Electronic Supplementary Information for:

Standard density functionals with small basis sets can accurately describe dispersion interactions

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Figure S1. Sample Gaussian-03 input file demonstrating the use of DCPs with B971/6-31G(d) and counterpoise corrections, for calculation of the methane dimer binding energy.

Table S1. Binding Energies (kcal/mol) for the set of non-covalently bound dimers. Comparison of counterpoise-corrected Method/Basis-DCP and M06-2X/6-31G(d) to high-level ab initio data.

Table S2. Deviations in monomer separations (Å), relative to high-level theoretical results, for the set of non-covalently bound dimers using counterpoise-corrected B971/Basis-DCP and M06-2X/6-31G(d).

Table S3. Binding Energies (kcal/mol) for the S22 set of non-covalently bound dimers. Comparison of counterpoise-corrected Method/6-31G(d)-DCP and M06-2X/6-31G(d) to high-level ab initio data.

Figure S5. Potential energy scan of the methane dimer using counterpoise-corrected method/6-31G(d).

Figure S6. Potential energy scan of the methane dimer using counterpoise-corrected method/6-31++G(d,p).

Figure S7. Potential energy scan of the ethene dimer using counterpoise-corrected method/6-31G(d).

Figure S8. Potential energy scan of the ethene dimer using counterpoise-corrected method/6-31++G(d,p).

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#B971 Gen OPT Pseudo=Read Counterpoise=2

Methane Dimer using optimised DCPs. The monomer is also calculated with the same DCPs.

0 1
C    0.000000    1.906281    0.000000 1
H   -0.981163    1.425134    0.000000 1
H    0.553375    1.602684    0.892189 1
H    0.553375    1.602684   -0.892189 1
H   -0.125117    2.992038    0.000000 1
C    0.000000   -1.906281    0.000000 2
H    0.125117   -2.992038    0.000000 2
H    0.981163   -1.425134    0.000000 2
H   -0.553375   -1.602684    0.892189 2
H   -0.553375   -1.602684   -0.892189 2

C H 0
6-31G(d)
****

C 0
C 3 0
     F and up
 3
   2      0.08  -0.001578
   2      0.12   0.003490
   2      0.009 -0.0000042
     S - F
 1
   2      1.0      0.0
     P - F
 1
   2      1.0      0.0
     D - F
 1
   2      1.0      0.0
```

Table S1. Binding Energies (kcal/mol) for the set of non-covalently bound dimers. Comparison of Method/Basis-DCP and M06-2X/6-31G(d) to high-level *ab initio* data.[a]

	B971		PBE		PBE1			
	3-21G(d)	6-31G(d)	3-21G(d)	6-31G(d)	3-21G(d)	6-31G(d)	M06-2X	high-level[b]
				Hydrocarbons				
$CH_4 \cdot C_6H_6$	1.11	1.14	1.02	1.06	1.04	1.08	1.05	1.23
$(CH_4)_2$	0.35	0.43	0.27	0.32	0.23	0.28	0.48	0.51
$CH_4 \cdot C_2H_4$	0.63	0.63	0.62	0.61	0.54	0.53	0.32	0.50
P-$(C_6H_6)_2$	0.72	1.35	0.78	1.38	0.55	1.23	*-0.34*[c]	1.70
SP-$(C_6H_6)_2$	1.80	2.30	1.85	2.45	1.93	2.45	1.24	2.63
T-$(C_6H_6)_2$	2.56	2.49	2.55	2.46	2.64	2.52	1.94	2.61
$(C_2H_4)_2$	1.42	1.43	1.31	1.31	1.30	1.26	1.42	1.42
$(C_2H_2)_2$	1.61	1.67	1.58	1.35	1.54	1.56	1.25	1.38
P-$(C_{10}H_8)_2$	2.67	3.83	2.73	4.08	2.48	3.95	0.36	3.78
PC-$(C_{10}H_8)_2$	4.43	5.53	4.73	6.04	5.16	6.16	2.81	5.28
T-$(C_{10}H_8)_2$	4.95	4.64	4.88	4.54	5.14	4.79	3.50	4.34
TC-$(C_{10}H_8)_2$	3.63	3.38	3.56	3.30	3.59	3.32	2.99	3.09
SD	-0.22	0.03	-0.22	0.04	-0.20	0.06	-0.95	
AD (%)	21.07	11.04	21.87	12.29	22.09	13.66	33.72	
				Heterodimers				
HCN·HF	8.17	6.85	8.11	6.91	8.50	6.98	6.60	7.49
$C_2H_4 \cdot HF$	5.08	5.19	5.36	5.58	5.19	5.28	4.69	4.50
$(CF_4)_2$	0.90	0.85	1.14	0.93	0.91	0.83	0.39	0.78
$(CH_3F)_2$	3.06	2.26	3.03	2.19	2.91	2.10	1.83	2.33
$CH_4 \cdot HF$	1.59	1.52	1.75	1.73	1.58	1.48	1.31	1.65
$CH_4 \cdot NH_3$	1.58	1.09	1.80	1.15	1.53	1.03	0.88	0.76
$(CO_2)_2$	1.66	1.39	1.51	1.28	1.64	1.33	1.33	1.37
$(H_2CO)_2$	3.25	3.26	3.00	2.98	3.16	3.16	3.15	3.72
$H_2O \cdot C_6H_6$	3.84	3.49	3.71	3.42	3.83	3.48	3.51	3.17
$(H_3CCN)_2$	5.05	5.65	4.96	5.52	5.06	5.63	5.80	6.16
SD	0.23	-0.04	0.24	-0.02	0.24	-0.06	-0.24	
AD (%)	25.41	11.81	31.20	15.81	24.87	12.34	15.90	
SD (Total)	-0.02	0.00	0.01	0.01	0.00	0.00	-0.63	
AD (%) (Total)	23.04	11.39	26.11	13.89	23.35	13.06	25.62	

[a] High-level data are generally of large basis set, CCSD(T) quality, with the exception of those for the naphthalene dimers.[b]For refs., see Full text. [c]not bound, error of 100 % assigned.

Table S2. Deviations in monomer separations (Å), relative to high-level theoretical results, for the set of non-covalently bound dimers using B971/Basis-DCP and M06-2X/6-31G(d).

		B971		PBE		PBE1			
		3-21G(d)	6-31G(d)	3-21G(d)	6-31G(d)	3-21G(d)	6-31G(d)	M06-2X	high-level[b]
					Hydrocarbons				
$CH_4 \cdot C_6H_6$	H_4C-CM(C_6H_6)	0.1	0.1	0.1	0	0.1	0	0	3.8
$(CH_4)_2$	C-C	0.1	0.1	0.3	0.2	0.3	0.1	-0.1	3.6
$CH_4 \cdot C_2H_4$	H_4C-CM(C_2H_4)	0	-0.1	0	-0.1	0	-0.1	0	4.2
P-$(C_6H_6)_2$	CM-CM	0.1	0	0.1	-0.1	0.2	-0.1	0	3.9
SP-$(C_6H_6)_2$	CM-CM	0.2	0.1	0.1	-0.1	0	-0.1	-0.1	3.9
T-$(C_6H_6)_2$	CM-CM	0	0	0	0	0	0	-0.1	5.0
$(C_2H_4)_2$	CM-CM	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.3	3.8
$(C_2H_2)_2$	CM-CM	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	4.3
P-$(C_{10}H_8)_2$	CM-CM	0	0	0	-0.1	0	-0.1	-0.2	3.8
PC-$(C_{10}H_8)_2$	CM-CM	0	-0.1	-0.2	-0.2	-0.3	-0.2	-0.1	3.6
T-$(C_{10}H_8)_2$	CM-CM	0.1	0.1	0.1	0.1	0	0.1	0	5.0
TC-$(C_{10}H_8)_2$	CM-CM	0.1	0.1	0.1	0	0	0	-0.1	5.2
MAD		0.07	0.07	0.10	0.09	0.09	0.08	0.10	
					Heterodimers				
HCN·HF	N-HF	0	0	0	0	-0.1	0	0	1.9
$C_2H_4 \cdot HF$	FH-CM(C_2H_4)	0.1	0	0	0	0	0	0	2.2
$(CF_4)_2$	C-C	-0.2	0	-0.2	0	-0.2	0	-0.1	4.0
$(CH_3F)_2$	C-C	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	3.9
$CH_4 \cdot HF$	C-HF	0.1	0.1	0.1	0.1	0.1	0.1	0.1	2.3
$CH_4 \cdot NH_3$	C-N	-0.3	-0.2	-0.3	-0.2	-0.3	-0.2	-0.2	3.9
$(CO_2)_2$	C-C	0	0	0	0	0	0	-0.2	3.6
$(H_2CO)_2$	C-C	0	0	0	0	-0.1	-0.1	0	3.6
$H_2O \cdot C_6H_6$	O-CM(C_6H_6)	0	0	0	0	0	0	-0.2	3.4
$(H_3CCN)_2$	C-C	0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	3.4
MAD		0.09	0.05	0.09	0.05	0.11	0.06	0.12	
MAD (Total)		0.08	0.06	0.09	0.07	0.10	0.07	0.11	

[a]CM = centre-of-mass of heavy atoms. [b]High-level data are generally of large basis set, CCSD(T) quality, with the exception of those for the naphthalene dimers. For refs., see Full text.

Table S3. Binding Energies (kcal/mol) for the S22 set of non-covalently bound dimers. Comparison of Method/6-31G(d)-DCP and M06-2X/6-31G(d) to high-level *ab initio* data.[a]

	B971	PBE	PBE1	M06-2X	high-level
Hydrogen bonded					
$(NH_3)_2$	3.54	3.68	3.56	4.14	3.17
$(H_2O)_2$	6.07	6.37	6.25	6.32	5.02
$(HCOOH)_2$	16.63	17.79	17.57	16.60	18.61
$(HCONH_2)_2$	14.70	15.48	15.29	14.72	15.96
uracil dimer (C_{2h})	18.11	18.83	18.93	17.72	20.65
2-$C_8H_{11}NO_3$·2-$(C_5H_6N_2)_2$	15.31	16.68	16.09	14.74	16.71
adenine·thymine WC	14.66	15.77	15.37	14.04	16.37
SD	-1.07	-0.27	-0.49	-1.17	
AD (%)	11.76	9.03	9.27	16.47	
Dispersion-dominated					
$(CH_4)_2$	0.43	0.32	0.28	0.48	0.51
$(C_2H_4)_2$	1.43	1.31	1.26	1.42	1.42
C_6H_6·CH_4	1.14	1.06	1.08	1.05	1.23
SP-$(C_6H_6)_2$	2.30	2.45	2.45	1.24	2.63
$(C_4H_4N_2)_2$	3.54	3.57	3.70	3.53	4.42
uracil dimer (C_2)	7.23	7.30	7.61	8.17	10.12
C_8H_7N·C_6H_6 (C_1)	3.89	4.19	4.31	2.81	5.22
adenine·thymine stack	8.81	8.96	9.42	10.10	12.23
SD	-1.13	-1.08	-0.96	-1.12	
AD (%)	17.35	19.95	19.61	22.07	
Mixed complexes					
C_2H_4·C_2H_2	2.02	2.05	1.94	1.55	1.53
H_2O·C_6H_6	3.49	3.42	3.48	3.51	3.17
NH_3·C_6H_6	1.99	1.91	1.93	2.10	2.35
HCN·C_6H_6	4.82	4.77	5.10	4.76	4.46
T-$(C_6H_6)_2$	2.49	2.46	2.52	1.94	2.61
T-C_8H_7N·C_6H_6	5.29	5.38	5.40	4.76	5.73
$(C_6H_5OH)_2$	6.99	7.03	7.17	7.04	7.05
SD	0.03	0.02	0.09	-0.18	
AD (%)	11.26	11.48	11.36	10.31	
SD (Total)	-0.74	-0.47	-0.47	-0.84	
AD (%) (Total)	13.63	13.78	13.70	16.55	

[a]For ref., see Full text; CCSD(T)/CBS energies.

Figure S5. Potential energy scan of the methane dimer using counterpoise-corrected method/6-31G(d).

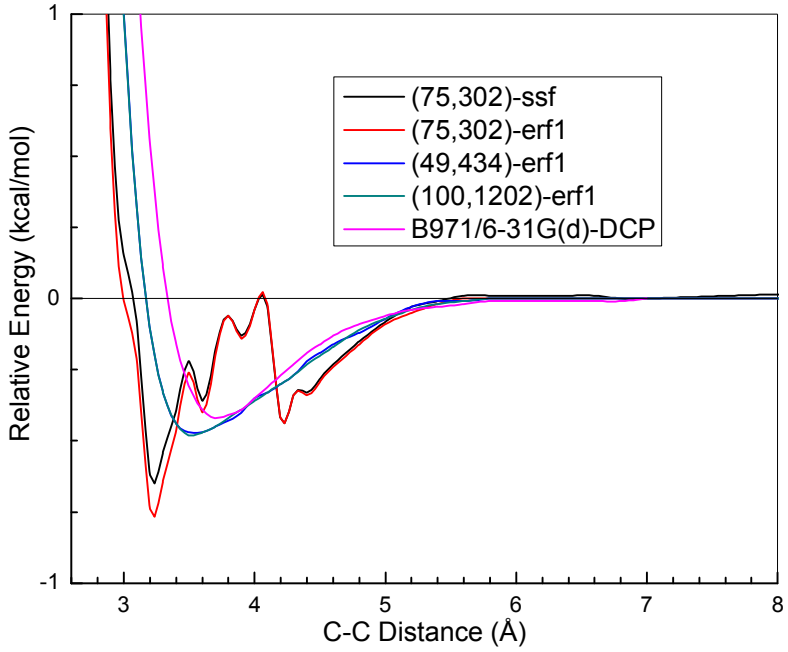

Figure S6. Potential energy scan of the methane dimer using counterpoise-corrected method/6-31++G(d,p).

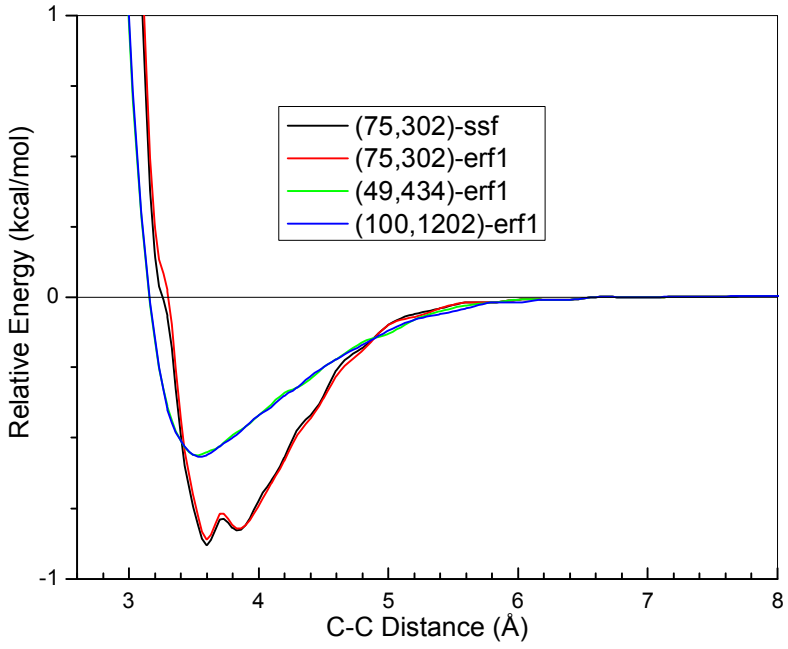

Figure S7. Potential energy scan of the ethene dimer using counterpoise-corrected method/6-31G(d).

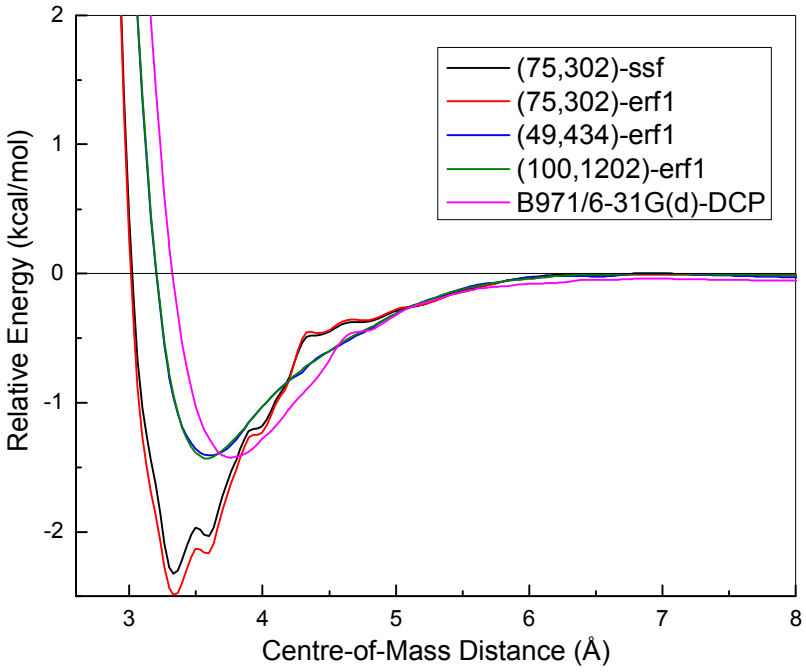

Figure S8. Potential energy scan of the ethene dimer using counterpoise-corrected method/6-31++G(d,p).