Electronic Supplementary Material for PCCP

Supporting Information

A fast correlated electronic structure method for computing interaction energies of large van der Waals complexes applied to the fullerene-porphyrin dimer

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SI 1. Absolute HF, opposite-spin correlation (OS-Corr), and X3LYP energies of different configurations of benzene dimer and monomer benzene (in Hartree).

		Benzene	S	T	PD
HF	cc-pVDZ	-230.7223	-461.4403	-461.4441	-461.4408
	cc-pVTZ	-230.7798	-461.5547	-461.5586	-461.5552
	cc-pVQZ	-230.7941	-461.5830	-461.5869	-461.5834
OS-Corr	cc-pVDZ	-0.5765	-1.1575	-1.1561	-1.1581
	cc-pVTZ	-0.7119	-1.4294	-1.4275	-1.4302
	cc-pVQZ	-0.7628	-1.5312	-1.5293	-1.5320
X3LYP	cc-pVQZ	-232.1274	-464.2517	-464.2549	-464.2524

SI 2. Relative HF and X3LYP (association) energies for different configurations of benzene dimer *without* CP correction in (kcal/mol) based on absolute energies in SI 1. Positive relative energies mean that they are not bound.

		S	T	PD
HF	cc-pVDZ	2.67	0.28	2.32
	cc-pVTZ	3.11	0.72	2.83
	cc-pVQZ	3.29	0.87	3.06
X3LYP	cc-pVQZ	1.89	0.01	1.55

SI 3. Absolute and relative HF, opposite-spin correlation (OS-Corr), and X3LYP energies of ethylene dimer with D_{2d} symmetry and monomer ethylene.

		Ethylene (Hartree)	D_{2d} Dimer (Hartree)	Relative E (kcal/mol)
HF	cc-pVDZ	-78.03990	-156.0797	0.09
	cc-pVTZ	-78.0635	-156.1265	0.36
	cc-pVQZ	-78.0688	-156.1369	0.49
OS-Corr	cc-pVDZ	-0.2145	-0.4302	a
	cc-pVTZ	-0.2647	-0.5309	a
	cc-pVQZ	-0.2828	-0.5673	a
X3LYP	cc-pVQZ	-78.54419	-157.0886	-0.16

a. Since these correlations enegies are raw opposite-spin correlation energies, appropriate scaling parameter has to be chosen for relative energies. (See the main text for more results.)

SI 4. Absolute and relative HF, opposite-spin correlation (OS-Corr), and X3LYP energies of stacked Uracil dimer and monomer.

		Uracil (Hartree)	Stacked dimer (Hartree)	Relative E (kcal/mol)
HF	cc-pVDZ	-412.5052	-825.0128	-1.51
	cc-pVTZ	-412.6194	-825.2386	0.11
	cc-pVQZ	-412.6487	-825.2961	0.81
OS-Corr	cc-pVDZ	-0.86152	-0.8634	-
	cc-pVTZ	-1.08665	-1.0881	-
	cc-pVQZ	-1.17499	-1.1759	-
X3LYP	cc-pVQZ	-414.66443	-829.332852	-2.50

SI 5. Absolute and relative HF and opposite-spin correlation (OS-Corr) energies of the C_{60}-Tetraphenylporphyrin dimer and individual monomers.

		C60 (Hartree)	Porphyrin (Hartree)	Complex (Hartree)	Relative E (kcal/mol)
HF	cc-pVDZ	-2271.9591	-1901.5619	-4173.5125	5.37
	cc-pVTZ	-2272.4139	-1901.9980	-4174.3982	8.57
OS-Corr	cc-pVDZ	-5.3652	-4.6380	-10.0437	-
	cc-pVTZ	-6.5541	-5.7094	-12.3109	-

SI 6. The equilibrium geometry for benzene dimer (S).
[Ref: M. O. Sinnokrot and C. D. Sherrill, J. Phys. Chem. A 108, 10200 (2004)]

C	0.000000000000	1.950000000000	1.391500000000
H	0.000000000000	1.950000000000	2.471500000000
C	1.205074349366	1.950000000000	0.695750000000
H	2.140381785453	1.950000000000	1.235750000000
C	1.205074349366	1.950000000000	-0.695750000000
H	2.140381785453	1.950000000000	-1.235750000000
C	-0.000000000000	1.950000000000	-1.391500000000
H	-0.000000000000	1.950000000000	-2.471500000000
C	-1.205074349366	1.950000000000	-0.695750000000
H	-2.140381785453	1.950000000000	-1.235750000000
C	-1.205074349366	1.950000000000	0.695750000000
H	-2.140381785453	1.950000000000	1.235750000000
C	-1.205074349366	-1.950000000000	-0.695750000000
H	-2.140381785453	-1.950000000000	-1.235750000000
C	-0.000000000000	-1.950000000000	-1.391500000000
H	-0.000000000000	-1.950000000000	-2.471500000000
C	1.205074349366	-1.950000000000	-0.695750000000
H	2.140381785453	-1.950000000000	-1.235750000000
C	1.205074349366	-1.950000000000	0.695750000000
H	2.140381785453	-1.950000000000	1.235750000000
C	-0.000000000000	-1.950000000000	1.391500000000
H	-0.000000000000	-1.950000000000	2.471500000000
C	-1.205074349366	-1.950000000000	0.695750000000
H	-2.140381785453	-1.950000000000	1.235750000000

SI 7. The equilibrium geometry for benzene dimer (PD)
[Ref: M. O. Sinnokrot and C. D. Sherrill, J. Phys. Chem. A 108, 10200 (2004)]

C	-0.800000000000	1.800000000000	1.391500000000
H	-0.800000000000	1.800000000000	2.471500000000
C	0.405074349366	1.800000000000	0.695750000000
H	1.340381785453	1.800000000000	1.235750000000
C	-2.005074349366	1.800000000000	0.695750000000
H	-2.940381785453	1.800000000000	1.235750000000
C	0.405074349366	1.800000000000	-0.695750000000
H	1.340381785453	1.800000000000	-1.235750000000
C	-2.005074349366	1.800000000000	-0.695750000000
H	-2.940381785453	1.800000000000	-1.235750000000
C	-0.800000000000	1.800000000000	-1.391500000000
H	-0.800000000000	1.800000000000	-2.471500000000
C	0.800000000000	-1.800000000000	-1.391500000000
C	2.005074349366	-1.800000000000	-0.695750000000

H	2.940381785453	-1.800000000000	-1.235750000000
H	0.800000000000	-1.800000000000	-2.471500000000
C	2.005074349366	-1.800000000000	0.695750000000
H	2.940381785453	-1.800000000000	1.235750000000
C	0.800000000000	-1.800000000000	1.391500000000
H	0.800000000000	-1.800000000000	2.471500000000
C	-0.405074349366	-1.800000000000	0.695750000000
H	-1.340381785453	-1.800000000000	1.235750000000
C	-0.405074349366	-1.800000000000	-0.695750000000
H	-1.340381785453	-1.800000000000	-1.235750000000

SI 8. The equilibrium geometry for benzene dimer (T).
[Ref: M. O. Sinnokrot and C. D. Sherrill, J. Phys. Chem. A 108, 10200 (2004)]

C	1.391500000000	-0.000000000000	2.495750000000
H	2.471500000000	-0.000000000000	2.495750000000
C	0.695750000000	1.205074349366	2.495750000000
H	1.235750000000	2.140381785453	2.495750000000
C	0.695750000000	-1.205074349366	2.495750000000
H	1.235750000000	-2.140381785453	2.495750000000
C	-0.695750000000	1.205074349366	2.495750000000
H	-1.235750000000	2.140381785453	2.495750000000
C	-0.695750000000	-1.205074349366	2.495750000000
H	-1.235750000000	-2.140381785453	2.495750000000
C	-1.391500000000	-0.000000000000	2.495750000000
H	-2.471500000000	-0.000000000000	2.495750000000
C	0.000000000000	0.000000000000	-1.104250000000
C	-0.000000000000	-1.205074349366	-1.800000000000
H	-0.000000000000	-2.140381785453	-1.260000000000
H	0.000000000000	0.000000000000	-0.024250000000
C	-0.000000000000	-1.205074349366	-3.191500000000
H	-0.000000000000	-2.140381785453	-3.731500000000
C	-0.000000000000	0.000000000000	-3.887250000000
H	-0.000000000000	0.000000000000	-4.967250000000
C	-0.000000000000	1.205074349366	-3.191500000000
H	0.000000000000	2.140381785453	-3.731500000000
C	0.000000000000	1.205074349366	-1.800000000000
H	0.000000000000	2.140381785453	-1.260000000000

SI 9. The equilibrium geometry for stacked Uracil dimer.
[Ref: I. Daabkowska, P. Jurecka and P. Hobza, J. Chem. Phys. **122**, (2005)]

N	2.0113587	-1.2132073	-0.0980673
C	2.0257076	-0.6971797	-1.3644029

H	2.2975208	-1.3910592	-2.1456459
C	1.7145226	0.5919651	-1.6124892
H	1.7272873	0.9908466	-2.6120050
C	1.3089605	1.4575340	-0.5205890
O	0.9205926	2.6110864	-0.6260457
N	1.3768885	0.8397454	0.7346356
H	1.0518040	1.3862229	1.5233710
C	1.6459909	-0.4852113	1.0187267
O	1.5611090	-0.9718061	2.1298059
H	2.1294635	-2.2015046	0.0568134
N	-2.0113587	1.2132073	-0.0980673
C	-2.0257076	0.6971797	-1.3644029
H	-2.2975208	1.3910592	-2.1456459
C	-1.7145226	-0.5919651	-1.6124892
H	-1.7272873	-0.9908466	-2.6120050
C	-1.3089605	-1.4575340	-0.5205890
O	-0.9205926	-2.6110864	-0.6260457
N	-1.3768885	-0.8397454	0.7346356
H	-1.0518040	-1.3862229	1.5233710
C	-1.6459909	0.4852113	1.0187267
O	-1.5611090	0.9718061	2.1298059
H	-2.1294635	2.2015046	0.0568134

SI 10. The equilibrium geometry for Uracil monomer.
[Ref: I. Daabkowska, P. Jurecka and P. Hobza, J. Chem. Phys. **122**, (2005)]

O	0.9982966	2.2585668	0.0000000
C	0.3689249	1.2195224	0.0000000
N	-1.0154905	1.1741836	0.0000000
C	-1.7364367	0.0091958	0.0000000
C	-1.1397741	-1.1995505	0.0000000
C	0.3108620	-1.2878827	0.0000000
N	0.9430099	-0.0350412	0.0000000
O	0.9687114	-2.3133449	0.0000000
H	-1.7132937	-2.1101183	0.0000000
H	-1.4725513	2.0705536	0.0000000
H	1.9537440	-0.0477638	0.0000000
H	-2.8098420	0.1264227	0.0000000

SI 11. The equilibrium geometry for ethylene dimer with D_{2d} symmetry.
[Ref: S. Tsuzuki, K. Honda, T. Uchimaru, M. Mikami and K. Tanabe, J. Am. Chem. Soc. 124, 104 (2002)]

C	.000000	-.667480	1.900000

C	.000000	.667480	1.900000
H	.000000	-1.237695	2.822832
H	.000000	-1.237695	.977168
H	.000000	1.237695	2.822832
H	.000000	1.237695	.977168
C	-.667480	.000000	-1.900000
C	.667480	.000000	-1.900000
H	-1.237695	.000000	-.977168
H	-1.237695	.000000	-2.822832
H	1.237695	.000000	-.977168
H	1.237695	.000000	-2.822832

SI 12. The equilibrium geometry for C_{60}-Tetraporphyrin dimer
[Ref.Y. B. Wang and Z. Y. Lin, J. Am. Chem. Soc. **125**, 6072 (2003)]

C	3.209884	0.611626	1.661426
C	-0.170402	-0.073605	0.764282
C	3.698286	-3.236510	-0.590125
C	-1.020293	-0.100818	-2.694088
C	3.576891	3.170462	-1.529195
C	4.706119	2.418516	-1.027367
C	5.503755	-1.600928	-0.916942
C	-0.580531	-2.038699	-1.237559
C	0.705421	1.324380	-4.444678
C	2.488473	-3.142504	0.196138
C	4.291080	-0.269992	1.280058
C	0.453582	-0.027665	-4.663110
C	3.957812	-1.162069	-4.693872
C	5.636129	-0.542009	-3.004292
C	2.697706	-2.145116	1.221064
C	4.579056	2.074049	-3.338830
C	5.325758	1.740620	-2.144942
C	3.497540	2.958518	-2.957634
C	0.043741	-2.706910	-2.352398
C	0.789861	0.865634	1.301711
C	0.084697	2.004879	-3.328833
C	0.988449	2.092705	0.671907
C	2.254787	2.847272	-3.577093
C	2.046535	1.845304	-4.601961
C	0.114900	-2.082619	-3.598051
C	3.088395	0.994852	-4.970450
C	3.753692	-2.386140	-4.059629
C	1.654338	-1.294449	1.584440
C	4.499935	-2.717436	-2.863509
C	1.246314	-3.245830	-0.426739
C	2.332927	-3.550360	-2.613394

C	4.039319	-1.622745	1.065785
C	3.622361	-3.440055	-1.969200
C	1.042941	2.945278	-2.791932
C	2.412332	-2.902692	-3.902911
C	-0.682363	1.520105	-1.040225
C	4.379563	1.111072	-4.326644
C	1.534395	-0.909756	-5.044164
C	1.918385	0.110221	1.808583
C	-0.893451	0.247762	-0.382727
C	1.323619	-2.179384	-4.385477
C	4.627043	1.787921	0.213304
C	-1.102020	-0.756210	-1.405477
C	5.424735	-1.813742	-2.346419
C	3.417787	1.884943	1.000443
C	2.409799	3.264587	-0.772472
C	1.119018	3.150311	-1.413732
C	5.845398	0.458064	-1.980616
C	2.328051	2.610827	0.514400
C	5.763955	-0.196117	-0.692083
C	0.239457	2.427761	-0.521494
C	2.827448	-0.410162	-5.196459
C	0.364921	-1.407066	0.938741
C	-0.426008	-0.753450	-3.772382
C	4.917220	-0.221810	-4.155172
C	0.161849	-2.372523	-0.042189
C	5.166834	0.456309	0.384862
C	-0.760736	1.304810	-2.468735
C	4.657459	-2.298506	-0.054695
C	1.172082	-3.450910	-1.854230
H	-0.553408	4.316742	4.374549
C	-3.601836	4.742079	0.276970
C	-2.575330	5.515132	-0.279857
C	-4.117293	7.345225	-0.628609
C	-5.145562	6.578447	-0.079757
C	-4.889354	5.284488	0.371646
H	-6.154626	6.991191	0.004049
H	-4.317892	8.361015	-0.979778
H	-2.022154	7.403449	-1.163066
H	-1.571036	5.089830	-0.367010
C	-4.652444	2.448727	-1.154984
C	-4.993360	1.199570	-1.562662
H	-5.530885	0.911880	-2.464217
H	-4.851174	3.394802	-1.655021
N	-3.213507	-1.767190	1.283683
N	-1.569333	-0.624042	3.399084
C	-4.568179	-1.109994	-0.679607

C	-3.992479	-2.045910	0.187982
C	-4.082490	-3.470205	0.094897
C	-3.349014	-4.008978	1.120556
C	-2.804250	-2.931022	1.886532
C	-1.989417	-3.033709	3.020147
C	-1.436359	-1.948318	3.725325
C	-0.656983	-2.118144	4.941166
C	-0.310163	-0.870068	5.347553
C	-4.458897	0.288069	-0.564020
C	-5.334702	-1.667562	-1.827943
C	-4.665412	-2.311405	-2.874968
C	-5.378789	-2.854715	-3.942467
C	-6.770567	-2.760268	-3.973802
C	-7.444524	-2.116114	-2.935204
C	-6.730554	-1.571312	-1.867869
C	-1.701373	-4.411089	3.502798
C	-2.724314	-5.197932	4.046998
C	-2.456727	-6.487005	4.506009
C	-1.162676	-7.003236	4.428453
C	-0.139523	-6.226518	3.883983
C	-0.406992	-4.939166	3.420389
H	-4.648033	-4.001988	-0.666411
H	-3.189643	-5.062531	1.337275
H	-0.437694	-3.065944	5.427782
H	0.254009	-0.585863	6.233352
H	-3.574575	-2.381551	-2.848929
H	-4.841963	-3.352911	-4.754117
H	-7.330479	-3.190398	-4.808556
H	-8.535173	-2.042276	-2.952151
H	-7.253701	-1.072354	-1.046717
H	-3.733964	-4.782720	4.119425
H	-3.262956	-7.089045	4.933557
H	-0.950632	-8.011805	4.793267
H	0.876281	-6.624696	3.816111
H	0.392056	-4.329718	2.989272
N	-3.805630	0.962529	0.432667
C	-3.912723	2.282374	0.086844
C	-3.335523	3.365837	0.774851
C	-2.509658	3.259865	1.900709
N	-2.132446	2.094439	2.522516
C	-1.318900	2.371511	3.593969
H	-2.013579	5.385112	2.375303
C	-0.749391	1.441413	4.470627
C	-0.882387	0.045703	4.374728
C	0.022204	2.002958	5.612962
C	-2.831589	6.810641	-0.728489

C	-0.657038	2.643062	6.656929
C	0.047493	3.180237	7.733348
C	1.438905	3.083638	7.775680
H	-5.687878	4.681024	0.813005
C	2.121587	2.445816	6.738806
C	1.417238	1.907467	5.661523
H	1.949902	1.412383	4.844034
H	3.211877	2.370456	6.765130
H	1.991928	3.507018	8.618500
H	-0.495626	3.673815	8.543736
H	-1.748578	2.707764	6.618380
C	-1.159640	3.790706	3.640942
C	-1.894041	4.332416	2.617879
H	-3.010234	-0.826837	1.631235
H	-2.461143	1.161714	2.259683

SI 13. The equilibrium geometry for C_{60}.

C	3.211150	0.620078	1.664715
C	-0.174642	-0.072889	0.770286
C	3.700682	-3.243639	-0.594056
C	-1.025763	-0.101166	-2.696438
C	3.581203	3.179093	-1.526814
C	4.712815	2.426975	-1.023368
C	5.508605	-1.600549	-0.915644
C	-0.588811	-2.041578	-1.242220
C	0.701893	1.326410	-4.449180
C	2.487796	-3.146027	0.193081
C	4.293485	-0.265332	1.283097
C	0.450558	-0.028848	-4.667915
C	3.957739	-1.164073	-4.693381
C	5.639639	-0.540980	-3.003825
C	2.698837	-2.143109	1.218039
C	4.583179	2.078847	-3.338931
C	5.331733	1.746628	-2.143314
C	3.500990	2.964635	-2.957890
C	0.030516	-2.721592	-2.361470
C	0.785559	0.869736	1.308845
C	0.082722	2.006693	-3.328930
C	0.989205	2.096711	0.675979
C	2.255999	2.851696	-3.577963
C	2.045081	1.848557	-4.603063
C	0.108186	-2.091155	-3.604837
C	3.087174	0.995913	-4.970197
C	3.754057	-2.391002	-4.060466

C	1.656609	-1.290195	1.584869
C	4.503071	-2.722721	-2.864653
C	1.242424	-3.258831	-0.427414
C	2.329963	-3.567640	-2.616229
C	4.042173	-1.620609	1.064056
C	3.622977	-3.449953	-1.972457
C	1.043012	2.949108	-2.790729
C	2.411015	-2.913174	-3.906651
C	-0.684853	1.521340	-1.038271
C	4.380288	1.113252	-4.325882
C	1.532519	-0.914440	-5.048954
C	1.917705	0.117238	1.812421
C	-0.895996	0.246897	-0.380819
C	1.321058	-2.188807	-4.391732
C	4.635019	1.796804	0.219568
C	-1.106976	-0.755990	-1.406247
C	5.427682	-1.815197	-2.346424
C	3.422513	1.894613	1.006820
C	2.413261	3.273203	-0.768581
C	1.120171	3.156132	-1.412380
C	5.850539	0.461632	-1.978975
C	2.332254	2.618846	0.521816
C	5.769466	-0.193059	-0.688292
C	0.239949	2.428958	-0.519898
C	2.826112	-0.411611	-5.197147
C	0.363753	-1.407809	0.940754
C	-0.429727	-0.756235	-3.775070
C	4.918470	-0.221548	-4.155090
C	0.160334	-2.373490	-0.046263
C	5.173512	0.461997	0.390175
C	-0.764728	1.306234	-2.469103
C	4.661154	-2.301325	-0.056013
C	1.161924	-3.473650	-1.858325

SI 14. The equilibrium geometry for tetraphenylporphyrin.

H	-0.584408	4.324215	4.392184
C	-3.604775	4.744434	0.275039
C	-2.578876	5.515592	-0.285103
C	-4.118097	7.347491	-0.633757
C	-5.146414	6.582884	-0.080409
C	-4.890830	5.289100	0.372620
H	-6.150671	6.997187	0.005694
H	-4.317172	8.359971	-0.985049
H	-2.028087	7.399220	-1.173694

H	-1.580743	5.085595	-0.373389
C	-4.655062	2.449899	-1.160489
C	-4.995935	1.201821	-1.567104
H	-5.530721	0.914968	-2.466066
H	-4.852409	3.391629	-1.660802
N	-3.207838	-1.766298	1.281419
N	-1.559613	-0.631839	3.395656
C	-4.567373	-1.110092	-0.681568
C	-3.989831	-2.044752	0.186793
C	-4.086030	-3.469601	0.097932
C	-3.353659	-4.008609	1.124118
C	-2.800427	-2.931089	1.885978
C	-1.986868	-3.035542	3.021644
C	-1.431430	-1.952107	3.727595
C	-0.663012	-2.119248	4.954093
C	-0.320810	-0.871049	5.358858
C	-4.451539	0.287501	-0.572437
C	-5.337808	-1.670220	-1.828896
C	-4.669429	-2.313452	-2.877594
C	-5.384995	-2.854632	-3.945172
C	-6.777020	-2.757203	-3.975947
C	-7.449094	-2.113196	-2.936019
C	-6.733238	-1.572828	-1.867448
C	-1.701691	-4.413700	3.508611
C	-2.722935	-5.200904	4.054481
C	-2.453385	-6.491533	4.508968
C	-1.159256	-7.007730	4.424959
C	-0.136535	-6.228058	3.882343
C	-0.406687	-4.938969	3.424745
H	-4.647156	-4.001231	-0.661647
H	-3.191690	-5.058333	1.337427
H	-0.447860	-3.062058	5.445180
H	0.233383	-0.585367	6.246472
H	-3.581140	-2.377563	-2.850697
H	-4.852819	-3.348600	-4.757955
H	-7.336552	-3.181376	-4.809749
H	-8.536028	-2.036541	-2.953061
H	-7.252513	-1.075634	-1.047731
H	-3.728307	-4.785770	4.130724
H	-3.254949	-7.091950	4.938916
H	-0.947791	-8.015225	4.783112
H	0.875221	-6.626858	3.809093
H	0.384704	-4.328243	2.989525
N	-3.791843	0.963392	0.418184
C	-3.905012	2.283619	0.077193
C	-3.333286	3.366620	0.771132

C	-2.509544	3.262500	1.899355
N	-2.120405	2.097860	2.515026
C	-1.319435	2.373781	3.596463
H	-2.039321	5.387398	2.395683
C	-0.752998	1.440137	4.472927
C	-0.884240	0.043399	4.375527
C	0.020162	2.001839	5.617821
C	-2.833780	6.810391	-0.735674
C	-0.652640	2.643574	6.664308
C	0.057638	3.181598	7.736781
C	1.449258	3.081997	7.774606
H	-5.686467	4.690098	0.816134
C	2.125988	2.441339	6.735429
C	1.415167	1.904329	5.661504
H	1.938144	1.409363	4.842664
H	3.212913	2.363502	6.758086
H	2.004859	3.502926	8.612537
H	-0.478538	3.675624	8.546947
H	-1.740534	2.710648	6.630763
C	-1.181754	3.796746	3.657982
C	-1.914493	4.337631	2.633085
H	-2.966511	-0.827555	1.603204
H	-2.407248	1.162041	2.222999