Supplementary information for: "Assessing the effect of regularization on the molecular properties predicted by SCAN and self-interaction corrected SCAN meta-GGA"

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S1 Polynomial used in rCAN

The polynomial function used in the rSCAN implementation is defined as

$$f(\alpha) = c_1 + c_2\alpha + c_3\alpha^2 + c_4\alpha^3 + c_5\alpha^4 + c_6\alpha^5 + c_7\alpha^6 + c_8\alpha^7 \tag{S1}$$

for $\alpha \in [0, 2.5]$ where the coefficients c's are as shown in Table S1. Those are the same as in Ref.[1]. The constraints used are $f^{(0,1,2)}(0)$ and $f^{(0,1,2,3)}(2.5)$ to be identical values as the $f(\alpha)$ in SCAN at these two points. In addition, $f(1) = 0$ was also used as a constraint. The plots of $f_x(\alpha)$ and $f_x'(\alpha)$ are shown in Fig. S1. The plot of $\partial\varepsilon_{XC}/\partial\rho$ for an Ar atom is shown in Fig. S2. We have also tested different choices of polynomials with the same constraints and found essentially the same results.

Table S1 The coefficients used for the rSCAN implementation (same as Ref. [1]).

Coef.	Exchange	Correlation
c_1	1.000	1.000
c_2	−0.677	−0.640
c_3	−0.44456	−0.4352
c_4	−0.62109	−1.53568
c_5	1.39690	3.06156
c_6	−0.85920	−1.91571
c_7	0.22746	0.51688
c_8	−0.02252	−0.05185

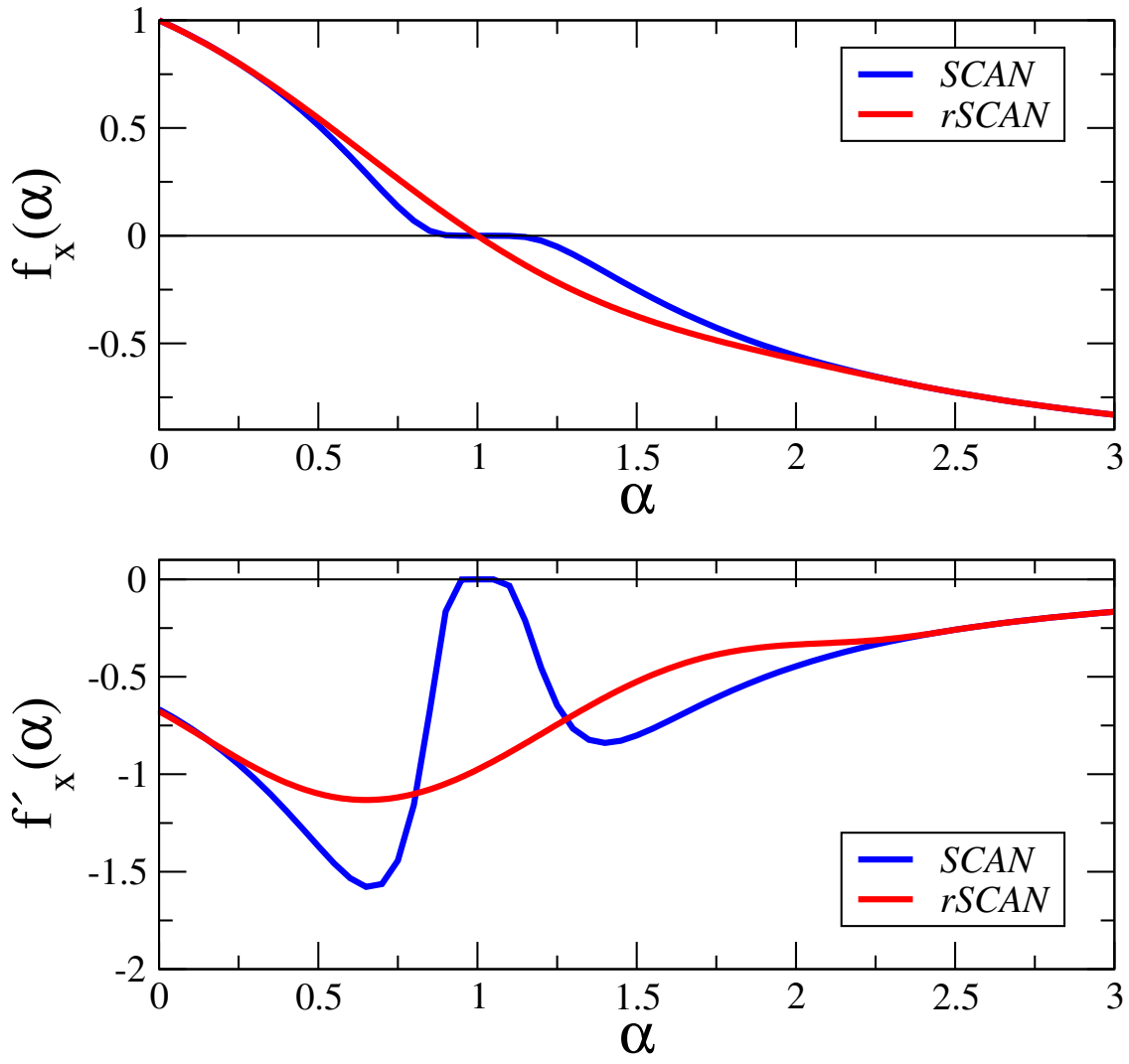

Figure S1 The switching function $f_x(\alpha)$ and $f'_x(\alpha)$ for SCAN and rSCAN.

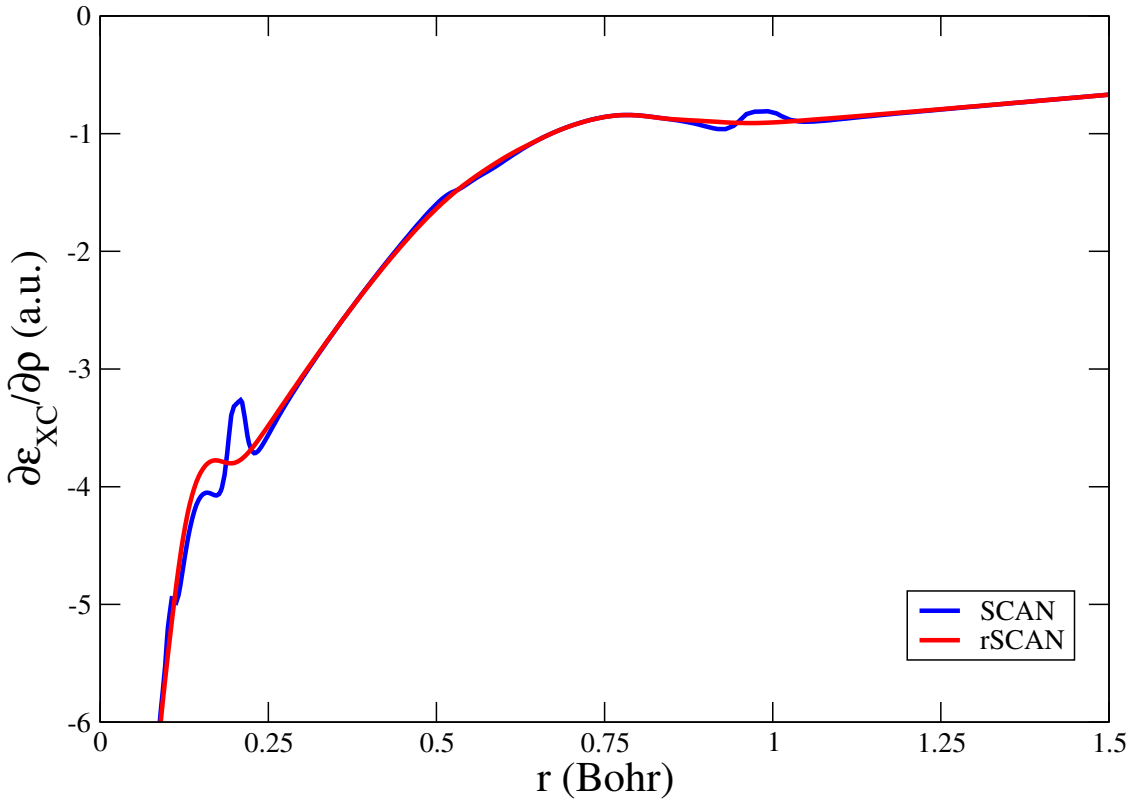

Figure S2 $\partial\varepsilon_{XC}/\partial\rho$ as a function of r for Ar atom with SCAN and rSCAN.

S2 Dipole moments, S22, and BH76

Table S2 Dipole moments of 152 benchmark molecules (in Debye).

System	SCAN	rSCAN	CCSD(T)[a]
AlF	1.31	1.31	1.47
AlH_2	0.40	0.40	0.40
BeH	0.58	0.58	0.23
BF	1.05	1.05	0.82
BH	1.58	1.59	1.41
BH_2	0.48	0.49	0.50
BH_2Cl	0.55	0.55	0.68
BH_2F	0.68	0.68	0.83
$BHCl_2$	0.56	0.56	0.67
BHF_2	0.83	0.83	0.96
BN	2.12	2.06	2.04
BO	2.35	2.33	2.32
BS	0.89	0.85	0.78
C_2H	0.76	0.74	0.76
C_2H_3	0.71	0.70	0.69
C_2H_5	0.34	0.34	0.31
CF	0.89	0.90	0.68
CF_2	0.72	0.72	0.54
CH	1.48	1.48	1.43
CH_2BH	0.56	0.57	0.62
CH_2BOH	2.31	2.31	2.26
CH_2F	1.27	1.27	1.38
CH_2NH	2.02	2.00	2.07
CH_2PH	1.02	0.99	0.87
CH_2-singlet	1.83	1.82	1.49
CH_2-triplet	0.59	0.59	0.59
CH_3BH_2	0.69	0.70	0.58
CH_3BO	3.77	3.78	3.68
CH_3Cl	1.94	1.91	1.90
CH_3F	1.72	1.71	1.81
CH_3Li	5.77	5.76	5.83
CH_3NH_2	1.36	1.35	1.39
CH_3O	2.11	2.09	2.04
CH_3OH	1.66	1.65	1.71
CH_3SH	1.65	1.66	1.59
ClCN	3.00	3.02	2.85
ClF	0.82	0.75	0.88

[a]Reference [2]

Dipole moments continued.

ClO_2	1.76	1.75	1.86
CN	1.41	1.41	1.43
CO	0.13	0.17	0.12
CS	1.92	1.96	1.97
CSO	0.79	0.79	0.73
FCN	2.33	2.35	2.18
FCO	0.85	0.84	0.77
FH-BH_2	3.03	3.03	2.97
FH-NH_2	4.67	4.67	4.63
FH-OH	3.40	3.40	3.38
FNO	1.54	1.51	1.70
H_2CN	2.52	2.50	2.49
H_2O	1.86	1.87	1.86
H_2O-Al	4.53	4.54	4.36
H_2O-Cl	3.04	3.05	2.24
H_2O-F	2.58	2.64	2.19
H_2O-H_2O	2.78	2.78	2.73
H_2O-Li	2.98	2.98	3.62
H_2O-NH_3	3.57	3.58	3.50
H_2S-H_2S	1.05	1.06	0.92
H_2S-HCl	2.36	2.36	2.13
HBH_2BH	0.85	0.88	0.84
HBO	2.72	2.71	2.73
HBS	1.43	1.40	1.38
HCCCl	0.31	0.28	0.50
HCCF	0.56	0.52	0.75
HCHO	2.37	2.32	2.39
HCHS	1.86	1.80	1.76
HCl	1.16	1.15	1.11
HCl-HCl	1.91	1.90	1.78
HCN	3.03	3.02	3.01
HCNO	2.60	2.57	2.96
HCO	1.67	1.65	1.69
HCOF	2.09	2.07	2.12
$HCONH_2$	3.96	3.95	3.92
HCOOH	1.48	1.47	1.38
HCP	0.48	0.45	0.35
HF	1.80	1.80	1.81
HF-HF	3.42	3.42	3.40
HN_3	1.77	1.79	1.66
HNC	3.05	3.07	3.08
HNCO	2.05	2.04	2.06
HNO	1.57	1.56	1.65
HNO_2	1.96	1.95	1.93

Dipole moments continued.

HNS	1.39	1.39	1.41
HO_2	2.17	2.21	2.17
HOCl	1.55	1.56	1.52
HOCN	3.97	3.99	3.80
HOF	1.92	1.89	1.92
HOOH	1.57	1.57	1.57
HPO	2.34	2.32	2.63
$LiBH_4$	6.11	6.11	6.13
LiCl	7.10	7.10	7.10
LiCN	6.99	7.00	6.99
LiF	6.28	6.28	6.29
LiH	5.82	5.82	5.83
LiN	6.84	6.83	7.06
LiOH	4.53	4.53	4.57
N_2H_2	2.83	2.83	2.88
N_2H_4	2.71	2.71	2.72
NaCl	8.85	8.85	9.01
NaCN	8.81	8.82	8.89
NaF	7.99	7.99	8.13
NaH	6.33	6.33	6.40
NaLi	0.23	0.25	0.48
NaOH	6.63	6.63	6.77
NCl	1.14	1.16	1.13
NCO	0.83	0.84	0.79
NF	0.15	0.18	0.07
NF_2	0.13	0.11	0.19
NH	1.54	1.54	1.54
NH_2	1.80	1.80	1.79
NH_2Cl	2.03	2.01	1.95
NH_2F	2.28	2.24	2.27
NH_2OH	0.70	0.67	0.70
NH_3	1.55	1.55	1.53
NH_3-BH_3	5.33	5.33	5.28
NH_3-NH_3	2.18	2.19	2.13
NH_3O	5.21	5.21	5.39
NO	0.17	0.19	0.13
NO_2	0.29	0.29	0.34
NOCl	1.86	1.83	2.08
NP	2.74	2.75	2.87
NS	1.77	1.79	1.82
O_3	0.63	0.64	0.57
OCl	1.43	1.43	1.28
OCl_2	0.50	0.48	0.56
OF	0.16	0.19	0.02

Dipole moments continued.

OF_2	0.33	0.31	0.33
OH	1.65	1.65	1.66
P_2H_4	1.06	1.08	1.00
PCl	0.42	0.38	0.57
PF	0.65	0.66	0.81
PH	0.50	0.49	0.44
PH_2	0.62	0.62	0.55
PH_2OH	1.89	1.92	0.68
PH_3	0.67	0.69	0.61
PH_3O	3.63	3.63	3.77
PO	1.89	1.85	1.96
PO_2	1.36	1.33	1.44
PPO	1.74	1.69	1.88
PS	0.55	0.52	0.68
S_2H_2	1.19	1.19	1.14
SCl	0.19	0.22	0.07
SCl_2	0.34	0.31	0.39
SF	0.63	0.59	0.81
SF_2	0.90	0.87	1.06
SH	0.83	0.83	0.77
SH_2	1.06	1.07	0.99
SiH	0.19	0.20	0.11
SiH_3Cl	1.28	1.28	1.36
SiH_3F	1.23	1.23	1.31
SiO	2.99	2.95	3.11
SO_2	1.54	1.52	1.63
SO-triplet	1.40	1.40	1.56

Table S3 Weak interaction energies of the S22 set of molecules (in kcal/mol).

System	SCAN	rSCAN	CCSD(T)[a]
2-pyridoxine–2-aminopyridine	17.0	17.1	17
Adenine–thymine stack	8.7	8.5	11.66
Adenine–thymine WC	16.0	16.2	16.74
Ammonia dimer	3.2	3.2	3.17
Benzene–ammonia	2.1	2.0	2.32
Benzene dimer C2h	1.0	0.9	2.62
Benzene dimer C2v	1.5	1.5	2.71
Benzene–HCN	4.2	4.1	4.55
Benzene–methane	0.9	0.9	1.45
Benzene–water	3.4	3.3	3.29
Ethene dimer	1.2	1.1	1.5
Ethene–ethyne	1.4	1.4	1.51
Formamide dimer	16.6	16.7	16.12
Formic acid dimer	21.0	20.9	18.8
Indole–benzene stack	2.1	1.9	4.59
Indole–benzene T-shape	4.2	4.1	5.62
Methane dimer	0.4	0.4	0.53
Phenol dimer	6.0	5.9	7.09
Pyrazine dimer	2.7	2.5	4.2
Uracil dimer HB	20.5	20.6	20.69
Uracil dimer stack	8.1	7.9	9.74
Water dimer	5.5	5.5	5.02

[a]Reference [3]

Table S4 Reaction barrier heights of the BH76 set of molecules (in kcal/mol).

Reaction	Direction	SCAN	rSCAN	W1[a]	W2-F12[b]
$H + HCl \rightarrow H_2 + Cl$	Forward	-1.4	-0.1	5.7	6.1
	Reverse	0.1	-0.3	8.7	8.0
$OH + H_2 \rightarrow H_2O + H$	Forward	-2.1	-2.6	5.1	5.2
	Reverse	11.1	13.2	21.2	21.6
$CH_3 + H_2 \rightarrow CH_4 + H$	Forward	7.2	6.9	12.1	11.9
	Reverse	7.0	8.0	15.3	15.0
$OH + CH_4 \rightarrow H_2O + CH_3$	Forward	-1.6	-1.9	6.7	6.3
	Reverse	11.8	12.7	19.6	19.5
$H + H_2 \rightarrow H_2 + H$	Forward	2.4	2.3	9.6	9.7
	Reverse	2.4	2.3	9.6	9.7
$OH + NH_3 \rightarrow H_2O + NH_2$	Forward	-7.4	-7.9	3.2	3.4
	Reverse	3.2	3.3	12.7	13.7
$HCl + CH_3 \rightarrow CH_4 + Cl$	Forward	-3.1	-3.3	1.7	1.8
	Reverse	-1.7	-2.3	7.9	6.8
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	Forward	-4.8	-5.3	3.4	3.5
	Reverse	13.0	14.0	19.9	20.4
$F + H_2 \rightarrow HF + H$	Forward	-7.7	-8.2	1.8	1.6
	Reverse	22.2	24.8	33.4	33.8
$O + CH_4 \rightarrow OH + CH_3$	Forward	2.2	2.1	13.7	14.4
	Reverse	3.3	2.9	8.1	8.9
$H + PH_3 \rightarrow H_2 + PH_2$	Forward	-3.2	-3.4	3.1	2.9
	Reverse	19.5	19.3	23.2	24.7
$H + HO \rightarrow H_2 + O$	Forward	3.2	3.0	10.7	10.9
	Reverse	2.1	1.1	13.1	13.2
$H + H_2S \rightarrow H_2 + HS$	Forward	-2.7	-2.7	3.5	3.9
	Reverse	11.1	10.1	17.3	17.2
$O + HCl \rightarrow OH + Cl$	Forward	-4.0	-5.0	9.8	10.4
	Reverse	-1.5	-3.2	10.4	9.9
$CH_3 + NH_2 \rightarrow CH_4 + NH$	Forward	4.5	3.9	8	8.9
	Reverse	12.5	12.8	22.4	22.0
$C_2H_5 + NH_2 \rightarrow C_2H_6 + NH$	Forward	6.0	5.5	7.5	9.8
	Reverse	9.5	9.6	18.3	19.4
$NH_2 + C_2H_6 \rightarrow NH_3 + C_2H_5$	Forward	4.8	4.5	10.4	11.3
	Reverse	12.0	12.6	17.4	17.8
$NH_2 + CH_4 \rightarrow NH_3 + CH_3$	Forward	7.7	7.6	14.5	13.9
	Reverse	10.4	11.0	17.8	16.9
s-trans cis-$C_5H_8 \rightarrow$ s-trans cis-C_5H_8	Forward	33.6	32.5	38.4	39.7
	Reverse	33.6	32.5	38.4	39.7

[a]Reference [4]
[b]Reference [5]

BH76 continued.

$H + N_2O \rightarrow OH + N_2$	Forward	18.7	19.2	18.14	17.7
	Reverse	66.1	62.6	83.22	82.6
$H + FH \rightarrow HF + H$	Forward	38.3	38.2	42.18	42.1
	Reverse	38.3	38.2	42.18	42.1
$H + ClH \rightarrow HCl + H$	Forward	19.5	19.3	18	17.8
	Reverse	19.5	19.3	18	17.8
$H + FCH_3 \rightarrow HF + CH_3$	Forward	29.2	28.3	30.38	30.5
	Reverse	46.3	46.4	57.02	56.9
$H + F_2 \rightarrow HF + F$	Forward	-1.6	-0.5	2.27	1.5
	Reverse	88.6	89.2	106.18	104.8
$CH_3 + FCl \rightarrow CH_3F + Cl$	Forward	-5.1	-4.7	7.43	7.1
	Reverse	45.9	45.4	60.17	59.8
$F^- + CH_3F \rightarrow FCH_3 + F^-$	Forward	-8.3	-7.8	-0.34	-0.6
	Reverse	-8.3	-7.8	-0.34	-0.6
$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	Forward	7.5	7.9	13.38	13.4
	Reverse	7.5	7.9	13.38	13.4
$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	Forward	-6.1	-4.6	3.1	2.5
	Reverse	-6.1	-4.6	3.1	2.5
$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	Forward	6.1	7.2	13.61	13.5
	Reverse	6.1	7.2	13.61	13.5
$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	Forward	-21.7	-20.5	-12.54	-12.3
	Reverse	14.3	14.2	20.11	19.8
$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	Forward	-2.1	-1.2	2.89	3.5
	Reverse	24.4	24.2	29.62	29.6
$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	Forward	-11.2	-10.7	-2.78	-2.7
	Reverse	9.8	10.8	17.33	17.6
$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	Forward	3.9	4.3	10.96	11.0
	Reverse	43.9	45.1	47.2	47.7
$H + N_2 \rightarrow HN_2$	Forward	13.9	13.7	14.69	14.6
	Reverse	9.8	9.3	10.72	10.9
$H + CO \rightarrow HCO$	Forward	5.9	6.1	3.17	3.2
	Reverse	24.2	24.2	22.68	22.8
$H + C_2H_4 \rightarrow CH_3CH_2$	Forward	5.2	6.4	1.72	2.0
	Reverse	43.3	43.2	41.75	42.0
$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	Forward	0.7	2.1	6.85	6.4
	Reverse	31.0	31.9	32.97	33.0
$HCN \rightarrow HNC$	Forward	46.1	46.1	48.16	48.1
	Reverse	32.0	31.6	33.11	33.0

S3 Infrared and Raman spectra of water cluster

Table S5 Infrared and Raman spectra of water monomer. Frequencies (in cm^{-1}), IR intensities (in km mol^{-1}), and Raman intensities (in $Å^4$ u^{-1}) and depolarization ratio are shown.

SCAN				rSCAN				CCSD(T)[a]
Freq.	IR	Raman	Depol.	Freq.	IR	Raman	Depol.	Freq.
1640	70.77	0.66	0.72	1636	71.72	0.66	0.71	1638.1
3802	2.96	100.86	0.05	3803	3.36	100.12	0.05	3786.8
3909	54.50	25.46	0.75	3911	55.89	25.03	0.75	3904.5

[a]Reference [6]

Table S6 Infrared and Raman spectra of water dimer. Frequencies (in cm^{-1}), IR intensities (in km mol^{-1}), and Raman intensities (in $Å^4$ u^{-1}) and depolarization ratio are shown.

SCAN				rSCAN				CCSD(T)[a]
Freq.	IR	Raman	Depol.	Freq.	IR	Raman	Depol.	Freq.
94	124.45	0.04	0.73	105	154.49	0.05	0.74	132.6
147	47.70	0.05	0.74	163	22.31	0.03	0.71	145.3
171	118.93	0.14	0.66	164	125.78	0.15	0.66	146.1
203	173.20	0.06	0.54	201	161.80	0.04	0.58	183.6
388	43.82	0.15	0.68	382	46.30	0.12	0.71	355.2
649	89.10	0.34	0.74	653	88.74	0.32	0.74	629.7
1639	85.86	0.92	0.75	1635	87.59	0.88	0.74	1639.6
1664	36.35	0.72	0.30	1660	37.28	0.69	0.31	1658.8
3654	386.50	151.68	0.14	3659	397.39	170.27	0.15	3712.1
3790	8.85	83.27	0.05	3799	8.71	80.66	0.05	3782.5
3876	74.56	51.35	0.26	3885	75.17	50.81	0.26	3875.5
3894	78.12	23.97	0.75	3903	79.83	23.69	0.75	3896.1

[a]Reference [6]

Table S7 Infrared and Raman spectra of water trimer. Frequencies (in cm^{-1}), IR intensities (in km mol^{-1}), and Raman intensities (in $Å^4$ u^{-1}) and depolarization ratio are shown.

SCAN				rSCAN				CCSD(T)[a]
Freq.	IR	Raman	Depol.	Freq.	IR	Raman	Depol.	Freq.
190	102.95	0.04	0.71	200	37.87	0.03	0.71	157
197	44.45	0.10	0.62	204	25.98	0.05	0.56	170
213	57.00	0.19	0.74	220	71.17	0.30	0.70	183
214	79.27	0.21	0.73	224	148.95	0.15	0.75	190.3
240	7.45	0.27	0.18	239	5.47	0.26	0.18	216.7
250	42.44	0.18	0.63	264	43.85	0.19	0.66	234.1
375	62.91	0.93	0.34	385	76.09	0.72	0.41	334.5
388	51.73	0.49	0.62	396	30.54	0.63	0.49	343.5
481	122.23	0.49	0.28	488	124.93	0.53	0.25	434.1
636	186.88	0.76	0.56	638	186.37	0.59	0.63	558.7
719	290.05	0.30	0.46	724	291.11	0.27	0.57	650.1
953	8.74	0.52	0.74	958	9.02	0.49	0.73	850.8
1649	57.25	1.28	0.65	1647	52.22	1.29	0.63	1647.8
1651	81.78	0.90	0.53	1649	89.09	0.88	0.52	1650.1
1674	14.87	0.98	0.75	1672	14.12	0.98	0.75	1671.7
3429	29.13	304.92	0.06	3427	26.38	300.24	0.06	3596.5
3515	754.03	37.68	0.74	3514	759.62	37.20	0.74	3647.8
3537	683.55	47.93	0.54	3533	687.80	38.67	0.59	3655
3864	78.86	53.18	0.22	3865	87.49	46.96	0.25	3865.7
3865	77.77	51.03	0.43	3866	70.63	62.53	0.32	3869.9
3867	42.63	114.89	0.08	3869	45.91	109.97	0.09	3871.4

[a]Reference [6]

Table S8 Infrared and Raman spectra of water tetramer. Frequencies (in cm^{-1}), IR intensities (in km mol^{-1}), and Raman intensities (in $Å^4$ u^{-1}) and depolarization ratio are shown.

SCAN				rSCAN				CCSD(T)[a]
Freq.	IR	Raman	Depol.	Freq.	IR	Raman	Depol.	Freq.
63	0.15	0.17	0.67	54	0.01	0.12	0.73	48.8
77	2.91	0.30	0.74	85	1.90	0.39	0.75	76.1
222	0.16	0.24	0.11	223	0.10	0.22	0.12	192.1
236	38.03	0.96	0.75	234	37.55	0.81	0.75	208.2
251	130.83	0.04	0.75	263	37.78	0.05	0.75	230.8
260	47.33	0.06	0.74	265	20.32	0.05	0.75	230.8
277	146.05	0.03	0.66	283	234.89	0.00	0.75	248.7
282	216.38	0.00	0.34	286	248.59	0.00	0.73	248.7
287	9.42	0.03	0.60	289	3.94	0.05	0.75	254.3
316	1.50	0.22	0.36	327	0.31	0.20	0.34	283.5
433	0.20	0.19	0.29	442	0.02	0.21	0.29	391
461	19.63	0.78	0.74	478	15.73	0.80	0.75	421
481	38.75	0.56	0.75	493	37.35	0.52	0.75	437.9
484	37.65	0.62	0.75	494	38.02	0.59	0.75	437.9
807	132.49	0.62	0.73	811	136.70	0.69	0.75	730.5
891	159.02	0.41	0.75	898	163.54	0.40	0.75	800.2
900	161.73	0.37	0.74	900	161.87	0.41	0.75	800.2
1074	0.02	0.68	0.01	1078	0.00	0.42	0.08	971
1649	83.66	0.66	0.75	1647	84.91	0.64	0.75	1653
1664	42.80	0.54	0.75	1663	42.73	0.53	0.75	1666.6
1665	42.21	0.54	0.74	1664	42.67	0.55	0.75	1666.6
1697	0.05	1.75	0.20	1696	0.00	1.91	0.19	1693.3
3161	0.21	360.22	0.08	3160	0.23	357.14	0.08	3446.4
3299	1886.40	2.13	0.73	3299	1893.09	2.10	0.74	3526.6
3303	1917.26	2.27	0.72	3300	1891.83	2.38	0.73	3526.6
3354	26.31	105.31	0.75	3353	26.84	106.52	0.75	3559.1
3860	67.22	48.06	0.35	3861	69.75	44.94	0.34	3860.9
3861	45.97	95.66	0.08	3862	73.59	39.86	0.34	3861.4
3862	71.11	43.90	0.45	3863	45.34	97.98	0.11	3861.4
3864	45.77	95.13	0.07	3865	46.19	95.84	0.09	3861.5

[a]Reference [6]

Table S9 Infrared and Raman spectra of water pentamer. Frequencies (in cm^{-1}), IR intensities (in km mol^{-1}), and Raman intensities (in $Å^4$ u^{-1}) and depolarization ratio are shown.

SCAN				rSCAN				CCSD(T)[a]
Freq.	IR	Raman	Depol.	Freq.	IR	Raman	Depol.	Freq.
30	4.38	0.02	0.75	30	4.57	0.02	0.74	22.5
44	0.06	0.18	0.62	43	0.03	0.20	0.61	41.4
68	0.10	0.22	0.74	67	0.15	0.25	0.75	60.6
78	1.84	0.29	0.66	71	1.45	0.26	0.75	63.5
189	2.21	0.21	0.22	191	0.91	0.22	0.15	179.2
203	31.05	0.59	0.74	206	31.14	0.60	0.75	190.1
213	31.08	0.62	0.74	219	39.08	0.59	0.75	196
238	115.26	0.17	0.70	244	95.34	0.17	0.73	226.6
255	4.33	0.01	0.73	258	6.82	0.01	0.71	232.3
267	146.94	0.03	0.74	266	148.96	0.04	0.71	236.9
286	270.53	0.09	0.29	288	276.54	0.05	0.59	265.1
321	82.37	0.18	0.74	324	76.91	0.17	0.75	291.8
330	11.90	0.06	0.75	331	19.75	0.04	0.73	295
336	1.11	0.04	0.70	338	1.52	0.02	0.72	297.7
449	48.52	0.84	0.39	453	50.97	0.62	0.46	400.5
463	14.93	0.31	0.22	467	10.20	0.30	0.16	420.7
490	15.64	0.81	0.74	495	15.78	0.75	0.74	443.9
500	17.78	0.79	0.73	507	19.11	0.79	0.73	456.7
559	62.28	0.99	0.35	561	62.38	0.89	0.40	503.1
771	23.74	1.31	0.65	778	24.16	1.32	0.70	702.5
848	128.11	1.18	0.69	852	126.67	1.07	0.74	766.2
934	130.17	0.62	0.69	941	130.08	0.59	0.75	843.9
955	124.66	0.26	0.73	960	123.33	0.22	0.73	860
1063	8.15	0.07	0.19	1068	8.54	0.15	0.11	963.7
1649	83.44	0.17	0.69	1647	83.94	0.18	0.74	1657.6
1662	20.27	0.72	0.58	1660	19.34	0.72	0.59	1667.9
1672	58.45	0.55	0.37	1671	61.06	0.49	0.42	1675.2
1696	34.66	0.48	0.05	1695	36.19	0.44	0.04	1694.4
1705	4.22	0.62	0.63	1703	3.96	0.73	0.49	1701.4
3095	50.75	495.91	0.08	3097	48.68	493.31	0.08	3413
3223	2923.51	4.41	0.74	3224	2857.86	4.04	0.74	3482.9
3235	2624.40	13.29	0.38	3237	2630.15	13.05	0.38	3490.2
3297	93.02	74.00	0.75	3298	79.76	73.89	0.74	3529.6
3317	113.31	79.85	0.72	3317	120.20	75.18	0.73	3535.5
3861	50.36	53.55	0.28	3867	56.87	60.48	0.19	3859.1
3862	67.18	61.22	0.15	3870	66.32	49.40	0.24	3861.1
3862	50.73	57.29	0.18	3871	49.89	88.56	0.12	3862.9
3864	52.53	87.50	0.12	3873	40.97	23.24	0.71	3862.9
3867	57.65	108.78	0.08	3875	67.76	142.57	0.05	3865.7

[a]Reference [6]

S4 FLOSIC-rCAN calculations

Table S10 Atoms: total energies (in Hartree).

Z	rSCAN	SIC-rSCAN	E_{Accu}[a]
1	-0.500	-0.500	-0.5
2	-2.905	-2.900	-2.90
3	-7.480	-7.474	-7.48
4	-14.650	-14.643	-14.67
5	-24.641	-24.628	-24.65
6	-37.841	-37.813	-37.85
7	-54.594	-54.538	-54.59
8	-75.076	-74.997	-75.07
9	-99.752	-99.640	-99.73
10	-128.963	-128.799	-128.94
11	-162.286	-162.100	-162.25
12	-200.082	-199.874	-200.05
13	-242.383	-242.147	-242.35
14	-289.404	-289.131	-289.36
15	-341.311	-340.993	-341.26
16	-398.164	-397.807	-398.11
17	-460.208	-459.802	-460.15
18	-527.606	-527.141	-527.54
19	-599.981	-599.467	
20	-677.627	-677.061	
21	-760.692	-760.077	
22	-849.446	-848.791	
23	-944.011	-943.254	
24	-1044.596	-1043.686	
25	-1151.143	-1150.196	
26	-1263.849	-1262.832	
27	-1382.936	-1381.869	
28	-1508.506	-1507.310	
29	-1640.748	-1639.332	
30	-1779.669	-1778.237	
31	-1925.102	-1923.629	
32	-2077.232	-2075.698	
33	-2236.145	-2234.541	
34	-2401.837	-2400.160	
35	-2574.471	-2572.710	
36	-2754.143	-2752.290	

[a]Reference [7]

Table S11 Atoms: ionization potentials (in eV).

Z	rSCAN	SIC-rSCAN	Expt.[a]
2	24.624	24.483	24.587
3	5.400	5.374	5.392
4	8.802	8.820	9.323
5	8.788	8.732	8.298
6	11.716	11.437	11.26
7	14.889	14.308	14.534
8	13.707	13.431	13.618
9	17.609	17.005	17.423
10	21.633	20.589	21.565
11	5.180	5.140	5.139
12	7.393	7.395	7.646
13	6.181	6.180	5.986
14	8.341	8.215	8.152
15	10.670	10.441	10.487
16	10.345	10.419	10.36
17	13.045	12.962	12.968
18	15.879	15.646	15.76
19	4.282	4.472	4.341
20	5.839	6.089	6.113
21	6.241	7.054	6.561
22	6.984	8.324	6.828
23	7.126	7.070	6.746
24	7.312	7.015	6.767
25	6.908	7.133	7.434
26	7.795	8.068	7.902
27	8.396	8.279	7.881
28	8.789	8.443	7.64
29	8.090	7.488	7.726
30	9.238	9.519	9.394
31	6.156	6.560	5.999
32	8.093	8.324	7.899
33	10.134	10.423	9.789
34	9.685	10.280	9.752
35	11.913	12.379	11.814
36	14.250	14.743	14

[a]Reference [8]

Table S12 Atoms: electron affinities (in eV).

Z	rSCAN	SIC-rSCAN	Expt.[a]
1	0.725	0.510	0.754
3	0.446	0.465	0.618
5	0.608	0.167	0.280
6	1.547	0.875	1.262
8	1.573	0.637	1.462
9	3.428	2.123	3.401
11	0.457	0.480	0.548
13	0.626	0.383	0.434
14	1.570	1.277	1.390
15	0.765	0.602	0.747
16	2.157	1.843	2.077
17	3.714	3.277	3.613
19	0.409	0.424	0.501
22	1.008	-1.211	0.087
29	1.178	1.061	1.236
31	0.544	0.187	0.43
32	1.540	1.274	1.233
33	0.830	0.659	0.814
34	2.135	1.806	2.021
35	3.584	3.232	3.364

[a]Reference [9]

Table S13 Mean absolute error (in eV) of ΔSCF electron affinities with respect to experiment.

Method	12 EAs	20 EAs
SCAN[a]	0.115	0.148
rSCAN[a]	0.135	0.173
SIC-SCAN[b]	0.364	0.341
SIC-rSCAN	0.329	0.314
Δ-DFA[c]	0.036	0.036
Δ-SIC[d]	0.036	0.032

[a]Based on total energies. The eigenvalue of the extra electron becomes positive.
[b]From reference [10]
[c]Δ-DFA is difference between rSCAN and SCAN
[d]Δ-SIC is difference between SIC-rSCAN and SIC-SCAN

Table S14 Atomization energies of the AE6 set of molecules (in kcal/mol).

System	rSCAN	SIC-rSCAN	Ref.[a]
$C_2O_2H_2$	643.0	589.5	634.0
CH_3CCH	710.2	678.3	705.1
C_4H_8	1160.8	1134.0	1149.4
S_2	109.6	98.7	104.3
SiH_4	322.4	326.9	325.0
SiO	188.8	157.8	193.1

[a]Reference [11]

Table S15 Reaction barrier heights of the BH6 set of molecules (in kcal/mol).

Reaction	Direction	rSCAN	SIC-rSCAN	Ref.[a]
$OH + CH_4 \rightarrow CH_3 + H_2O$	Forward	-14.6	11.6	6.7
	Reverse	12.6	14.2	19.6
$H + OH \rightarrow H_2 + O$	Forward	2.1	10.6	10.7
	Reverse	12.8	14.0	13.1
$H + H_2S \rightarrow H_2 + HS$	Forward	-2.7	1.6	3.6
	Reverse	4.3	14.3	17.3

[a]Reference [11]

Table S16 Dissociation and reaction energies of the SIE4×4 and SIE11 sets of molecules (in kcal/mol).

Reaction	rSCAN	SIC-rSCAN	Ref.[a]
$H_2^+ \rightarrow H + H^+$			
$R/R_e = 1.0$	67.8	64.4	64.4
$R/R_e = 1.25$	64.9	58.9	58.9
$R/R_e = 1.5$	57.8	48.7	48.7
$R/R_e = 1.75$	50.8	38.2	38.3
$He_2^+ \rightarrow He + He^+$			
$R/R_e = 1.0$	74.4	56.5	56.9
$R/R_e = 1.25$	71.5	44.6	46.9
$R/R_e = 1.5$	63.4	27.5	31.3
$R/R_e = 1.75$	58.5	14.3	19.1
$(NH_3)_2^+ \rightarrow NH_3 + NH_3^+$			
$R/R_e = 1.0$	43.4	36.3	35.9
$R/R_e = 1.25$	38.3	25.4	25.9
$R/R_e = 1.5$	30.9	11.6	13.4
$R/R_e = 1.75$	27.2	4.1	4.9
$(H_2O)_2^+ \rightarrow H_2O + H_2O^+$			
$R/R_e = 1.0$	52.9	36.3	39.7
$R/R_e = 1.25$	48.8	22.8	29.1
$R/R_e = 1.5$	42.7	11.9	16.9
$R/R_e = 1.75$	40.1	6.2	9.3
$C_4H_{10}^+ \rightarrow C_2H_5 + C_2H_5^+$	42.0	34.3	35.28
$(CH_3)_2CO^+ \rightarrow CH_3 + CH_3CO^+$	30.1	40.5	22.57
$ClFCl \rightarrow ClClF$	-22.3	-2.9	-1.01
$C_2H_4...F_2 \rightarrow C_2H_4 + F_2$	2.5	0.5	1.08
$C_6H_6...Li \rightarrow Li + C_6H_6$	7.7	12.1	9.5
$NH_3...ClF \rightarrow NH_3 + ClF$	17.1	12.0	10.5
$NaOMg \rightarrow MgO + Na$	75.7	95.3	69.56
$FLiF \rightarrow Li + F_2$	120.4	92.4	94.36

[a]Reference [12]

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