	-5.0821
3.70	-1.1892	6.4745	-2.3727	2.0046	-10.8106	0.8832	-5.0102
4.40	0.5780	0.8136	-0.3162	0.1470	-4.1486	0.1304	-2.7959
5.00	0.5988	0.1224	-0.0947	0.0152	-2.0143	0.0235	-1.3492
5.12	0.5762	0.0822	-0.0793	0.0100	-1.7618	0.0166	-1.1562
aug-cc-pVTZ basis set							
3.60	-1.9341	8.5574	-3.3360	2.9524	-12.9382	1.1848	-5.5137
Graphite configuration							
aug-cc-pVDZ basis set							
3.00	-16.8011	44.9052	-20.9110	20.2837	-30.3004	4.9540	2.1306
3.20	-8.7936	25.5038	-11.2194	10.7170	-22.1621	3.0636	-2.8907
3.50	-2.9301	10.8298	-4.4134	3.9844	-14.0575	1.4499	-5.1369
3.58	-2.0728	8.5880	-3.4372	3.0301	-12.4784	1.1795	-5.1909
3.60	-1.8897	8.1025	-3.2292	2.8278	-12.1143	1.1197	-5.1831
3.70	-1.1283	6.0514	-2.3645	1.9933	-10.4603	0.8616	-5.0469
4.30	0.5295	1.0209	-0.4076	0.2137	-4.5710	0.1700	-3.0446
5.00	0.5936	0.1133	-0.0963	0.0157	-1.9495	0.0234	-1.2998
aug-cc-pVTZ basis set							
3.58	-2.0208	8.4959	-3.5404	3.1473	-12.9203	1.2223	-5.6162
Slipped-parallel configuration							
aug-cc-pVDZ basis set							
3.00	-15.6136	42.0185	-19.6337	19.0035	-28.8170	4.6592	1.6169
3.20	-8.1686	23.8585	-10.5236	10.0042	-21.1207	2.8856	-3.0645
3.40	-4.0260	13.5064	-5.6643	5.1963	-15.5971	1.7626	-4.8221
3.50	-2.7159	10.1407	-4.1608	3.7199	-13.4385	1.3698	-5.0847
3.55	-2.1958	8.7796	-3.5666	3.1407	-12.4807	1.2054	-5.1174
3.60	-1.7500	7.5989	-3.0581	2.6476	-11.5960	1.0596	-5.0981
3.70	-1.0432	5.6850	-2.2520	1.8740	-10.0245	0.8165	-4.9442
4.40	0.5484	0.7188	-0.3142	0.1432	-3.8742	0.1225	-2.6555
5.00	0.5551	0.1079	-0.0960	0.0156	-1.8919	0.0224	-1.2869
aug-cc-pVTZ basis set							
3.55	-2.1512	8.7092	-3.6999	3.2892	-12.9281	1.2485	-5.5323
T-shape configuration							
aug-cc-pVDZ basis set							
4.30	-18.0848	50.6206	-20.3068	17.7951	-25.2866	4.3606	9.0980
4.60	-8.4747	22.5523	-8.0827	7.0436	-16.0086	2.2512	-0.7189
4.90	-4.0641	9.7573	-3.1413	2.6001	-10.1806	1.0981	-3.9305
5.00	-3.2210	7.3390	-2.2917	1.8408	-8.7743	0.8551	-4.2522
5.10	-2.5763	5.5059	-1.6755	1.2962	-7.5731	0.6627	-4.3602
5.12	-2.4668	5.1966	-1.5744	1.2075	-7.3547	0.6294	-4.3623
5.20	-2.0827	4.1188	-1.2287	0.9073	-6.5466	0.5111	-4.3208
5.80	-0.7686	0.6803	-0.2254	0.0981	-2.8579	0.1002	-2.9734
6.50	-0.3953	0.0723	-0.0570	0.0078	-1.2160	0.0136	-1.5746
aug-cc-pVTZ basis set							
5.12	-2.4324	5.1764	-1.6745	1.3107	-7.5717	0.6514	-4.5401

B. Anthracene dimer

TABLE V: SAPT(DFT) results for the anthracene dimer in aug-cc-pVDZ MC$^+$BS basis set. R—distance between the rings (in Å) for all configurations except for the T-shape where R corresponds to the distance between centers of mass, 'elst'—$E^{(1)}_{\rm elst}$(KS), 'exch'—$E^{(1)}_{\rm exch}$(KS), 'ind'—$E^{(2)}_{\rm ind}$(CKS), 'ex-ind'—$\tilde{E}^{(2)}_{\rm exch-ind}$(CKS), 'disp'—$E^{(2)}_{\rm disp}$(CKS), 'ex-disp'—$\tilde{E}^{(2)}_{\rm exch-disp}$(CKS), $E_{\rm int}$—total interaction energy. Energies in kcal/mol

R	elst	exch	ind	ex-ind	disp	ex-disp	$E_{\rm int}$
Crossed configuration							
3.00	-18.3495	46.0230	-21.3470	20.5893	-35.1658	4.9779	-3.2721
3.20	-10.0541	25.9784	-11.4287	10.8017	-26.0657	3.0655	-7.7030
3.40	-5.3815	14.5928	-6.1247	5.5514	-19.4882	1.8581	-8.9920
3.45	-4.5744	12.6101	-5.2344	4.6757	-18.1391	1.6340	-9.0281
3.50	-3.8805	10.8866	-4.4735	3.9309	-16.8892	1.4348	-8.9909
3.60	-2.7504	8.0995	-3.2638	2.7569	-14.6640	1.1027	-8.7191
4.40	0.2032	0.7034	-0.3306	0.1188	-5.2175	0.1233	-4.3994
5.00	0.4124	0.0947	-0.1178	0.0126	-2.6692	0.0224	-2.2449
Graphite configuration							
3.00	-24.1146	63.4173	-29.7420	29.0151	-43.4885	6.8351	1.9223
3.20	-12.7073	35.9648	-15.9651	15.3704	-31.9290	4.2115	-5.0547
3.50	-4.3462	15.2862	-6.2892	5.7513	-20.4207	1.9899	-8.0286
3.57	-3.2736	12.4740	-5.0491	4.5313	-18.4286	1.6591	-8.0869
3.60	-2.8739	11.4289	-4.5957	4.0873	-17.6399	1.5337	-8.0596
3.70	-1.7783	8.5307	-3.3582	2.8837	-15.2702	1.1779	-7.8143
4.40	0.7149	1.0575	-0.4311	0.2032	-6.0021	0.1739	-4.2838
5.00	0.7674	0.1551	-0.1299	0.0202	-2.9813	0.0313	-2.1372
Slipped-parallel configuration							
3.00	-21.6122	57.3190	-26.8534	26.1072	-40.4147	6.2263	0.7723
3.20	-11.4453	32.5447	-14.4990	13.8635	-29.7566	3.8436	-5.4492
3.40	-5.7744	18.4609	-7.8500	7.2521	-22.1243	2.3485	-7.6872
3.50	-3.9689	13.8532	-5.7643	5.1932	-19.1182	1.8225	-7.9825
3.53	-3.5216	12.7007	-5.2511	4.6896	-18.3018	1.6868	-7.9972
3.60	-2.6291	10.3606	-4.2245	3.6877	-16.5391	1.4059	-7.9385
4.40	0.6272	0.9649	-0.4159	0.1844	-5.6988	0.1613	-4.1769
5.00	0.6855	0.1424	-0.1299	0.0193	-2.8540	0.0294	-2.1073
T-shape configuration							
4.30	-26.4668	75.1822	-30.7656	27.0600	-37.1346	6.3023	14.1775
4.60	-12.4042	33.6642	-12.4345	10.9203	-23.6834	3.2687	-0.6689
5.00	-4.7181	11.0121	-3.5678	2.9097	-13.1323	1.2505	-6.2459
5.10	-3.7736	8.2736	-2.6135	2.0584	-11.3710	0.9710	-6.4550
5.14	-3.4609	7.3743	-2.3093	1.7896	-10.7395	0.8764	-6.4695
5.20	-3.0500	6.2006	-1.9203	1.4484	-9.8631	0.7506	-6.4338
5.80	-1.1197	1.0397	-0.3504	0.1607	-4.4027	0.1489	-4.5235
6.50	-0.5783	0.1137	-0.0868	0.0128	-1.9248	0.0204	-2.4430

C. Pyrene dimer

TABLE VI: SAPT(DFT) results for the pyrene dimer in aug-cc-pVDZ MC$^+$BS basis set. R—distance between the rings (in Å), 'elst'—$E^{(1)}_{\rm elst}$(KS), 'exch'—$E^{(1)}_{\rm exch}$(KS), 'ind'—$E^{(2)}_{\rm ind}$(CKS), 'ex-ind'—$\tilde{E}^{(2)}_{\rm exch-ind}$(CKS), 'disp'—$E^{(2)}_{\rm disp}$(CKS), 'ex-disp'—$\tilde{E}^{(2)}_{\rm exch-disp}$(CKS), $E_{\rm int}$—total interaction energy. Energies in kcal/mol

R	elst	exch	ind	ex-ind	disp	ex-disp	$E_{\rm int}$
Graphite configuration							
2.80	-49.0626	122.7306	-61.2779	59.9926	-67.0632	11.8925	17.2120
3.00	-26.7895	69.9715	-33.0334	32.3459	-49.1816	7.4728	0.7857
3.20	-14.2202	39.6457	-17.8024	17.2040	-36.1960	4.5902	-6.7786
3.40	-7.2372	22.4599	-9.6128	9.0197	-26.9185	2.7932	-9.4958
3.50	-5.0113	16.8398	-7.0411	6.4616	-23.2631	2.1627	-9.8515
3.53	-4.4632	15.4343	-6.4096	5.8364	-22.2700	2.0003	-9.8718
3.60	-3.3628	12.5823	-5.1433	4.5880	-20.1253	1.6643	-9.7967
3.80	-1.2652	7.0046	-2.7525	2.2620	-15.1837	0.9789	-8.9560
4.00	-0.1496	3.8997	-1.4974	1.0819	-11.6058	0.5742	-7.6971
4.50	0.7478	0.8536	-0.3822	0.1491	-6.1647	0.1421	-4.6542
5.00	0.7846	0.1683	-0.1519	0.0219	-3.4904	0.0338	-2.6335
5.50	0.6723	0.0282	-0.0843	0.0043	-2.0936	0.0082	-1.4649
Slipped-parallel L configuration							
2.80	-51.4933	128.1942	-64.4403	63.1072	-69.1066	12.3685	18.6298
3.00	-28.0471	73.0144	-34.5720	33.8742	-50.6333	7.7704	1.4065
3.20	-14.8373	41.3203	-18.5383	17.9380	-37.2251	4.7715	-6.5708
3.40	-7.5235	23.3815	-9.9810	9.3897	-27.6393	2.8998	-9.4728
3.50	-5.2003	17.5363	-7.3111	6.7332	-23.8756	2.2458	-9.8717
3.54	-4.4494	15.6176	-6.4519	5.8822	-22.5251	2.0244	-9.9022
3.60	-3.4816	13.1176	-5.3475	4.7927	-20.6514	1.7301	-9.8400
3.70	-2.2191	9.7954	-3.9116	3.3873	-17.8993	1.3278	-9.5195
3.80	-1.2970	7.3122	-2.8675	2.3777	-15.5593	1.0172	-9.0169
4.00	-0.1407	4.0729	-1.5592	1.1438	-11.8710	0.5952	-7.7590
5.00	0.8221	0.1744	-0.1527	0.0223	-3.5512	0.0347	-2.6503
6.00	0.5743	0.0036	-0.0529	0.0011	-1.3321	0.0021	-0.8040
Slipped-parallel S configuration							
2.80	-50.2622	126.5267	-62.8196	61.5614	-68.4041	12.1557	18.7580
3.00	-27.3733	72.1175	-33.8247	33.1714	-50.1088	7.6304	1.6126
3.20	-14.4745	40.9786	-18.2591	17.6795	-36.9064	4.7005	-6.2813
3.40	-7.3448	23.1611	-9.8205	9.2446	-27.3723	2.8480	-9.2838
3.50	-5.0709	17.3779	-7.1870	6.6206	-23.6530	2.2062	-9.7062
3.55	-4.1660	15.0412	-6.1448	5.5869	-22.0021	1.9387	-9.7462
3.60	-3.3886	13.0090	-5.2520	4.7048	-20.4744	1.7015	-9.6996
3.70	-2.1516	9.7131	-3.8340	3.3146	-17.7539	1.3064	-9.4055
4.00	-0.1185	4.0255	-1.5156	1.1039	-11.7757	0.5846	-7.6959
4.50	0.7808	0.8825	-0.3841	0.1521	-6.2466	0.1445	-4.6707
5.00	0.8105	0.1752	-0.1519	0.0224	-3.5351	0.0345	-2.6445
6.00	0.5652	0.0039	-0.0525	0.0012	-1.3303	0.0021	-0.8105
Crossed configuration							
3.00	-29.8312	79.9155	-37.1649	36.6138	-53.0019	8.2478	4.7791
3.20	-15.6754	45.2560	-19.8830	19.3781	-38.9373	5.0763	-4.7852
3.40	-7.8459	25.5297	-10.6487	10.1186	-28.8053	3.0730	-8.5785
3.50	-5.3785	19.1430	-7.7823	7.2496	-24.8664	2.3800	-9.2547
3.60	-3.5598	14.3256	-5.6795	5.1562	-21.5062	1.8354	-9.4283
3.70	-2.2277	10.6903	-4.1403	3.6379	-18.6279	1.4081	-9.2597
4.40	0.8063	1.3163	-0.5116	0.2484	-7.3404	0.2047	-5.2763
5.00	0.8828	0.1900	-0.1533	0.0234	-3.6636	0.0366	-2.6842