New intermolecular benchmark calculations on the water dimer:
SAPT and supermolecular post-Hartree-Fock approaches
(Supplementary material)

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I. Geometries

I.1. atomic positions (cartesian coordinates in Angstroms)

system No 1

H	0.287800	0.000000	-2.003704
H	0.287800	0.000000	-0.489804
O	0.873683	0.000000	-1.246754
H	-0.666591	0.756950	1.706755
H	-0.666591	-0.756950	1.706754
O	-0.778985	0.000000	1.131754

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system No 2

H	0.251288	-0.110365	-2.046327
H	0.251288	-0.110365	-0.532426
O	0.837171	-0.110365	-1.289376
H	-1.592086	0.092239	1.467635
H	-0.208172	0.565711	1.858013
O	-0.674961	0.055713	1.196014

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system No 3

H	0.225672	0.000000	-2.070873
H	0.225672	0.000000	-0.556973
O	0.811554	0.000000	-1.313923
H	-0.086106	0.000000	1.964049
H	-1.547467	0.000000	1.568676
O	-0.663775	0.000000	1.200813

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system No 4

H	-0.681313	-0.656527	-1.972502
H	-0.681313	-0.656527	-0.458601
O	-0.095431	-0.656527	-1.215551
H	0.681313	0.656527	0.458601
H	0.681313	0.656527	1.972502
O	0.095431	0.656527	1.215551

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system No 5

H	-0.856322	0.362638	-2.053897
H	-0.856322	0.362638	-0.539996
O	-0.270440	0.362638	-1.296947
H	0.682418	-0.875997	1.961938
H	0.839693	-0.406742	0.531218
O	0.294256	-0.292955	1.309539

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system No 6

H	-0.925346	0.000000	-2.081528
H	-0.925346	0.000000	-0.567627
O	-0.339463	0.000000	-1.324577
H	0.925345	0.000000	0.567627
H	0.925346	0.000000	2.081528
O	0.339463	0.000000	1.324577

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system No 7

H	-1.209230	0.000000	0.455450
H	-1.209230	0.000000	1.969351
O	-0.623348	0.000000	1.212401
H	0.855026	-0.756950	-0.757896
H	0.855025	0.756951	-0.757896
O	0.711899	0.000000	-1.326027

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system No 8

H	0.467631	1.322676	-0.756950
H	0.467631	1.322676	0.756951
O	1.053513	1.322676	0.000000
H	-0.467631	-1.322675	-0.756951
H	-0.467631	-1.322675	0.756950
O	-1.053513	-1.322677	0.000000

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system No 9

H	0.990354	0.000000	-0.756951
H	0.990354	0.000000	0.756950
O	1.576236	0.000000	0.000000
H	-1.927765	0.756950	0.000000
H	-1.927765	-0.756951	0.000000
O	-1.341883	0.000000	0.000000

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system No 10

H	-2.021005	0.000000	-0.756950
H	-2.021005	0.000000	0.756951
O	-1.435122	0.000000	0.000000
H	1.083593	0.000000	-0.756951
H	1.083593	0.000000	0.756950
O	1.669475	0.000000	0.000000

I.2. basic energies (in a.u.)

system	nuclear(dimer)	HF(water 1)	HF(water 2)	HF(dimer)
1	36.713473	-76.060662	-76.060683	-152.126966
2	36.487778	-76.060659	-76.060665	-152.126359
3	36.446679	-76.060659	-76.060658	-152.126385
4	37.467960	-76.060664	-76.060664	-152.125498
5	37.484346	-76.060659	-76.060659	-152.125204
6	37.511658	-76.060662	-76.060662	-152.125211
7	36.932667	-76.060655	-76.060655	-152.124567
8	34.499326	-76.060633	-76.060633	-152.122393
9	36.491690	-76.060638	-76.060663	-152.124484
10	35.412786	-76.060651	-76.060630	-152.123712

differences in the monomer total energies are entirely due to
the Hartree-Fock basis-set superposition error.

II. SAPT results (all in kcal/mol, 1 a.u. = 627.51 kcal/mol)

II.1. SAPT contributions in principle taken into account in Hartree-Fock

#	E10pol	E100ex	E200Ind	E200Ind,r	E200ExInd	E200ExInd,r	E300Ind	E300ExInd*
1	-8.23	6.93	-2.42	-2.94	1.30	1.61	-2.75	1.47
2	-7.02	5.76	-2.00	-2.40	1.01	1.24	-2.16	1.09
3	-6.85	5.51	-1.91	-2.29	0.95	1.16	-2.04	1.01
4	-6.81	5.28	-1.64	-2.02	1.05	1.31	-2.06	1.33
5	-5.95	4.45	-1.29	-1.58	0.76	0.94	-1.46	0.87
6	-5.67	4.12	-1.17	-1.41	0.66	0.80	-1.26	0.71
7	-4.93	3.42	-1.08	-1.31	0.79	0.97	-1.64	1.21
8	-1.49	0.91	-0.28	-0.34	0.20	0.24	-3.91	2.79
9	-4.95	3.61	-1.10	-1.30	0.72	0.86	-1.53	1.01
10	-2.94	1.79	-0.58	-0.68	0.33	0.39	-0.71	0.41

* : approximated

#	SCFlike(2)	SCFlike,r(2)	SCFlike(3)	SCFlike(Paris)	E_HF
1	-2.43	-2.63	-3.71	-3.91	-3.53
2	-2.25	-2.43	-3.32	-3.50	-3.16
3	-2.31	-2.48	-3.34	-3.51	-3.18
4	-2.11	-2.24	-2.84	-2.97	-2.62
5	-2.02	-2.14	-2.62	-2.73	-2.44
6	-2.06	-2.16	-2.60	-2.71	-2.44
7	-1.80	-1.85	-2.23	-2.29	-2.04
8	-0.66	-0.68	-1.79	-1.81	-0.71
9	-1.72	-1.78	-2.25	-2.31	-2.00
10	-1.39	-1.43	-1.69	-1.73	-1.53

#

SCFlike(2) = E100pol + E100ex + E200Ind + E200ExInd

SCFlike,r(2) = E100pol + E100ex + E200Ind,r + E200ExInd,r

# SCFlike(3) = E100pol + E100ex + E200Ind + E200ExInd +
E300Ind(1+E200ExInd/E200Ind)

# SCFlike,r(3) = E100pol + E100ex + E200Ind,r + E200ExInd,r +
E300Ind(1+E200ExInd/E200Ind)

SCFlike(Paris) = SCFlike,r(3)

II.2. SAPT correlation contributions

#	eps1	eps2	E1exch	E22	E22	E20	E2	E30
#	pol,r	disp	(CCSD)	Ind	ExInd*	ExDisp	Disp	IndDisp
1	0.27	-0.40	1.08	-0.41	0.23	0.45	-2.94	-0.62
2	0.31	-0.34	0.86	-0.30	0.16	0.38	-2.63	-0.49
3	0.35	-0.32	0.80	-0.28	0.14	0.36	-2.57	-0.45
4	0.18	-0.34	0.84	-0.35	0.23	0.39	-2.77	-0.48
5	0.24	-0.27	0.61	-0.22	0.13	0.32	-2.56	-0.35
6	0.29	-0.25	0.53	-0.17	0.10	0.29	-2.49	-0.31
7	0.06	-0.34	0.84	-0.35	0.26	0.29	-2.23	-0.35
8	0.00	-0.21	0.37	-0.12	0.09	0.09	-1.00	-0.10
9	0.19	-0.33	0.74	-0.27	0.18	0.30	-2.16	-0.31
10	0.21	-0.22	0.43	-0.13	0.08	0.16	-1.43	-0.14

* : approximated

eps1pol,r = E12pol,r + E13pol,r
E22ExInd = E22Ind * E20ExInd/E20Ind
E2Disp = E20Disp + E21Disp + E22Disp
eps2Disp = E21Disp + E22Disp = E2Disp - E20Disp
#
Corr,r
1 -1.32
2 -1.23
3 -1.19
4 -1.49
5 -1.47
6 -1.46
7 -1.12
8 -0.57
9 -1.03
10 -0.69

Corr,r = eps1pol,r + E1exch(CCSD) + E22Ind + E22ExInd + E20ExDisp + E2Disp

II.3. SAPT total interaction energies

#	SAPT(2)	SAPT(2),r	SAPT(3)	SAPT(Paris)	SAPT(Hybrid)
1	-3.75	-3.95	-5.03	-5.23	-4.85
2	-3.48	-3.65	-4.55	-4.72	-4.39
3	-3.50	-3.67	-4.53	-4.70	-4.37
4	-3.60	-3.73	-4.34	-4.46	-4.11
5	-3.50	-3.61	-4.10	-4.21	-3.91
6	-3.52	-3.62	-4.06	-4.17	-3.90
7	-2.92	-2.98	-3.36	-3.41	-3.17
8	-1.23	-1.25	-2.35	-2.37	-1.28
9	-2.75	-2.81	-3.28	-3.34	-3.02
10	-2.08	-2.12	-2.38	-2.42	-2.22

SAPT = SCFlike + Corr,r
SAPT(Hybrid) = E_HF + Corr,r

III. Interaction energies with supermolecular correlation methods

III.A. Perturbation theory and Coupled Cluster

all electrons correlated
aug-cc-pvtz basis set

n	RHF	MP2	MP4(SDTQ)	CCSD	CCSD(T)
1	-3.53	-4.65	-4.66	-4.46	-4.68
2	-3.16	-4.17	-4.17	-3.99	-4.19
3	-3.18	-4.15	-4.14	-3.98	-4.16
4	-2.62	-3.94	-3.97	-3.76	-3.98
5	-2.44	-3.74	-3.75	-3.55	-3.75
6	-2.44	-3.72	-3.72	-3.52	-3.72
7	-2.04	-2.94	-3.04	-2.91	-3.08
8	-0.71	-1.10	-1.20	-1.14	-1.24
9	-2.00	-2.72	-2.81	-2.72	-2.86
10	-1.53	-1.94	-2.02	-1.97	-2.06

O1s core electrons not correlated
aug-cc-pvtz basis set

# n	RHF	MP2	MP4(SDTQ)	CCSD	CCSD(T)
1	-3.53	-4.62	-4.63	-4.44	-4.66
2	-3.16	-4.15	-4.15	-3.98	-4.17
3	-3.18	-4.12	-4.12	-3.95	-4.14
4	-2.62	-3.92	-3.96	-3.75	-3.97
5	-2.44	-3.72	-3.74	-3.53	-3.73
6	-2.44	-3.70	-3.70	-3.51	-3.70
7	-2.04	-2.93	-3.03	-2.90	-3.07
8	-0.71	-1.10	-1.20	-1.14	-1.23
9	-2.00	-2.71	-2.80	-2.70	-2.85
10	-1.53	-1.93	-2.00	-1.96	-2.05

III.B. CI-based correlation methods

all electrons correlated
aug-cc-pvtz basis set

# n	RHF	CISD	CEPA-0	ACPF	AQCC
1	-3.53	12.95	-4.58	-4.57	-4.28
2	-3.16	13.41	-4.09	-4.09	-3.80
3	-3.18	13.42	-4.06	-4.06	-3.78
4	-2.62	13.72	-3.90	-3.87	-3.57
5	-2.44	13.93	-3.66	-3.64	-3.34
6	-2.44	13.95	-3.62	-3.60	-3.31
7	-2.04	14.56	-3.03	-3.00	-2.70
8	-0.71	16.32	-1.22	-1.20	-0.91
9	-2.00	14.71	-2.82	-2.80	-2.51
10	-1.53	15.44	-2.03	-2.02	-1.74

O1s core electrons not correlated

aug-cc-pvtz basis set

# n	RHF	CISD	CEPA-0	ACPF	AQCC
1	-3.53	12.16	-4.56	-4.55	-4.12
2	-3.16	12.62	-4.07	-4.07	-3.64
3	-3.18	12.63	-4.04	-4.04	-3.62
4	-2.62	12.93	-3.88	-3.85	-3.41
5	-2.44	13.14	-3.64	-3.62	-3.18
6	-2.44	13.16	-3.61	-3.59	-3.15
7	-2.04	13.77	-3.02	-2.99	-2.55
8	-0.71	15.53	-1.22	-1.19	-0.76
9	-2.00	13.93	-2.80	-2.78	-2.35
10	-1.53	14.66	-2.01	-2.01	-1.58