Application of Spin-Ratio Scaled MP2 for the prediction of intermolecular interactions in chemical systems

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Supplementary Information

Table S1. c_{OS} and c_{SS} coefficients in the SRS-MP2 method with best performing basis sets, cc-pVTZ and cc-pVQZ.

Basis set	$\epsilon_{\Delta s}$	c_{OS}	c_{SS}
cc-pVTZ	≥ 1	1.640	-
	< 1	0.660	1.140
cc-pVQZ	≥ 1	1.689	-
	< 1	0.671	1.119

Table S2. Error statistics for SRS-MP2/cc-pVQZ in kJ mol^{-1}.

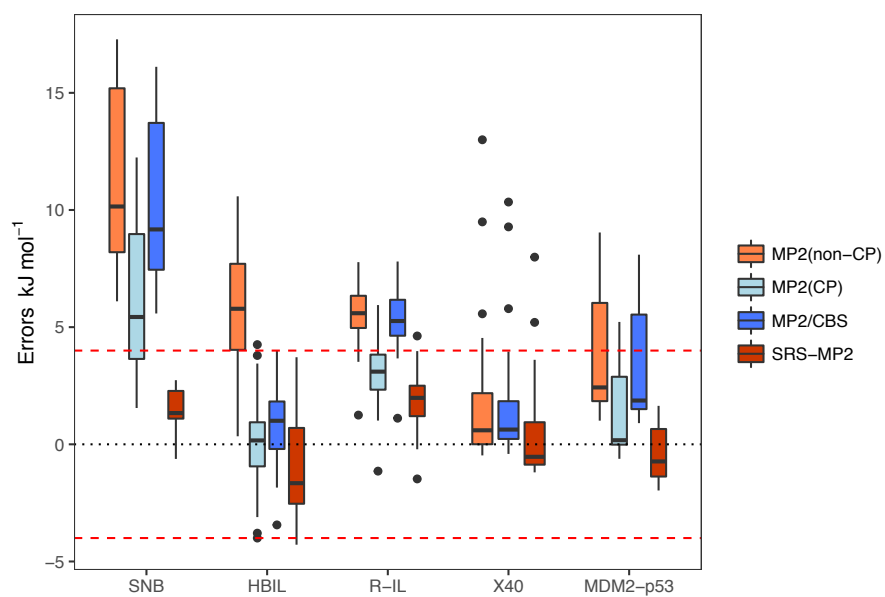| Dataset	MAE[a]	SD[b]	Min	Max
SNB	1.6	1.1	-0.6	2.7
HBIL	2.2	2.3	-4.3	3.7
R-IL	1.9	1.0	-1.5	4.6
X40	1.4	2.1	-1.2	8.0
MDM2-p53	1.2	1.4	-2.0	1.6

[a] Mean Absolute Error. [b] Standard Deviation

Table S3. Percentage error statistics for SRS-MP2/cc-pVQZ.

| Dataset	MAE	SD	Max
SNB	3.0	1.9	6.1
HBIL	6.9	3.6	15.8
R-IL	9.7	5.9	28.8
X40	11.6	5.9	27.9
MDM2-p53	3.8	2.1	6.9
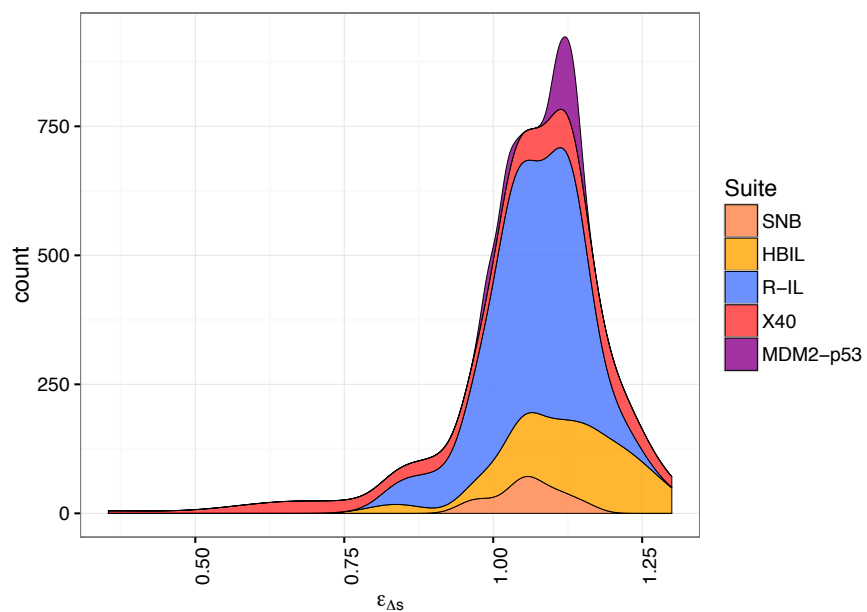
Figure S1. Ratio distributions for the different datasets.

Figure S2. Error distributions for SRS-MP2 and original MP2 methods using the cc-pVQZ basis set across different datasets.

Table S4. CCSD(T)/CBS interaction correlation energies for the different datasets in kJ mol^{-1}.

| Dataset	Mean[J]	SD	Min	Max
SNB	-54.0	10.4	-72.1	-39.4
HBIL	-33.2	7.1	-46.3	-14.9
R-IL	-21.6	5.2	-34.9	-11.5
X40	-11.8	7.6	-35.9	-3.7
MDM2-p53	-34.7	14.0	-56.7	-15.0
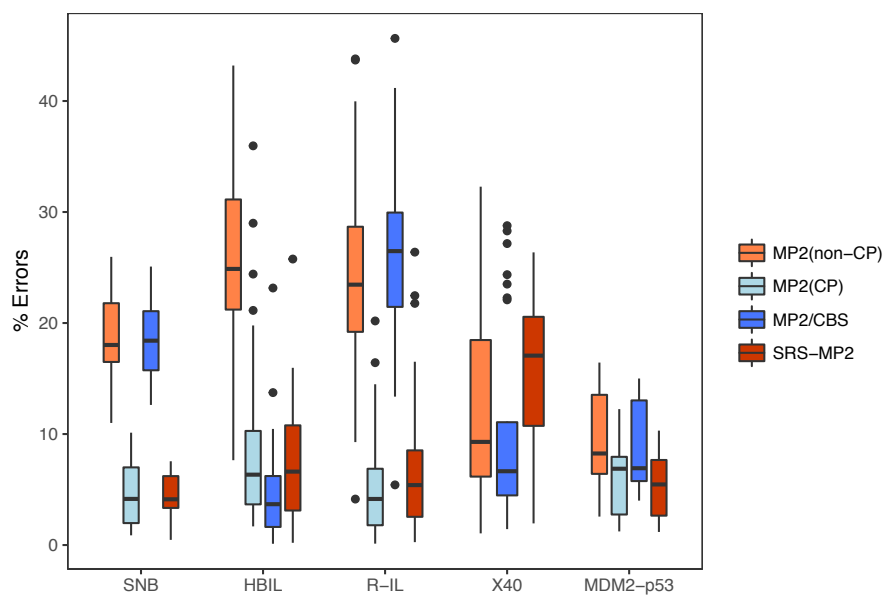
Figure S3. Percentage error distributions for SRS-MP2 and original MP2 methods using the cc-pVTZ basis set across different datasets.

Table S5. Error statistics (all numbers are in kJ mol^{-1}) of MP2, SCS-MP2, SCS(MI), SCSN and SRS-MP2 for cc-pVTZ and cc-pVQZ basis sets, with cc-pVTZ used for SCSN. Error statistics for MP2/CBS are given for comparison.

Basis set	Dataset	Method	Mean[j]	SD	Min	Max
cc-pVTZ	SNB	MP2 (non-CP)	10.6	10.6	4.38	4.87
		MP2(CP)	0.64	2.67	3.41	-4.36
		MP2/CBS	10.32	10.32	3.87	5.58
		SCS-MP2	-13.28	13.28	2.76	-17.27
		SCS(MI)	0.6	1.41	1.74	-1.74
		SCSN	-3.52	3.52	0.84	-4.55
		SRS-MP2	-1.86	2.36	1.8	-3.8
	HBIL	MP2 (non-CP)	8.64	8.64	3.5	1.36
		MP2(CP)	-1.91	2.61	2.45	-7.49
		MP2/CBS	0.84	1.44	1.59	-3.44
		SCS-MP2	-10	10	2.33	-14.1
		SCS(MI)	-1.73	2.44	2.44	-6.38
		SCSN	-4.07	4.21	2.48	-9.68
		SRS-MP2	-0.94	2.22	2.45	-5.2
	R-IL	MP2 (non-CP)	4.98	4.98	1.05	0.85
		MP2(CP)	0.01	1	1.29	-4.15
		MP2/CBS	5.35	5.35	1.14	1.11
		SCS-MP2	-5.62	5.62	1.88	-11.27
		SCS(MI)	0.23	1.16	1.49	-4.12
		SCSN	-1.37	1.75	1.64	-5.35
		SRS-MP2	0.85	1.2	1.18	-2.01
	X40	MP2 (non-CP)	1.05	1.75	2.85	-1.82
		MP2/CBS	1.6	1.68	2.6	-0.41
		SRS-MP2	-0.26	1.65	2.04	-2.97
	MDM2-p53	MP2 (non-CP)	3.76	3.76	3.2	0.58
		MP2(CP)	-1.5	1.82	1.56	-4.26
		MP2/CBS	3.48	3.48	2.93	0.9
		SCS-MP2	-9.65	9.65	3.7	-16.1
		SCS(MI)	-2.11	2.11	0.94	-3.00
		SCSN	-4.69	4.69	0.83	-5.16
		SRS-MP2	-1.45	1.61	1.22	-2.96
cc-pVQZ	SNB	MP2 (non-CP)	11.29	11.29	4.16	6.1
		MP2(CP)	6.39	6.39	3.62	1.55
		MP2/CBS	10.32	10.32	3.87	5.58
		SCS-MP2	-8.49	8.49	2.27	-11.9

	SCS(MI)	0.51	1.12	1.39	-1.19
	SRS-MP2	1.36	1.55	1.14	-0.62
HBIL	MP2 (non-CP)	5.7	5.7	2.54	0.34
	MP2(CP)	0.17	1.51	1.96	-4.00
	MP2/CBS	0.84	1.44	1.59	-3.44
	SCS-MP2	-8.24	8.24	1.83	-11.2
	SCS(MI)	-2.83	2.96	1.72	-5.44
	SRS-MP2	-1.06	2.23	2.26	-4.28
R-IL	MP2 (non-CP)	5.65	5.65	1.01	1.25
	MP2(CP)	3.16	3.18	1.15	-1.14
	MP2/CBS	5.35	5.35	1.14	1.11
	SCS-MP2	-2.94	2.94	1.5	-7.62
	SCS(MI)	0.75	1.22	1.36	-3.2
	SRS-MP2	1.86	1.89	1.00	-1.48
X40	MP2 (non-CP)	1.79	1.9	3.01	-0.47
	MP2/CBS	1.60	1.68	2.6	-0.41
	SRS-MP2	0.49	1.43	2.12	-1.2
MDM2-p53	MP2 (non-CP)	4.00	4.00	3.16	1.01
	MP2(CP)	1.38	1.59	2.16	-0.62
	MP2/CBS	3.48	3.48	2.93	0.9
	SCS-MP2	-7.19	7.19	2.58	-11.56
	SCS(MI)	-2.58	2.58	0.74	-3.43
	SRS-MP2	-0.35	1.23	1.38	-1.97
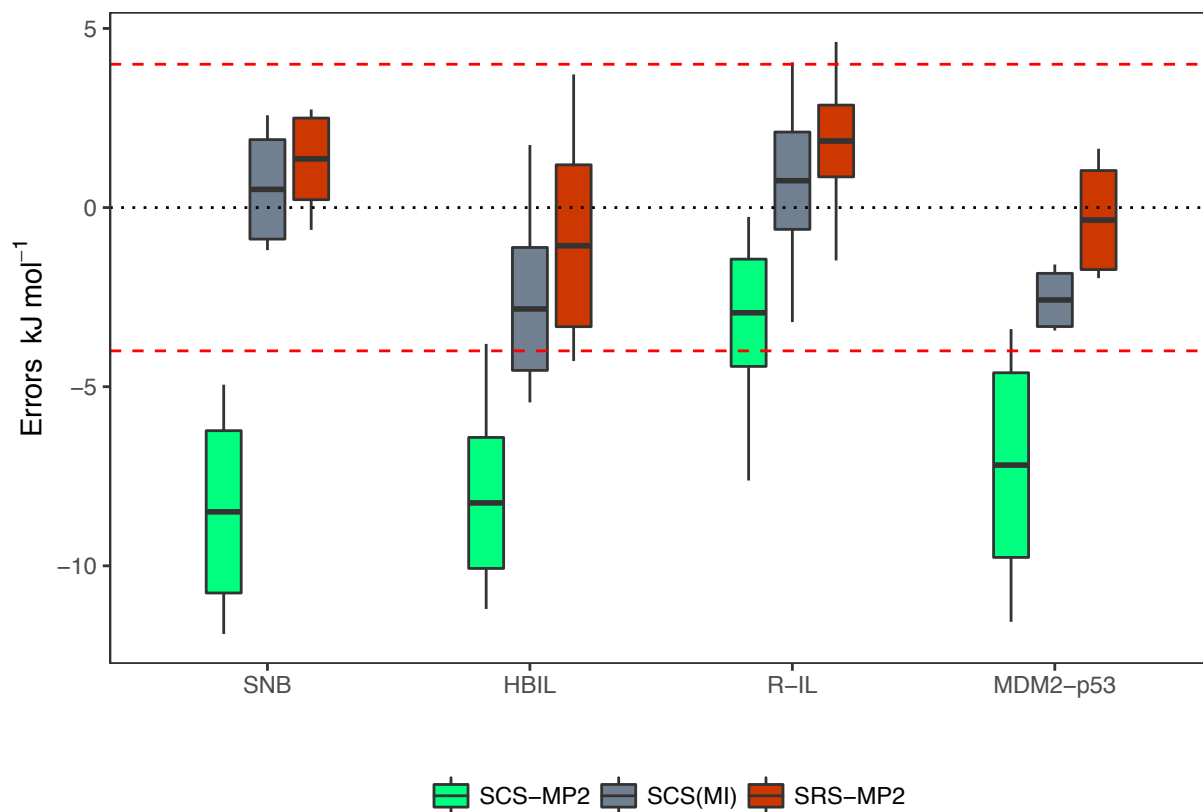
Figure S4. Comparison of SCS-MP2, SCS(MI) and SRS-MP2 performance for the four datasets studied for cc-pVQZ basis set, except SCSN, which is only available for aug-cc-pVTZ. SCS-MP2, SCS(MI) and SCSN used counterpoise corrected energies. The following scaling coefficients were used: 1) c_{OS}=1.2 and c_{SS} = 1/3 for SCS-MP2; 2) c_{OS}=0.31 and c_{SS} = 1.46 for SCS(MI).

Table S5. Error statistics (all numbers are in kJ mol^{-1}) of the SRS-MP2 for all basis sets and all Separations for the S66x8 dataset.

Basis set	Separation	Mean[1]	SD	Min	Max
aug-cc-pVQZ	0.90	2.79	2.72	-9.01	1.95
cc-pVQZ	0.90	1.95	2.24	-7.48	2.21
cc-pVTQZ	0.90	3.18	3.13	-9.69	2.48
aug-cc-pVQZ	0.95	2.17	2.09	-7.26	1.33
cc-pVQZ	0.95	1.49	1.81	-6.10	1.42
cc-pVTQZ	0.95	2.47	2.50	-7.94	1.65
aug-cc-pVQZ	1.00	1.68	1.64	-5.85	0.92
cc-pVQZ	1.00	1.15	1.46	-4.98	1.15
cc-pVTQZ	1.00	1.96	1.99	-6.52	1.30
aug-cc-pVQZ	1.05	1.30	1.30	-4.72	0.79
cc-pVQZ	1.05	0.91	1.18	-4.07	1.03
cc-pVTQZ	1.05	1.50	1.60	-5.36	1.19
aug-cc-pVQZ	1.10	0.99	1.04	-3.81	0.69
cc-pVQZ	1.10	0.73	0.96	-3.32	0.95
cc-pVTQZ	1.10	1.22	1.30	-4.39	1.09
aug-cc-pVQZ	1.25	0.53	0.67	-2.03	1.59
cc-pVQZ	1.25	0.47	0.60	-1.82	0.94
cc-pVTQZ	1.25	0.67	0.76	-2.42	0.86
aug-cc-pVQZ	1.50	0.25	0.32	-0.76	0.99
cc-pVQZ	1.50	0.23	0.28	-0.69	0.50
cc-pVTQZ	1.50	0.30	0.37	-0.92	0.65
aug-cc-pVQZ	2.00	0.10	0.10	-0.15	0.37
cc-pVQZ	2.00	0.09	0.09	-0.13	0.24
cc-pVTQZ	2.00	0.10	0.12	-0.19	0.37