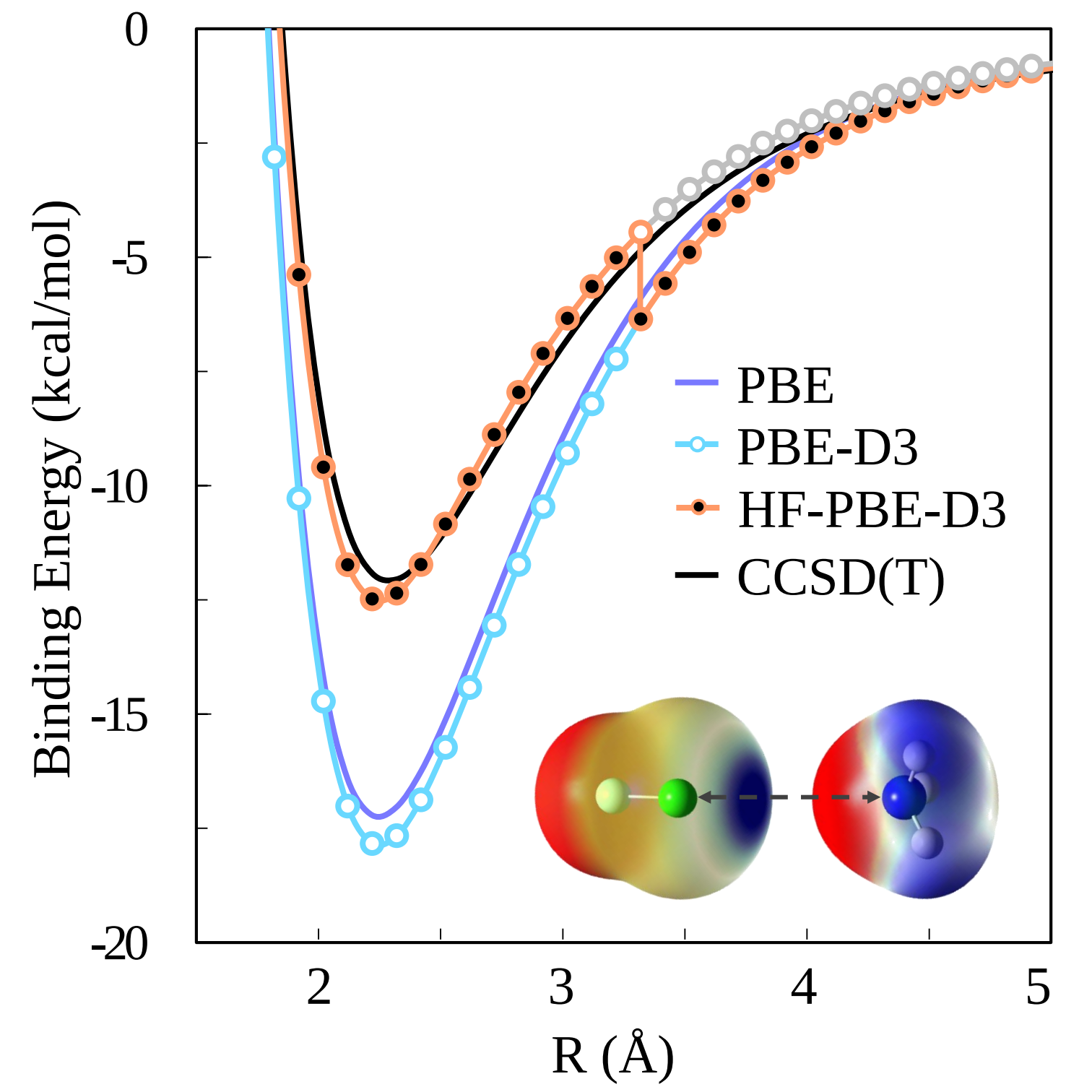
0
-5
-10
-15
-20
Binding Energy (kcal/mol)
2
3
4
5
R (Å)
PBE
PBE-D3
HF-PBE-D3
CCSD(T)

Halogen and Chalcogen Binding Dominated by Density-Driven Errors

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Abstract

Dispersion corrections of various kinds usually improve DFT energetics of weak non-covalent interactions. But in some cases involving molecules or halides, especially those with σ-hole interactions, the density-driven errors of uncorrected DFT are larger *than the dispersion corrections. In these abnormal situations, HF-DFT (using Hartree-Fock densities instead of self-consistent densities) greatly improves bond energies, while dispersion corrections can even worsen the results. On the other hand, pnictogen bonds and the S22 dataset are normal and are not improved by this procedure. Such effects should be accounted for when parametrizing dispersion interactions.*

It has long been recognized that standard semilocal density functionals are usually inaccurate for non-covalent interactions.[1, 2] About 15 years ago, a variety of dispersion correction methods were introduced.[3, 4, 5, 6, 7] These typically reduce the errors on the binding energies of the S22 dataset of weakly bonded systems.[8] But not all non-covalent interactions are weak or can be fixed by dispersion correction. Interactions between small molecules and/or ions involving nonmetals are relatively strong and are known to be significantly overestimated by density functional theory (DFT).[9, 10] Halogen bonds, such as R$-$X$\cdots$B where X is halogen atom and B is a Lewis base, have an anisotropic distribution of charge around the halogen (the σ-hole interaction) and are said to have a large self-interaction error.[11] Although not as strong as halogen bonds, chalcogen and pnictogen bonds exhibit similar behavior.[12, 13] While pure generalized gradient approximation (GGA), meta-GGA (mGGA), and hybrid functionals with small amounts of exact exchange are inaccurate due to the delocalization error, BHandHLYP (HH in short) and M06-2X, which includes more than 50% exact exchange, are recommended for these systems.[14, 11] The addition of dispersion corrections to pure functionals is not useful for the calculation of these complexes, because it further contributes to the overestimation of binding energies. Here we show that the main cause of inaccurate DFT binding energies for the non-covalent σ-hole interaction is, in fact, their self-consistent density and present a practical but simple solution to improve the DFT calculation and obtain reliable results.

In the last few years, the theory of density-corrected DFT (DC-DFT) has been introduced to separate the sources of error in such calculations, into contributions driven by the energy functional and those due to errors in the self-consistent density.[15] Such density-driven errors have been found to dominate DFT errors in a variety of situations, including reaction barrier heights, electronegativities, stretched bonds, etc.[15, 16, 17, 18, 19, 20] These calculations are denoted abnormal, and can be detected by calculating the density sensitivity, which is (roughly) the magnitude of the change in exchange-correlation energy when the density is changed.[21] In abnormal calculations, with a simple script[22] and at no additional computational cost, energetics are much improved by evaluation of the functional on Hartree-Fock (HF) densities in place of self-consistent ones.

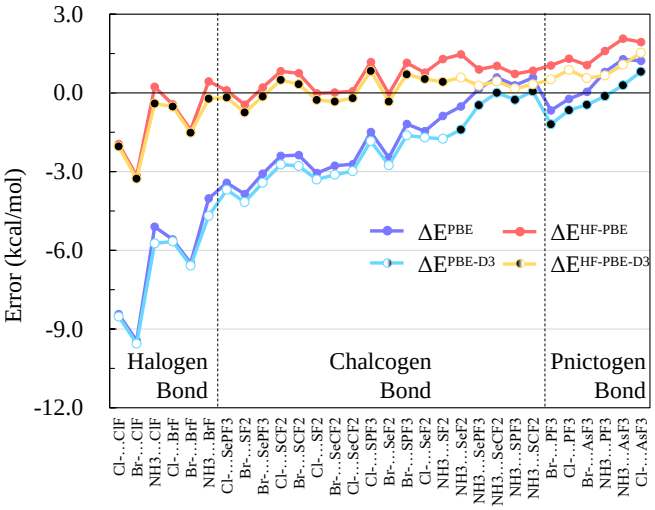

Figure 1: *Binding energy errors of the PBE functional for halogen, chalcogen, and pnictogen bonds: With and without D3 corrections, and on the self-consistent and HF densities. Black dots denote the results of HF-PBE-D3 applied only to abnormal calculations (see text).*

But most applications of DC-DFT have so far been limited to strong bonds. When the theory is applied to weak bonds, we find the energetics of the S22 dataset to be normal (almost always), but that halogen bonds are almost always abnormal, and many chalcogen bonds are as well (depending on the functional). The halogen bonds have large errors that

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are almost unchanged by typical dispersion schemes, but are fixed by using the HF density (HF-DFT), in which the DFT energy is evaluated on a HF density ($E^{DFT}[n^{\mathrm{HF}}]$), instead of on the usual self-consistent one. This behavior occurs for many different semilocal approximations and many different dispersion schemes. A typical case is illustrated in Fig. 1, in which we plot the binding energy errors using the PBE[23] GGA, corrected by the D3 scheme[24], for the B30 dataset.[14] The B30 includes 6 halogen-, 18 chalcogen-, and 6 pnictogen bonds, and is listed later.[14] The molecules have been grouped by type, and ordered by decreasing density sensitivity (defined later). The dark blue curve is the plain PBE self-consistent curve, with light blue being dispersion corrected. The red is the same on the HF density, with yellow indicating dispersion corrections. Clearly, at the far left, the error for the halogen bonds is very large (several kcal/mol), is barely affected by dispersion correction (in fact, always worsened), and largely cured by HF-DFT. Moving from left to right, this error shrinks. At molecule 20, the density sensitivity drops below 2 kcal/mol, and we classify the calculation as normal, and do not recommend using HF-DFT. The black circles denote the results of HF-DFT-D3, matching HF-PBE-D3 for molecules to the left of 20, and matching PBE-D3 to the right. The mean absolute error of PBE-D3 on the entire set is 2.5 kcal/mol without D3, 2.8 kcal/mol with D3, while that of HF-DFT is 0.7 kcal/mol without D3 and 0.6 kcal/mol with D3. Thus, HF-DFT can be crucial for finding accurate non-covalent binding energies, and all datasets used for determining dispersion coefficients should be tested for density-sensitivity. Any scheme ignoring this effect risks fitting the density-driven error with dispersion coefficients.

To demonstrate that this is not some specific deficiency of PBE or the D3 scheme, in Table 1 we list mean average errors over the B30 dataset, broken up into the different types of bonds, for several different functionals and disperion correction schemes. Table 1 presents the mean absolute error (MAE) of 12 functionals chosen to represent a standard set of approximate functionals from the level of GGA, mGGA, global hybrids, long-range corrected, and relatively recent Minnesota functionals. They are BP86, PBE, PW86PBE, BLYP, TPSS, SCAN, B3LYP, PBE0, M06, M06-2X, CAM-B3LYP, and LC-ωPBE, while SVWN, revTPSS, HH, M11, and MN15 are presented in the supporting information. HF-DFT results only differ when the sensitivity (defined below) with the given functional is above 2.0 kcal/mol, in which case the HF density is used instead.

In the first set (no dispersion correction), we see the greatest improvement in the GGA functionals, with the exception of BLYP, where HF worsens the halogen results. The mGGAs are also improved. Typically, one finds greatly reduced variance among GGAs for abnormal systems in HF-GGA. This appears true here also, with the exception of BLYP, which is unusually accurate at the self-consistent level. For the hybrids there is mild improvement in B3LYP and PBE0, but none for M06 and M06-2X, because their density sensitivity is so low for the B30 set that none of the systems are abnormal. This is understandable for M06-2X, as its 54% HF contribution makes its density much closer to HF, but less so for M06. However, this has the corrollary that such functionals cannot be improved with HF-DFT, leaving M06 the worst performing hybrid for the halogens. To an even greater extent, range-separated hybrids using 100% HF, obviously yield densities very close to HF for these systems, and so perform extremely well without correction (all systems are normal).

The results of averaging over several functionals (those for which we can do all dispersion corrections) are also represented in Fig. 2. We clearly see an overall improvement in going to HF-DFT, with the most extreme case being the halogen bonds, some effects on the chalcogens, and none on the pnictogens. Moreover, for the halogens where HF-DFT gives great improvement, we see a much reduced dependence on the choice

	Halogen		Chalcogen		Pnictogen		B30	
DFT	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**
BP86	5.06	1.02	1.16	1.59	1.91	1.91	2.09	1.54
PBE	6.51	1.27	1.85	0.50	0.70	0.70	2.55	0.69
PW86PBE	4.35	1.20	1.33	0.87	1.52	1.52	1.97	1.07
BLYP	1.77	3.32	1.21	2.74	3.85	3.85	1.85	3.08
TPSS	5.11	0.68	1.20	0.83	1.00	1.00	1.94	0.83
SCAN	7.87	3.19	2.26	1.10	1.51	1.51	3.23	1.60
B3LYP	1.71	1.58	0.86	0.86	2.29	2.29	1.31	1.29
PBE0	4.84	2.14	1.06	1.06	0.44	0.44	1.69	1.15
M06	3.38	3.38	1.36	1.36	0.81	0.81	1.65	1.65
M06-2X	1.77	1.77	0.53	0.53	1.42	1.42	0.96	0.96
CAM-B3LYP	1.23	1.23	1.00	1.00	1.33	1.33	1.11	1.11
LC-ωPBE	0.66	0.66	1.67	1.65	1.38	1.38	1.41	1.40
DFT-D3	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**
BP86	5.65	0.58	1.44	0.88	0.67	0.67	2.13	0.78
PBE	6.79	1.33	2.12	0.43	0.59	0.59	2.75	0.64
PW86PBE	4.68	0.92	1.52	0.61	0.90	0.90	2.03	0.73
BLYP	2.40	2.69	0.83	1.86	2.40	2.40	1.46	2.14
TPSS	5.51	0.75	1.49	0.68	0.36	0.36	2.07	0.63
B3LYP	2.25	1.04	0.35	0.35	1.10	1.10	0.88	0.64
PBE0	5.16	2.45	1.29	1.29	0.88	0.88	1.98	1.44
M06	3.43	3.43	1.42	1.42	0.92	0.92	1.72	1.72
M06-2X	1.78	1.78	0.54	0.54	1.44	1.44	0.97	0.97
CAM-B3LYP	1.61	1.61	0.62	0.62	0.79	0.79	0.85	0.85
LC-ωPBE	0.87	0.87	1.14	1.12	0.55	0.55	0.97	0.96
DFT-D3(BJ)	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**
BP86	6.60	1.10	2.26	0.49	0.65	0.65	2.81	0.64
PBE	7.34	1.87	2.55	0.60	0.81	0.81	3.16	0.90
PW86PBE	5.19	0.71	1.87	0.45	0.63	0.63	2.29	0.54
BLYP	3.68	1.44	1.24	0.85	1.18	1.18	1.71	1.03
TPSS	6.19	1.36	2.04	0.80	0.70	0.70	2.60	0.89
B3LYP	3.31	0.52	0.84	0.84	0.42	0.42	1.25	0.69
PBE0	5.60	2.90	1.66	1.66	1.31	1.31	2.38	1.84
CAM-B3LYP	1.99	1.99	0.31	0.31	0.43	0.43	0.67	0.67
LC-ωPBE	1.35	1.35	0.74	0.73	0.15	0.15	0.75	0.74
DFT-XDM	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**	**SC**	**HF**
PBE	7.30	1.80	2.66	0.68	0.88	0.88	3.23	0.94
PW86PBE	5.08	0.79	1.75	0.43	0.74	0.74	2.21	0.56
BLYP	3.71	1.36	1.07	0.90	1.45	1.45	1.68	1.10
B3LYP	3.15	0.64	0.75	0.75	0.47	0.47	1.17	0.67
PBE0	5.60	2.88	1.79	1.79	1.31	1.31	2.46	1.91
CAM-B3LYP	2.24	2.24	0.33	0.33	0.33	0.33	0.71	0.71
LC-ωPBE	1.06	1.06	1.05	1.02	0.51	0.51	0.94	0.93

Table 1: *Mean absolute error (MAE, kcal/mol) for the B30 dataset: DFT, HF-DFT, and their dispersion corrected calculations. Reds denote MAE<1.0 kcal/mol. Structures and reference CCSD(T)/CBS values are from Ref. [14].*

of dispersion correction.

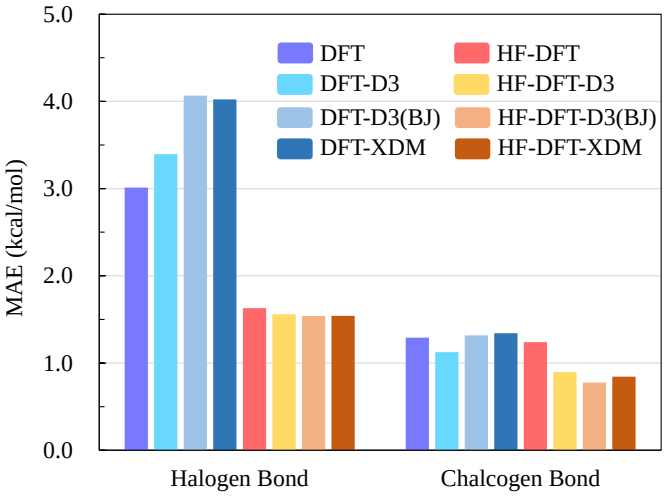

Figure 2: *Mean absolute error (MAE) and of the halogen-, and chalcogen-bonds in B30 dataset. The averages were taken for the functionals (PBE, PW86PBE, BLYP, B3LYP, PBE0, CAM-B3LYP, and LC-ωPBE) listed in Table 1.*

The rest of this paper is devoted to explaining how and why HF-DFT is working to improve these bonds. The general theory of [19] DC-DFT begins by classifying the energy errors in a Kohn-Sham DFT calculation with an approximate functional, say PBE:

$$\Delta E^{\rm PBE} = E^{\rm PBE}[n^{\rm PBE}] - E[n], \qquad (1)$$

where $E^{\rm PBE}$ is the energy evaluated with the PBE functional, $n^{\rm PBE}(\mathbf{r})$ is its self-consistent minimizing density, and quantities without a superscript are exact. The functional error is defined as

$$\Delta E_F^{\rm PBE}[n] = E_{\rm XC}^{\rm PBE}[n] - E_{\rm XC}[n] = \Delta E_{\rm XC}^{\rm PBE}[n], \qquad (2)$$

i.e., the error in energy made if PBE were evaluated on the exact density. The density-driven error is defined as the difference between total energy error and functional error:

$$\Delta E_D^{\rm PBE} = \Delta E^{\rm PBE} - \Delta E_{\rm XC}[n] = E^{\rm PBE}[n^{\rm PBE}] - E^{\rm PBE}[n]. \qquad (3)$$

Most DFT calculations produce highly accurate densities,[21] so that their energetic errors are dominated by the functional error. We call such calculations normal.

But certain classes of calculation tend to produce sufficiently inaccurate densities with semilocal functionals that their resulting energy error is substantially increased. We denote these as abnormal calculations. By definition, the energetics of such calculations can be improved by using the exact density in place of the self-consistent one. In practice, calculating the exact density will eliminate the cost-benefits of DFT, but experience shows that in many cases, the self-consistent HF density suffices to greatly reduce the density-driven error. In fact, since the local density approximation (LDA), is non-empirical and should have the largest density delocalization error, we can use the density sensitivity of an approximate functional, say again for PBE

$$S^{\rm PBE} = |E_{\rm XC}^{\rm PBE}[n^{\rm LDA}] - E_{\rm XC}^{\rm PBE}[n^{\rm HF}]| \qquad (4)$$

as a test of the density-driven error. Whenever $S >$ 2.0 kcal/mol, we classify the calculation as abnormal, and typically better results are found with HF densities.[21] Thus HF-DFT consists of using HF densities in place of self-consistent ones whenever S reaches this threshold. The philosophy of HF-DFT presumes the HF density is, in terms of energetic consequences, much closer to the exact density than the self-consistent density is, but *only* for abnormal calculations.[25]

#	complex	[a]	Density Sensitivity, S					
			PBE	PW86PBE	BLYP	B3LYP	PBE0	M06
	Halogen bonds							
1	$Cl^- \cdots ClF$	A	6.4	6.2	5.9	3.5	3.3	1.7
2	$Br^- \cdots ClF$	A	6.3	6.2	5.9	3.5	3.2	1.8
3	$NH_3 \cdots ClF$	A	5.3	5.0	4.7	2.4	2.3	0.8
4	$Cl^- \cdots BrF$	A	5.1	4.8	4.7	2.6	2.4	0.2
5	$Br^- \cdots BrF$	A	5.1	4.9	4.8	2.7	2.4	0.1
6	$NH_3 \cdots BrF$	A	4.4	4.1	3.9	2.0	1.9	0.2
	Chalcogen bonds							
7	$Cl^- \cdots SePF_3$	A	3.5	3.3	3.3	1.6	1.3	0.2
8	$Br^- \cdots SF_2$	A	3.4	3.3	3.0	1.8	1.7	0.6
9	$Br^- \cdots SePF_3$	A	3.3	3.3	3.2	1.5	1.1	0.2
10	$Cl^- \cdots SCF_2$	A	3.2	3.1	3.0	1.5	1.1	0.7
11	$Br^- \cdots SCF_2$	A	3.1	3.2	3.1	1.5	1.0	0.8
12	$Cl^- \cdots SF_2$	A	3.0	2.7	2.5	1.4	1.5	0.5
13	$Br^- \cdots SeCF_2$	A	2.8	2.8	2.8	1.4	1.0	0.0
14	$Cl^- \cdots SeCF_2$	A	2.7	2.6	2.6	1.2	1.0	0.2
15	$Cl^- \cdots SPF_3$	A	2.6	2.6	2.5	0.9	0.6	0.1
16	$Br^- \cdots SeF_2$	A	2.4	2.2	2.1	1.2	1.2	0.5
17	$Br^- \cdots SPF_3$	A	2.3	2.4	2.3	0.8	0.4	0.0
18	$Cl^- \cdots SeF_2$	A	2.2	1.9	1.8	0.9	1.1	0.5
19	$NH_3 \cdots SF_2$	A	2.1	1.9	1.6	0.7	0.9	0.1
20	$NH_3 \cdots SeF_2$	N	1.9	1.6	1.4	0.6	0.9	0.3
21	$NH_3 \cdots SePF_3$	N	0.7	0.8	0.6	0.2	0.1	0.0
22	$NH_3 \cdots SeCF_2$	N	0.4	0.5	0.3	0.1	0.1	0.1
23	$NH_3 \cdots SPF_3$	N	0.4	0.4	0.4	0.1	0.0	0.1
24	$NH_3 \cdots SCF_2$	N	0.2	0.3	0.2	0.0	0.0	0.1
	Pnictogen bonds							
25	$Br^- \cdots PF_3$	N	1.7	1.6	1.4	0.6	0.7	0.1
26	$Cl^- \cdots PF_3$	N	1.5	1.2	1.0	0.5	0.7	0.0
27	$Br^- \cdots AsF_3$	N	0.9	0.8	0.7	0.3	0.4	0.8
28	$NH_3 \cdots PF_3$	N	0.7	0.6	0.4	0.0	0.2	0.2
29	$NH_3 \cdots AsF_3$	N	0.6	0.5	0.3	0.0	0.2	0.4
30	$Cl^- \cdots AsF_3$	N	0.6	0.4	0.3	0.1	0.3	0.5

Table 2: *Density sensitivity (kcal/mol) of DFT calculations for the B30 dataset. [a] S^{PBE} was used to determine normal (N, < 2kcal/mol) and abnormal (A) classes shown here.*

Table 2 lists S values for the B30 molecular binding energies for several approximate functionals, of both GGA and hybrid type. Indeed, the first 19 are abnormal for every GGA listed (two are on borderline for a few functionals), while the remaining 11 are normal. This corresponds with experience, that abnormality is (roughly) a generic feature of semilocal approximations, independent of precisely which functional is used. On the other hand, the degree of sensitivity is much less when hybrids are involved, due to the admixture of HF exchange. (This effect is also seen in stronger bonds, but not as pronounced as here). Thus only the halogens are ab-

normal in hybrid calculations, no chalcogens are. The B30 molecules are ordered in all figures in decreasing order of PBE sensitivity. Thus HF-PBE uses HF densities for the first 19 molecules, while HF-B3LYP uses HF densities for the halogens only. On the other hand, almost none of the functionals on the S22 dataset have sensitivities reaching 2.0 kcal/mol in Table S3. The chief exception is PBE and other GGAs for the interaction energy of the formic acid dimer, where it just reaches 2.2 kcal/mol. We thus generically classify all S22 cases as normal, and HF-DFT has nothing to say to improve their energies.

Most chemistry applications use B3LYP for the semilocal functional and a dispersion correction. We thus include its performance for B30, and the effect of HF-DFT. It is clear that HF-DFT only improves the halogens in this case as they are the only abnormal cases. But the improvements remain signficant, as the B3LYP lines of Table 1 and Fig. 3 show. For the halogen bonds, the MAE of B3LYP is 1.7 kcal/mol, and is *increased* to 2.2 kcal/mol with D3 corrections, while HF-B3LYP has 1.6 kcal/mol without dispersion, and 1.0 kcal/mol with D3.

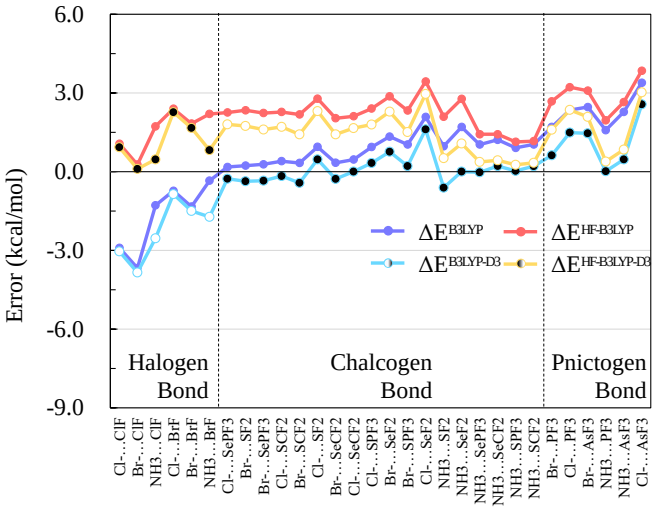

Figure 3: *Binding energy errors of B3LYP functional for the B30 dataset: With and without D3 corrections, and on the self-consistent and HF densities. Black dots denote the results of HF-PBE-D3 applied only to abnormal calculations (see text).*

With the assumption that the HF density yields energetics negligibly different from those of the exact density, we can use Eqs. (2) and (3) to extract the separate functional and density-driven errors to each binding energy. These are shown in Fig. 4(a) for the $H_3N\cdots ClF$ complex, which is highly abnormal. It is clear that overall HF-DFT reduces MAE (mean of blue bars relative to mean of greens). But we also find that semilocal functionals that include B88 exchange tend to perform better self-consistently than PBE and other Perdew functionals. In turn, this means less improvement when HF densities are used in abnormal calculations with B88. For both BLYP and B3LYP, the blue bars are larger than the green in magnitude, so HF-DFT slightly worsens those specific numbers. Finally, we make an important point about the last four functionals on the right. With the assumptions behind HF-DFT[21] and Fig. 4(a), the density sensitivity should match the magnitude of the density-driven error. We have thus plotted the (negative of the) sensitivity with red filled black circles. Until the last four functionals, they match very well the red bars, but not in the last four. For the range-separated hybrids, their densities are sufficiently similar to HF densities that we believe the assumptions are no longer valid. This means that some more accurate density must be used in the analysis to really distinguish density-driven from functional errors, and possibly even to determine the density-sensitivity. It appears that such an analysis would also be needed for the M06 and M06-2X functionals.

We also show that HF-DFT does not work just at equilibrium. Fig. 4(b) shows again the $H_3N\cdots ClF$ complex, but now as a function of separation. The improvement in PBE by using the HF density is excellent near equilibrium, and remains so out to about 4.0 Å. Contrary to covalent heteroatomic bonds, although the difference is small, it appears that the self-consistent curve is best for distances beyond that value. Also, the S^{PBE} value goes down less than 2.0 kcal/mol after 3.3 Å. To understand this, note that when an artificial charge transfer occurs in a self-consistent semilocal DFT calculation, the bond energy curve tends to become overstabilized at the stretched limit, as can be seen from the self-consistent DFT dissociation curve of NaCl. The inversion between HOMO of the electropositive species and LUMO of the electronegative species causes this unphysical phenomenon.[26, 18] Unlike covalent heteroatomic bonds, the HOMO of electropositive species (e.g., NH_3) lies below the LUMO of the electronegative one (e.g., ClF), so that that the calculations are normal for the complexes in the B30 dataset.

The substantial reduction of errors by HF-DFT-D demonstrates that the DFT error of σ-hole interaction originates from the error in the density, and so cannot be overcome by dispersion correction alone. In particular, halogen bonds are *abnormal* with a large density-driven error. Non-empirical functionals with the HF density substantially reduce the error of halogen-bonds regardless of the type of dispersion correction. Chalcogen bonds with small anion ligands can also be *abnormal* and HF-DFT may reduce the error by a factor of 2. However, classical non-covalent interactions such as hydrogen-bond, van der Waals dispersion, $\pi-$electron interaction, and pnictogen-bonds are normal calculations. HF-DFT-D is the most practical and accurate for the B30 dataset while DFT-D and HF-DFT-D are equally useful for the S22 dataset. (See Figure S1, where we rank calculation methods according to MAE.) In any event, it is clear that errors in self-consistent density must be accounted for when training any dispersion correction scheme.

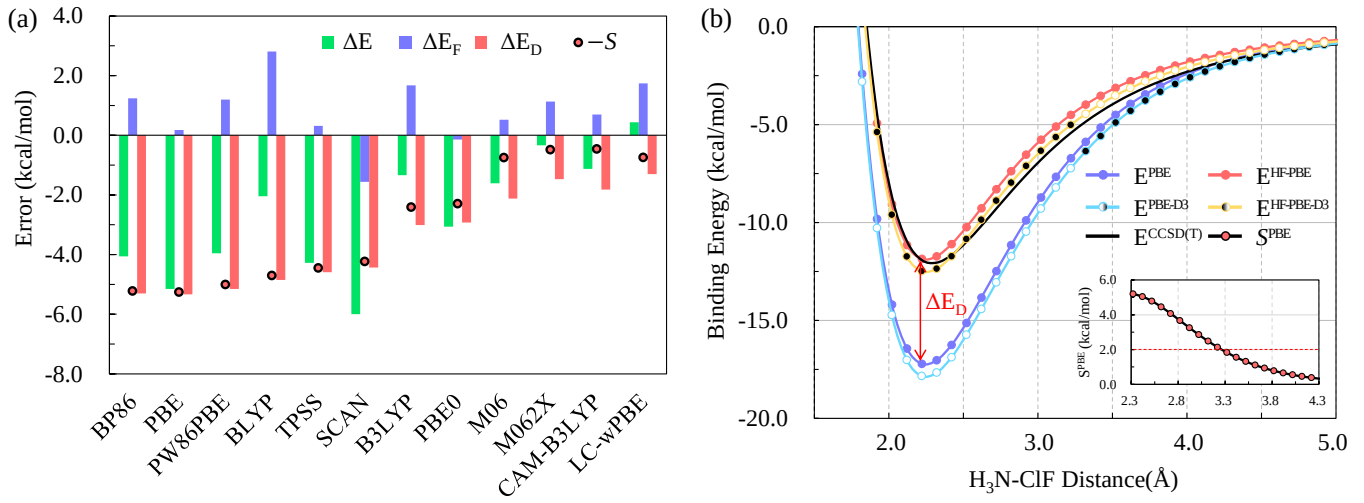

Figure 4: *Error decomposition at equilibrium geometry (a) and binding energy curve (b) of $H_3N\cdots ClF$ complex. In (a), green is the total error, blue is the functional error, and the red is the density-driven error, assuming HF density is much more accurate than self-consistent density. In (b), black dots denote HF-PBE-D3 values with respect to the density sensitivity (S^{PBE}). The red filled black circles in both (a) and the inset of (b) indicate the density sensitivity.*

Computational Details

All HF, DFT (SVWN [27, 28], BP86[29, 30], PBE[23], PW86PBE[31], BLYP[30, 32], B3LYP[33], PBE0[34], M06[35], CAM-B3LYP[36], and LC-ωPBE[37].) HF-DFT, results are performed with Gaussian16 package [38] and for SCAN[39], CCSD(T) are performed in TURBOMOLE 7.2.1 package[40]. In addition, dispersion correction D3 and D3(BJ) calculations are performed with the latest version of dftd3 program[24, 41], and XDM calculations are performed with postg program[42, 43]. Dunning's augmented correlation-consistent quadruple zeta basis set (aug-cc-pVQZ)[44] is used for the calculations in Fig 1, Fig 2, Fig 3, Fig. 4(a), Table 1, and Table 2. For Fig 4(b), aug-cc-pVTZ basis set[45, 46] was used for all calculation. To perform every calculation at their given orientation, molecular symmetry within the calculation was not considered. For the energy convergence criteria, SCF=tight option for the Gaussian16 while scfconv=7 and denconv=1.0d-6 are used for TURBOMOLE.

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Supporting Information

Halogen and Chalcogen Binding Dominated by Density-Driven Errors

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Abstract

Dispersion corrections of various kinds usually improve DFT energetics of weak non-covalent interactions. But in some cases involving molecules or halides, especially those with σ-hole interactions, the density-driven errors of uncorrected DFT are *larger* than the dispersion corrections. In these abnormal situations, HF-DFT (using Hartree-Fock densities instead of self-consistent densities) greatly improves bond energies, while dispersion corrections can even worsen the results. On the other hand, pnictogen bonds and the S22 dataset are all normal and are not improved by this procedure.

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1. B30 Dataset

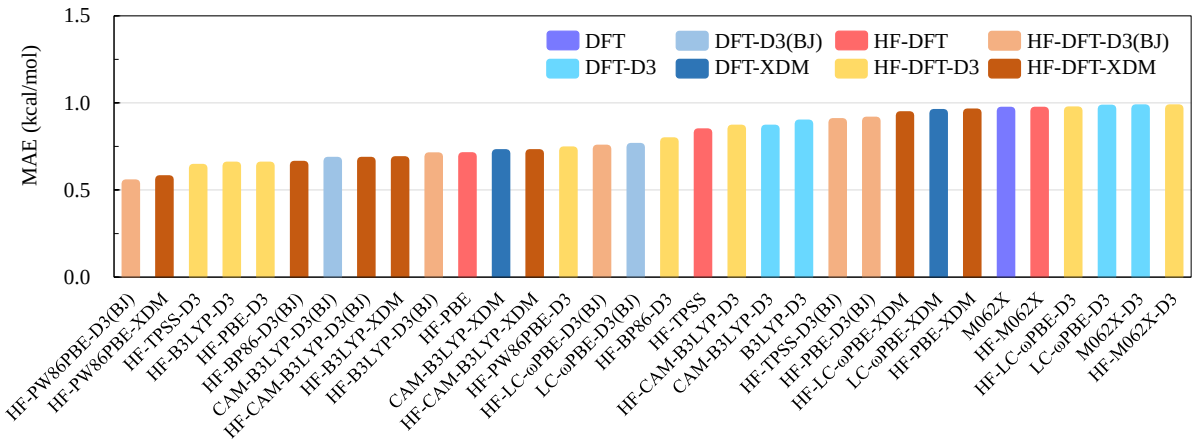

Figure S1: Performance of DFT calculations with MAE less than 1.0 kcal/mol for the B30 dataset. Out of the 78 methods in Table 1, the top 32 are shown. CCSD(T)/Ave-CBS[1] values are used as reference value. The structures are from σ-hole interaction dataset.[2]

Functionals employed for figures

Figure 1: PBE, PW86PBE, BLYP, B3LYP, PBE0, CAM-B3LYP, LC-ωPBE

Figure S1: Top 32 ranks are shown out of 78 methods – self-consistent calculations of BP86, PBE, PW86PBE, TPSS, SCAN, PBE0, M06, M06-2X, CAM-B3LYP, LC-ωPBE, BLYP, B3LYP and their dispersion corrected ones (D3, D3(BJ), XDM) if available.

Notation

If not self-consistent density, the used density is denoted by []. For example, LDA[HF] means that the LDA energy is calculated on the HF density while LDA means self-consistent calculation.

Table S1: DFT, HF-DFT with Disp3, Disp3BJ, XDM dispersion correction results (in kcal/-mol) for the B30 dataset. Structures and reference CCSD(T)/Ave-CBS energies are from Ref.[1,2]

	MAE								ME							
	Halogen		Chalcogen		Pnictogen		B30		Halogen		Chalcogen		Pnictogen		B30	
DFT	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
SVWN	16.26	10.06	7.38	4.70	6.68	5.89	9.01	6.01	-16.26	-10.06	-7.38	-4.70	-6.68	-5.89	-9.01	-6.01
BP86	5.06	1.02	1.16	1.59	1.91	1.91	2.09	1.54	-5.06	0.45	-0.49	1.59	1.91	1.91	-0.93	1.43
PBE	6.51	1.27	1.85	0.50	0.70	0.70	2.55	0.69	-6.51	-1.05	-1.67	0.38	0.41	0.41	-2.22	0.10
PW86PBE	4.35	1.20	1.33	0.87	1.52	1.52	1.97	1.07	-4.35	0.93	-0.94	0.85	1.52	1.52	-1.13	1.00
BLYP	1.77	3.32	1.21	2.74	3.85	3.85	1.85	3.08	-1.77	3.32	1.01	2.74	3.85	3.85	1.02	3.08
TPSS	5.11	0.68	1.20	0.83	1.00	1.00	1.94	0.83	-5.11	-0.27	-0.81	0.56	1.00	1.00	-1.31	0.48
revTPSS	5.25	0.65	1.29	0.82	0.61	0.61	1.95	0.74	-5.25	-0.51	-0.96	0.36	0.61	0.61	-1.50	0.24
SCAN	7.87	3.19	2.26	1.10	1.51	1.51	3.23	1.60	-7.87	-3.19	-2.15	-0.83	-1.51	-1.51	-3.16	-1.44
B3LYP	1.71	1.58	0.86	0.86	2.29	2.29	1.31	1.29	-1.71	1.58	0.86	0.86	2.29	2.29	0.63	1.29
PBE0	4.84	2.14	1.06	1.06	0.44	0.44	1.69	1.15	-4.84	-2.14	-0.81	-0.81	-0.18	-0.18	-1.49	-0.95
M06	3.38	3.38	1.36	1.36	0.81	0.81	1.65	1.65	-3.38	-3.38	-1.28	-1.28	-0.81	-0.81	-1.61	-1.61
HH	0.49	0.49	1.32	1.32	1.26	1.26	1.14	1.14	-0.39	-0.39	1.32	1.32	1.26	1.26	0.96	0.96
M06-2X	1.77	1.77	0.53	0.53	1.42	1.42	0.96	0.96	-1.77	-1.77	-0.46	-0.46	-1.42	-1.42	-0.91	-0.91
CAM-B3LYP	1.23	1.23	1.00	1.00	1.33	1.33	1.11	1.11	-1.23	-1.23	1.00	1.00	1.33	1.33	0.62	0.62
LC-ωPBE	0.66	0.66	1.67	1.65	1.38	1.38	1.41	1.40	-0.47	-0.47	1.67	1.65	1.38	1.38	1.18	1.17
M11	0.99	0.99	0.79	0.93	0.41	0.41	0.75	0.84	-0.04	-0.04	0.78	0.92	-0.39	-0.39	0.38	0.47
MN15	1.27	1.27	0.46	0.46	0.75	0.75	0.68	0.68	-1.27	-1.27	-0.27	-0.27	-0.75	-0.75	-0.57	-0.57
	Halogen		Chalcogen		Pnictogen		B30		Halogen		Chalcogen		Pnictogen		B30	
DFT-D3	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
BP86	5.65	0.58	1.44	0.88	0.67	0.67	2.13	0.78	-5.65	-0.14	-1.36	0.73	0.58	0.58	-1.83	0.52
PBE	6.79	1.33	2.12	0.43	0.59	0.59	2.75	0.64	-6.79	-1.33	-2.11	-0.05	-0.22	-0.22	-2.67	-0.34
PW86PBE	4.68	0.92	1.52	0.61	0.90	0.90	2.03	0.73	-4.68	0.60	-1.44	0.35	0.79	0.79	-1.64	0.49
BLYP	2.40	2.69	0.83	1.86	2.40	2.40	1.46	2.14	-2.40	2.69	0.09	1.82	2.40	2.40	0.06	2.11
TPSS	5.51	0.75	1.49	0.68	0.36	0.36	2.07	0.63	-5.51	-0.68	-1.43	-0.06	0.06	0.06	-1.95	-0.16
revTPSS	5.65	0.92	1.60	0.72	0.54	0.54	2.20	0.72	-5.65	-0.92	-1.58	-0.26	-0.33	-0.33	-2.14	-0.41
B3LYP	2.25	1.04	0.35	0.35	1.1	1.1	0.88	0.64	-2.25	1.04	0.07	0.07	1.1	1.1	-0.19	0.47
PBE0	5.16	2.45	1.29	1.29	0.88	0.88	1.98	1.44	-5.16	-2.45	-1.28	-1.28	-0.88	-0.88	-1.98	-1.44
M06	3.43	3.43	1.42	1.42	0.92	0.92	1.72	1.72	-3.43	-3.43	-1.38	-1.38	-0.92	-0.92	-1.70	-1.70
HH	0.83	0.83	0.82	0.82	0.77	0.77	0.81	0.81	-0.83	-0.83	0.68	0.68	0.29	0.29	0.30	0.30
M06-2X	1.78	1.78	0.54	0.54	1.44	1.44	0.97	0.97	-1.78	-1.78	-0.49	-0.49	-1.44	-1.44	-0.94	-0.94
CAM-B3LYP	1.61	1.61	0.62	0.62	0.79	0.79	0.85	0.85	-1.61	-1.61	0.46	0.46	0.50	0.50	0.05	0.05
LC-ωPBE	0.87	0.87	1.14	1.12	0.55	0.55	0.97	0.96	-0.87	-0.87	1.09	1.08	0.50	0.50	0.58	0.57
	Halogen		Chalcogen		Pnictogen		B30		Halogen		Chalcogen		Pnictogen		B30	
DFT-D3(BJ)	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
BP86	6.60	1.10	2.26	0.49	0.65	0.65	2.81	0.64	-6.60	-1.10	-2.20	-0.12	-0.33	-0.33	-2.71	-0.36
PBE	7.34	1.87	2.55	0.6	0.81	0.81	3.16	0.90	-7.34	-1.87	-2.55	-0.50	-0.79	-0.79	-3.16	-0.83
PW86PBE	5.19	0.71	1.87	0.45	0.63	0.63	2.29	0.54	-5.19	0.09	-1.87	-0.08	0.27	0.27	-2.10	0.03
BLYP	3.68	1.44	1.24	0.85	1.18	1.18	1.71	1.03	-3.68	1.41	-0.98	0.75	1.14	1.14	-1.10	0.96
TPSS	6.19	1.36	2.04	0.80	0.70	0.70	2.60	0.89	-6.19	-1.36	-2 .00	-0.63	-0.60	-0.6	-2.56	-0.77
revTPSS	6.33	1.60	2.16	0.92	0.99	0.99	2.76	1.07	-6.33	-1.60	-2.14	-0.83	-0.99	-0.99	-2.75	-1.01
B3LYP	3.31	0.52	0.84	0.84	0.42	0.42	1.25	0.69	-3.31	-0.02	-0.81	-0.81	0.04	0.04	-1.14	-0.48
PBE0	5.60	2.90	1.66	1.66	1.31	1.31	2.38	1.84	-5.60	-2.90	-1.66	-1.66	-1.31	-1.31	-2.38	-1.84
HH	1.77	1.77	0.33	0.33	0.65	0.65	0.68	0.68	-1.77	-1.77	-0.11	-0.11	-0.65	-0.65	-0.55	-0.55
CAM-B3LYP	1.99	1.99	0.31	0.31	0.43	0.43	0.67	0.67	-1.99	-1.99	0.11	0.11	0.19	0.19	-0.29	-0.29
LC-ωPBE	1.35	1.35	0.74	0.73	0.15	0.15	0.75	0.74	-1.35	-1.35	0.67	0.65	0.08	0.08	0.15	0.14
	Halogen		Chalcogen		Pnictogen		B30		Halogen		Chalcogen		Pnictogen		B30	
DFT-XDM	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
PBE	7.30	1.80	2.66	0.68	0.88	0.88	3.23	0.94	-7.30	-1.80	-2.65	-0.56	-0.75	-0.75	-3.20	-0.85
PW86PBE	5.08	0.79	1.75	0.43	0.74	0.74	2.21	0.56	-5.08	0.19	-1.74	0.03	0.49	0.49	-1.96	0.15
BLYP	3.71	1.36	1.07	0.90	1.45	1.45	1.68	1.10	-3.71	1.26	-0.78	0.80	1.45	1.45	-0.92	1.02
B3LYP	3.15	0.64	0.75	0.75	0.47	0.47	1.17	0.67	-3.15	0.14	-0.68	-0.68	0.34	0.34	-0.97	-0.31
PBE0	5.60	2.88	1.79	1.79	1.31	1.31	2.46	1.91	-5.6	-2.88	-1.77	-1.77	-1.31	-1.31	-2.45	-1.90
HH	1.41	1.41	0.27	0.27	0.35	0.35	0.51	0.51	-1.41	-1.41	0.14	0.14	-0.19	-0.19	-0.24	-0.24
CAM-B3LYP	2.24	2.24	0.33	0.33	0.33	0.33	0.71	0.71	-2.24	-2.24	-0.29	-0.29	-0.18	-0.18	-0.66	-0.66
LC-ωPBE	1.06	1.06	1.05	1.02	0.51	0.51	0.94	0.93	-1.06	-1.06	1.05	1.02	0.51	0.51	0.52	0.50

Table S2: Reference CCSD(T)/Ave-CBS value (in kcal/mol) for the B30 dataset from Ref.[1]

	CCSD(T)/Ave-CBS
Halogen Bonds	
$Cl^- \cdots ClF$	-43.91
$Br^- \cdots ClF$	-42.61
$Cl^- \cdots BrF$	-46.42
$Br^- \cdots BrF$	-43.67
$NH_3 \cdots ClF$	-12.1
$NH_3 \cdots BrF$	-16.03
Chalcogen Bonds	
$Cl^- \cdots SF_2$	-31.52
$Br^- \cdots SF_2$	-25.8
$Cl^- \cdots SeF_2$	-40.96
$Br^- \cdots SeF_2$	-35.5
$NH_3 \cdots SF_2$	-7.98
$NH_3 \cdots SeF_2$	-13.23
$Cl^- \cdots SCF_2$	-9.54
$Br^- \cdots SCF_2$	-7.8
$Cl^- \cdots SeCF_2$	-13.61
$Br^- \cdots SeCF_2$	-11.22
$NH_3 \cdots SCF_2$	-1.67
$NH_3 \cdots SeCF_2$	-2.73
$Cl^- \cdots SPF_3$	-8.42
$Br^- \cdots SPF_3$	-6.76
$Cl^- \cdots SePF_3$	-15.45
$Br^- \cdots SePF_3$	-12.48
$NH_3 \cdots SPF_3$	-1.42
$NH_3 \cdots SePF_3$	-2.84
Pnictogen Bonds	
$Cl^- \cdots PF_3$	-21.37
$Br^- \cdots PF_3$	-15.73
$Cl^- \cdots AsF_3$	-34.25
$Br^- \cdots AsF_3$	-27.42
$NH_3 \cdots PF_3$	-4.85
$NH_3 \cdots AsF_3$	-9.31

Table S3: LDA, LDA[HF] interaction energy results (in hartree) for the B30 dataset.

	LDA	LDA[HF]
Halogen Bonds		
$Cl^- \cdots ClF$	-0.100853	-0.089401
$Br^- \cdots ClF$	-0.099805	-0.088923
$Cl^- \cdots BrF$	-0.099771	-0.09011
$Br^- \cdots BrF$	-0.096236	-0.086961
$NH_3 \cdots ClF$	-0.039717	-0.030126
$NH_3 \cdots BrF$	-0.045319	-0.036983
Chalcogen Bonds		
$Cl^- \cdots SF_2$	-0.070576	-0.064444
$Br^- \cdots SF_2$	-0.061238	-0.054756
$Cl^- \cdots SeF_2$	-0.083802	-0.078765
$Br^- \cdots SeF_2$	-0.075634	-0.070553
$NH_3 \cdots SF_2$	-0.024044	-0.01952
$NH_3 \cdots SeF_2$	-0.034503	-0.030167
$Cl^- \cdots SCF_2$	-0.027548	-0.021551
$Br^- \cdots SCF_2$	-0.023831	-0.018127
$Cl^- \cdots SeCF_2$	-0.035505	-0.030113
$Br^- \cdots SeCF_2$	-0.030927	-0.025713
$NH_3 \cdots SCF_2$	-0.004361	-0.003578
$NH_3 \cdots SeCF_2$	-0.006821	-0.005691
$Cl^- \cdots SPF_3$	-0.02333	-0.018044
$Br^- \cdots SPF_3$	-0.019295	-0.014718
$Cl^- \cdots SePF_3$	-0.040287	-0.033447
$Br^- \cdots SePF_3$	-0.033873	-0.027611
$NH_3 \cdots SPF_3$	-0.004558	-0.003463
$NH_3 \cdots SePF_3$	-0.008235	-0.00653
Pnictogen Bonds		
$Cl^- \cdots PF_3$	-0.047033	-0.043297
$Br^- \cdots PF_3$	-0.036461	-0.032693
$Cl^- \cdots AsF_3$	-0.067242	-0.064556
$Br^- \cdots AsF_3$	-0.056516	-0.053666
$NH_3 \cdots PF_3$	-0.013526	-0.011288
$NH_3 \cdots AsF_3$	-0.023013	-0.020612

Table S4: BP86, BP86[HF], BP86[LDA], Disp3, Disp3BJ interaction energy results (in hartree) for the B30 dataset.

	BP86	BP86[HF]	BP86[LDA]	Disp3	Disp3BJ
Halogen Bonds					
$Cl^- \cdots ClF$	-0.080798	-0.070454	-0.080722	-0.000235	-0.002051
$Br^- \cdots ClF$	-0.080214	-0.070158	-0.080187	-0.000287	-0.002465
$Cl^- \cdots BrF$	-0.080429	-0.07207	-0.080349	-0.000218	-0.002398
$Br^- \cdots BrF$	-0.077403	-0.069164	-0.077377	-0.000279	-0.002847
$NH_3 \cdots ClF$	-0.025675	-0.017228	-0.025549	-0.002232	-0.002226
$NH_3 \cdots BrF$	-0.030126	-0.022936	-0.030004	-0.00237	-0.002751
Chalcogen Bonds					
$Cl^- \cdots SF_2$	-0.052406	-0.047555	-0.052289	-0.00082	-0.002791
$Br^- \cdots SF_2$	-0.044642	-0.03924	-0.044574	-0.001019	-0.003306
$Cl^- \cdots SeF_2$	-0.064989	-0.061309	-0.064867	-0.00082	-0.003064
$Br^- \cdots SeF_2$	-0.057899	-0.053927	-0.057837	-0.000995	-0.003617
$NH_3 \cdots SF_2$	-0.012325	-0.008851	-0.012156	-0.002897	-0.002851
$NH_3 \cdots SeF_2$	-0.019911	-0.016677	-0.019739	-0.003037	-0.003445
$Cl^- \cdots SCF_2$	-0.017302	-0.01211	-0.01721	-0.000993	-0.002512
$Br^- \cdots SCF_2$	-0.014478	-0.009487	-0.014415	-0.001305	-0.002905
$Cl^- \cdots SeCF_2$	-0.024161	-0.019536	-0.024083	-0.000773	-0.002718
$Br^- \cdots SeCF_2$	-0.020451	-0.015873	-0.020408	-0.001039	-0.003136
$NH_3 \cdots SCF_2$	-0.000491	-0.000032	-0.000405	-0.001512	-0.00156
$NH_3 \cdots SeCF_2$	-0.002113	-0.001357	-0.002033	-0.001841	-0.002031
$Cl^- \cdots SPF_3$	-0.014117	-0.009808	-0.014034	-0.001034	-0.002413
$Br^- \cdots SPF_3$	-0.010977	-0.007241	-0.010919	-0.001377	-0.002764
$Cl^- \cdots SePF_3$	-0.028185	-0.022476	-0.028118	-0.000763	-0.002792
$Br^- \cdots SePF_3$	-0.022914	-0.017624	-0.02288	-0.001048	-0.003223
$NH_3 \cdots SPF_3$	-0.000547	0.000184	-0.00046	-0.001587	-0.001655
$NH_3 \cdots SePF_3$	-0.002955	-0.001702	-0.002871	-0.001954	-0.002211
Pnictogen Bonds					
$Cl^- \cdots PF_3$	-0.031736	-0.0293	-0.031577	-0.0015	-0.003318
$Br^- \cdots PF_3$	-0.023662	-0.020972	-0.023557	-0.00188	-0.003789
$Cl^- \cdots AsF_3$	-0.049991	-0.048733	-0.049826	-0.001444	-0.003534
$Br^- \cdots AsF_3$	-0.040929	-0.03933	-0.040781	-0.001745	-0.004107
$NH_3 \cdots PF_3$	-0.0046	-0.003267	-0.004378	-0.002943	-0.003041
$NH_3 \cdots AsF_3$	-0.010738	-0.009398	-0.010493	-0.003294	-0.003717

Table S5: PBE, PBE[HF], PBE[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	PBE	PBE[HF]	PBE[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.083418	-0.073084	-0.083351	-0.000143	-0.001108	-0.001173	-0.001099	-0.001183
$Br^- \cdots ClF$	-0.082962	-0.072943	-0.082938	-0.000168	-0.00124	-0.001441	-0.00136	-0.001449
$Cl^- \cdots BrF$	-0.082875	-0.074677	-0.082802	-0.00013	-0.001209	-0.001402	-0.001333	-0.001411
$Br^- \cdots BrF$	-0.07993	-0.071852	-0.079912	-0.000158	-0.001339	-0.001738	-0.001663	-0.001744
$NH_3 \cdots ClF$	-0.027415	-0.018919	-0.027295	-0.001008	-0.001373	-0.000797	-0.00077	-0.000807
$NH_3 \cdots BrF$	-0.031959	-0.024847	-0.031846	-0.001053	-0.001593	-0.000988	-0.000956	-0.000997
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.055102	-0.050263	-0.055001	-0.000393	-0.0015	-0.001538	-0.001451	-0.001557
$Br^- \cdots SF_2$	-0.047266	-0.041832	-0.047219	-0.000479	-0.001651	-0.001892	-0.001796	-0.001908
$Cl^- \cdots SeF_2$	-0.067602	-0.064046	-0.067487	-0.000388	-0.001563	-0.001732	-0.001649	-0.001752
$Br^- \cdots SeF_2$	-0.06051	-0.056634	-0.060462	-0.000465	-0.00172	-0.002152	-0.002059	-0.002168
$NH_3 \cdots SF_2$	-0.014123	-0.01067	-0.013972	-0.001381	-0.001734	-0.001079	-0.001027	-0.001095
$NH_3 \cdots SeF_2$	-0.021905	-0.018745	-0.021748	-0.001412	-0.002015	-0.001263	-0.001208	-0.001278
$Cl^- \cdots SCF_2$	-0.019029	-0.013892	-0.018944	-0.000525	-0.001299	-0.001624	-0.00154	-0.001637
$Br^- \cdots SCF_2$	-0.016207	-0.011239	-0.016159	-0.000664	-0.001403	-0.001932	-0.001848	-0.001937
$Cl^- \cdots SeCF_2$	-0.026025	-0.021588	-0.02596	-0.000422	-0.00134	-0.001811	-0.001743	-0.001824
$Br^- \cdots SeCF_2$	-0.022308	-0.017863	-0.022286	-0.000541	-0.001446	-0.002175	-0.002109	-0.002179
$NH_3 \cdots SCF_2$	-0.00174	-0.001315	-0.001662	-0.000826	-0.000889	-0.000782	-0.000747	-0.000792
$NH_3 \cdots SeCF_2$	-0.003414	-0.002715	-0.003348	-0.000933	-0.0011	-0.000991	-0.000956	-0.001
$Cl^- \cdots SPF_3$	-0.015804	-0.011547	-0.015714	-0.00054	-0.001231	-0.001515	-0.001435	-0.001534
$Br^- \cdots SPF_3$	-0.012663	-0.008953	-0.012607	-0.000692	-0.001319	-0.001769	-0.001693	-0.001782
$Cl^- \cdots SePF_3$	-0.030084	-0.024471	-0.030025	-0.000424	-0.001371	-0.001809	-0.001741	-0.00183
$Br^- \cdots SePF_3$	-0.024796	-0.019561	-0.02478	-0.000552	-0.001479	-0.002157	-0.002094	-0.00217
$NH_3 \cdots SPF_3$	-0.001806	-0.001114	-0.001727	-0.000882	-0.000945	-0.000821	-0.00078	-0.000834
$NH_3 \cdots SePF_3$	-0.004282	-0.003099	-0.004211	-0.000994	-0.001206	-0.001056	-0.001014	-0.001069
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.034421	-0.031981	-0.034286	-0.000681	-0.001773	-0.001799	-0.001695	-0.001821
$Br^- \cdots PF_3$	-0.026128	-0.023403	-0.026059	-0.000845	-0.001872	-0.002172	-0.002056	-0.002191
$Cl^- \cdots AsF_3$	-0.052637	-0.051493	-0.052474	-0.000656	-0.001821	-0.001946	-0.001849	-0.001968
$Br^- \cdots AsF_3$	-0.043638	-0.042011	-0.043505	-0.000787	-0.001966	-0.002414	-0.002284	-0.002428
$NH_3 \cdots PF_3$	-0.006458	-0.005192	-0.006264	-0.001475	-0.00182	-0.001245	-0.001167	-0.001263
$NH_3 \cdots AsF_3$	-0.012796	-0.011546	-0.012572	-0.001585	-0.002176	-0.001433	-0.001355	-0.001449

Table S6: PW86PBE, PW86PBE[HF], PW86PBE[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	PW86PBE	PW86PBE[HF]	PW86PBE[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.079317	-0.069219	-0.079102	-0.000157	-0.001126	-0.001055	-0.00107	-0.001072
$Br^- \cdots ClF$	-0.079153	-0.069226	-0.079049	-0.000186	-0.001269	-0.001228	-0.001239	-0.001247
$Cl^- \cdots BrF$	-0.078614	-0.070852	-0.078432	-0.000144	-0.001232	-0.001171	-0.001204	-0.001189
$Br^- \cdots BrF$	-0.075871	-0.068112	-0.075844	-0.000178	-0.001372	-0.001382	-0.001412	-0.001401
$NH_3 \cdots ClF$	-0.025512	-0.017298	-0.025275	-0.001189	-0.001404	-0.001008	-0.001018	-0.001019
$NH_3 \cdots BrF$	-0.02944	-0.022695	-0.029224	-0.001261	-0.001633	-0.001139	-0.001148	-0.001152
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.051748	-0.047185	-0.051507	-0.000459	-0.001535	-0.001297	-0.001349	-0.001331
$Br^- \cdots SF_2$	-0.044468	-0.039155	-0.044376	-0.000565	-0.001707	-0.001508	-0.001549	-0.001545
$Cl^- \cdots SeF_2$	-0.063838	-0.060661	-0.063605	-0.000455	-0.001602	-0.001393	-0.001467	-0.001433
$Br^- \cdots SeF_2$	-0.057108	-0.05348	-0.057054	-0.000549	-0.001776	-0.001653	-0.001716	-0.001694
$NH_3 \cdots SF_2$	-0.013027	-0.009824	-0.012786	-0.001588	-0.001797	-0.001358	-0.001354	-0.001379
$NH_3 \cdots SeF_2$	-0.019845	-0.017	-0.019584	-0.00165	-0.002075	-0.001502	-0.001506	-0.001528
$Cl^- \cdots SCF_2$	-0.018476	-0.01336	-0.018337	-0.000596	-0.001375	-0.001185	-0.001236	-0.001218
$Br^- \cdots SCF_2$	-0.015845	-0.010723	-0.015802	-0.000764	-0.001505	-0.001373	-0.001409	-0.001405
$Cl^- \cdots SeCF_2$	-0.025171	-0.020884	-0.025042	-0.000478	-0.001406	-0.001261	-0.001348	-0.001297
$Br^- \cdots SeCF_2$	-0.021667	-0.017199	-0.021654	-0.000622	-0.001532	-0.001486	-0.001557	-0.001519
$NH_3 \cdots SCF_2$	-0.001613	-0.001128	-0.001565	-0.000918	-0.000972	-0.000903	-0.000864	-0.00091
$NH_3 \cdots SeCF_2$	-0.003358	-0.002601	-0.003321	-0.001054	-0.001199	-0.001089	-0.001052	-0.001098
$Cl^- \cdots SPF_3$	-0.015555	-0.011266	-0.01542	-0.00062	-0.001316	-0.001015	-0.001099	-0.001056
$Br^- \cdots SPF_3$	-0.012476	-0.008629	-0.012431	-0.000805	-0.001429	-0.001166	-0.001243	-0.001207
$Cl^- \cdots SePF_3$	-0.029268	-0.0238	-0.029122	-0.000478	-0.001444	-0.001211	-0.001301	-0.001257
$Br^- \cdots SePF_3$	-0.024206	-0.018958	-0.024183	-0.000634	-0.001575	-0.001425	-0.001504	-0.001467
$NH_3 \cdots SPF_3$	-0.001702	-0.000946	-0.001649	-0.000976	-0.001036	-0.000943	-0.000898	-0.00095
$NH_3 \cdots SePF_3$	-0.004254	-0.003012	-0.004205	-0.001121	-0.001312	-0.001158	-0.001115	-0.001168
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.032221	-0.030031	-0.031974	-0.000808	-0.001832	-0.001431	-0.001501	-0.001478
$Br^- \cdots PF_3$	-0.024623	-0.02203	-0.024537	-0.001005	-0.001966	-0.001613	-0.001672	-0.001665
$Cl^- \cdots AsF_3$	-0.049771	-0.0489	-0.049502	-0.000776	-0.001878	-0.001559	-0.00163	-0.001605
$Br^- \cdots AsF_3$	-0.041145	-0.039753	-0.041007	-0.000934	-0.002051	-0.001833	-0.001851	-0.001881
$NH_3 \cdots PF_3$	-0.00599	-0.004782	-0.005759	-0.001662	-0.001921	-0.001585	-0.001534	-0.001606
$NH_3 \cdots AsF_3$	-0.011676	-0.010562	-0.011378	-0.001822	-0.002265	-0.001815	-0.001776	-0.001837

Table S7: BLYP, BLYP[HF], BLYP[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	BLYP	BLYP[HF]	BLYP[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.074844	-0.06523	-0.074648	-0.000242	-0.002587	-0.002698	-0.002925	-0.002823
$Br^- \cdots ClF$	-0.0746	-0.065049	-0.074508	-0.000295	-0.002984	-0.003099	-0.003321	-0.003248
$Cl^- \cdots BrF$	-0.074036	-0.066411	-0.073874	-0.000224	-0.002921	-0.002998	-0.003305	-0.003149
$Br^- \cdots BrF$	-0.07128	-0.063563	-0.071239	-0.000286	-0.003323	-0.003498	-0.003801	-0.003671
$NH_3 \cdots ClF$	-0.022456	-0.01473	-0.022225	-0.002426	-0.00293	-0.002926	-0.002981	-0.002962
$NH_3 \cdots BrF$	-0.025998	-0.01953	-0.025778	-0.002541	-0.003544	-0.003288	-0.003344	-0.003345
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.047235	-0.043026	-0.046983	-0.000871	-0.003488	-0.003129	-0.003491	-0.003333
$Br^- \cdots SF_2$	-0.040182	-0.035227	-0.040053	-0.001079	-0.003953	-0.00357	-0.003885	-0.003793
$Cl^- \cdots SeF_2$	-0.059159	-0.056158	-0.058939	-0.000875	-0.003722	-0.003336	-0.003783	-0.003575
$Br^- \cdots SeF_2$	-0.052549	-0.04906	-0.052464	-0.001056	-0.004207	-0.003912	-0.00432	-0.004167
$NH_3 \cdots SF_2$	-0.010083	-0.00729	-0.00981	-0.003146	-0.003641	-0.003657	-0.003613	-0.003708
$NH_3 \cdots SeF_2$	-0.016383	-0.013848	-0.016089	-0.003267	-0.004407	-0.004181	-0.004204	-0.004277
$Cl^- \cdots SCF_2$	-0.015567	-0.010601	-0.015443	-0.001036	-0.002944	-0.002391	-0.002711	-0.002569
$Br^- \cdots SCF_2$	-0.013031	-0.008077	-0.012988	-0.001358	-0.003263	-0.0027	-0.002966	-0.002886
$Cl^- \cdots SeCF_2$	-0.02165	-0.01733	-0.021538	-0.000799	-0.003153	-0.002656	-0.003152	-0.002895
$Br^- \cdots SeCF_2$	-0.018258	-0.013785	-0.018238	-0.001073	-0.003489	-0.003086	-0.003525	-0.003328
$NH_3 \cdots SCF_2$	-0.000389	-0.0001	-0.000354	-0.001601	-0.001727	-0.001806	-0.001643	-0.001782
$NH_3 \cdots SeCF_2$	-0.001757	-0.001233	-0.00172	-0.001956	-0.002276	-0.002293	-0.002137	-0.002283
$Cl^- \cdots SPF_3$	-0.012721	-0.008617	-0.012617	-0.001075	-0.002785	-0.002104	-0.002532	-0.00233
$Br^- \cdots SPF_3$	-0.009818	-0.006144	-0.009788	-0.00143	-0.00306	-0.002314	-0.002717	-0.002553
$Cl^- \cdots SePF_3$	-0.025478	-0.020126	-0.02537	-0.000787	-0.003219	-0.002779	-0.003241	-0.003055
$Br^- \cdots SePF_3$	-0.020606	-0.015479	-0.020593	-0.00108	-0.003562	-0.003157	-0.003598	-0.00344
$NH_3 \cdots SPF_3$	-0.000398	0.000185	-0.000367	-0.001676	-0.001817	-0.001861	-0.001685	-0.001839
$NH_3 \cdots SePF_3$	-0.002474	-0.00145	-0.002429	-0.00208	-0.002486	-0.002472	-0.002308	-0.002477
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.027951	-0.026078	-0.027694	-0.001612	-0.004094	-0.003247	-0.003618	-0.003494
$Br^- \cdots PF_3$	-0.020825	-0.018554	-0.020704	-0.002016	-0.004431	-0.003451	-0.003764	-0.003717
$Cl^- \cdots AsF_3$	-0.045325	-0.044661	-0.045077	-0.001556	-0.004279	-0.003581	-0.003937	-0.003821
$Br^- \cdots AsF_3$	-0.036994	-0.035775	-0.036853	-0.001871	-0.004743	-0.004097	-0.004264	-0.004335
$NH_3 \cdots PF_3$	-0.003488	-0.002667	-0.00324	-0.003198	-0.003708	-0.00381	-0.003573	-0.003833
$NH_3 \cdots AsF_3$	-0.008562	-0.007822	-0.008252	-0.003576	-0.004645	-0.004737	-0.004565	-0.004793

Table S8: TPSS, TPSS[HF], TPSS[LDA], Disp3, Disp3BJ interaction energy results (in hartree) for the B30 dataset.

	TPSS	TPSS[HF]	TPSS[LDA]	Disp3	Disp3BJ
Halogen Bonds					
$Cl^- \cdots ClF$	-0.080504	-0.071272	-0.080283	-0.000183	-0.001455
$Br^- \cdots ClF$	-0.079579	-0.070556	-0.079498	-0.000219	-0.00166
$Cl^- \cdots BrF$	-0.080777	-0.073473	-0.080541	-0.000167	-0.001613
$Br^- \cdots BrF$	-0.077403	-0.070192	-0.077309	-0.000208	-0.001818
$NH_3 \cdots ClF$	-0.026019	-0.018702	-0.025792	-0.001527	-0.001755
$NH_3 \cdots BrF$	-0.030817	-0.02469	-0.030582	-0.001602	-0.002072
Chalcogen Bonds					
$Cl^- \cdots SF_2$	-0.052983	-0.049037	-0.052674	-0.000572	-0.001981
$Br^- \cdots SF_2$	-0.044977	-0.040539	-0.044781	-0.000705	-0.00223
$Cl^- \cdots SeF_2$	-0.066006	-0.063101	-0.065695	-0.000569	-0.002087
$Br^- \cdots SeF_2$	-0.058575	-0.055419	-0.058397	-0.000686	-0.002342
$NH_3 \cdots SF_2$	-0.013319	-0.010423	-0.013055	-0.002044	-0.002236
$NH_3 \cdots SeF_2$	-0.021329	-0.018742	-0.021055	-0.002109	-0.002617
$Cl^- \cdots SCF_2$	-0.017796	-0.013016	-0.017563	-0.000727	-0.00176
$Br^- \cdots SCF_2$	-0.014879	-0.010362	-0.014695	-0.000936	-0.001946
$Cl^- \cdots SeCF_2$	-0.024838	-0.020601	-0.024612	-0.00057	-0.001824
$Br^- \cdots SeCF_2$	-0.020986	-0.016844	-0.020822	-0.000748	-0.002009
$NH_3 \cdots SCF_2$	-0.001107	-0.000828	-0.000903	-0.001131	-0.001186
$NH_3 \cdots SeCF_2$	-0.002674	-0.002158	-0.002485	-0.001338	-0.001492
$Cl^- \cdots SPF_3$	-0.014143	-0.010454	-0.013886	-0.000747	-0.001682
$Br^- \cdots SPF_3$	-0.011034	-0.007936	-0.010805	-0.000976	-0.001846
$Cl^- \cdots SePF_3$	-0.028147	-0.023133	-0.027919	-0.000566	-0.001872
$Br^- \cdots SePF_3$	-0.02282	-0.018282	-0.022642	-0.000758	-0.002063
$NH_3 \cdots SPF_3$	-0.001051	-0.000526	-0.000845	-0.001195	-0.001259
$NH_3 \cdots SePF_3$	-0.003344	-0.002379	-0.003157	-0.001422	-0.001629
Pnictogen Bonds					
$Cl^- \cdots PF_3$	-0.03314	-0.031195	-0.032827	-0.001025	-0.002358
$Br^- \cdots PF_3$	-0.024782	-0.022593	-0.02457	-0.001281	-0.002559
$Cl^- \cdots AsF_3$	-0.051639	-0.0509	-0.051268	-0.000988	-0.002435
$Br^- \cdots AsF_3$	-0.04245	-0.041191	-0.042138	-0.00119	-0.00269
$NH_3 \cdots PF_3$	-0.005876	-0.004822	-0.005592	-0.00213	-0.002371
$NH_3 \cdots AsF_3$	-0.012531	-0.011512	-0.012222	-0.002326	-0.002837

Table S9: revTPSS, revTPSS[HF], revTPSS[LDA] interaction energy results (in hartree) for the B30 dataset.

	revTPSS	revTPSS[HF]	revTPSS[LDA]
Halogen Bonds			
$Cl^- \cdots ClF$	-0.080574	-0.071585	-0.080349
$Br^- \cdots ClF$	-0.079454	-0.070664	-0.079313
$Cl^- \cdots BrF$	-0.081326	-0.074064	-0.081088
$Br^- \cdots BrF$	-0.077815	-0.070661	-0.077666
$NH_3 \cdots ClF$	-0.026132	-0.019076	-0.025893
$NH_3 \cdots BrF$	-0.031136	-0.025107	-0.030902
Chalcogen Bonds			
$Cl^- \cdots SF_2$	-0.053278	-0.049389	-0.052973
$Br^- \cdots SF_2$	-0.045119	-0.040831	-0.044875
$Cl^- \cdots SeF_2$	-0.066779	-0.063802	-0.066474
$Br^- \cdots SeF_2$	-0.059189	-0.056007	-0.058966
$NH_3 \cdots SF_2$	-0.013834	-0.011022	-0.013579
$NH_3 \cdots SeF_2$	-0.022051	-0.019448	-0.021798
$Cl^- \cdots SCF_2$	-0.017857	-0.013337	-0.017591
$Br^- \cdots SCF_2$	-0.014863	-0.010674	-0.014618
$Cl^- \cdots SeCF_2$	-0.024926	-0.020788	-0.024696
$Br^- \cdots SeCF_2$	-0.02097	-0.017009	-0.020772
$NH_3 \cdots SCF_2$	-0.00129	-0.001004	-0.00112
$NH_3 \cdots SeCF_2$	-0.002887	-0.002355	-0.00273
$Cl^- \cdots SPF_3$	-0.014291	-0.010756	-0.013994
$Br^- \cdots SPF_3$	-0.011148	-0.008245	-0.010856
$Cl^- \cdots SePF_3$	-0.028136	-0.023224	-0.027895
$Br^- \cdots SePF_3$	-0.022751	-0.018394	-0.022521
$NH_3 \cdots SPF_3$	-0.001228	-0.000707	-0.001055
$NH_3 \cdots SePF_3$	-0.003554	-0.002592	-0.003391
Pnictogen Bonds			
$Cl^- \cdots PF_3$	-0.033606	-0.03157	-0.033296
$Br^- \cdots PF_3$	-0.025081	-0.022904	-0.024835
$Cl^- \cdots AsF_3$	-0.052569	-0.051672	-0.052215
$Br^- \cdots AsF_3$	-0.043086	-0.041813	-0.042811
$NH_3 \cdots PF_3$	-0.006473	-0.005372	-0.00624
$NH_3 \cdots AsF_3$	-0.013348	-0.012231	-0.013095

Table S10: SCAN, SCAN[HF], SCAN[LDA] interaction energy results (in hartree) for the B30 dataset.

	SCAN	SCAN[HF]	SCAN[LDA]
Halogen Bonds			
$Cl^- \cdots ClF$	-0.085723	-0.077555	-0.085462
$Br^- \cdots ClF$	-0.084689	-0.076713	-0.084554
$Cl^- \cdots BrF$	-0.085925	-0.078295	-0.085687
$Br^- \cdots BrF$	-0.082386	-0.075008	-0.082191
$NH_3 \cdots ClF$	-0.028836	-0.021772	-0.028512
$NH_3 \cdots BrF$	-0.033977	-0.027389	-0.033751
Chalcogen Bonds			
$Cl^- \cdots SF_2$	-0.058113	-0.053851	-0.057868
$Br^- \cdots SF_2$	-0.049501	-0.044687	-0.049317
$Cl^- \cdots SeF_2$	-0.071389	-0.06811	-0.071143
$Br^- \cdots SeF_2$	-0.063541	-0.060047	-0.063334
$NH_3 \cdots SF_2$	-0.016321	-0.013495	-0.016031
$NH_3 \cdots SeF_2$	-0.024942	-0.022215	-0.02465
$Cl^- \cdots SCF_2$	-0.018735	-0.014165	-0.018565
$Br^- \cdots SCF_2$	-0.015749	-0.011468	-0.015591
$Cl^- \cdots SeCF_2$	-0.026414	-0.022277	-0.026165
$Br^- \cdots SeCF_2$	-0.02232	-0.018264	-0.022115
$NH_3 \cdots SCF_2$	-0.001939	-0.00167	-0.001716
$NH_3 \cdots SeCF_2$	-0.003874	-0.003404	-0.003601
$Cl^- \cdots SPF_3$	-0.014906	-0.011868	-0.014438
$Br^- \cdots SPF_3$	-0.011625	-0.00912	-0.011173
$Cl^- \cdots SePF_3$	-0.029024	-0.024707	-0.028696
$Br^- \cdots SePF_3$	-0.023555	-0.019729	-0.023206
$NH_3 \cdots SPF_3$	-0.001762	-0.001312	-0.001527
$NH_3 \cdots SePF_3$	-0.004515	-0.003612	-0.004214
Pnictogen Bonds			
$Cl^- \cdots PF_3$	-0.037648	-0.035527	-0.037272
$Br^- \cdots PF_3$	-0.028407	-0.026133	-0.028095
$Cl^- \cdots AsF_3$	-0.056953	-0.056183	-0.056534
$Br^- \cdots AsF_3$	-0.0468	-0.045645	-0.046454
$NH_3 \cdots PF_3$	-0.008624	-0.00767	-0.008277
$NH_3 \cdots AsF_3$	-0.015964	-0.015135	-0.015551

Table S11: B3LYP, B3LYP[HF], B3LYP[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	B3LYP	B3LYP[HF]	B3LYP[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.074602	-0.068281	-0.07379	-0.000217	-0.002153	-0.002087	-0.002082	-0.00212
$Br^- \cdots ClF$	-0.073758	-0.067477	-0.073099	-0.000265	-0.002512	-0.002465	-0.002454	-0.002501
$Cl^- \cdots BrF$	-0.075137	-0.070154	-0.074299	-0.000208	-0.00246	-0.002406	-0.002427	-0.002434
$Br^- \cdots BrF$	-0.071718	-0.066678	-0.071038	-0.000266	-0.002836	-0.002873	-0.002889	-0.002903
$NH_3 \cdots ClF$	-0.021331	-0.016534	-0.020369	-0.002005	-0.002392	-0.00181	-0.0018	-0.001827
$NH_3 \cdots BrF$	-0.026096	-0.022043	-0.025207	-0.002193	-0.002909	-0.002133	-0.00212	-0.002155
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.048728	-0.045799	-0.048058	-0.000758	-0.002899	-0.002619	-0.002642	-0.002666
$Br^- \cdots SF_2$	-0.040752	-0.03739	-0.040178	-0.000948	-0.00332	-0.00307	-0.003077	-0.003126
$Cl^- \cdots SeF_2$	-0.061956	-0.059801	-0.061301	-0.000756	-0.003126	-0.002873	-0.002923	-0.002919
$Br^- \cdots SeF_2$	-0.054444	-0.052007	-0.053919	-0.000924	-0.003576	-0.00343	-0.003465	-0.003482
$NH_3 \cdots SF_2$	-0.011177	-0.009383	-0.010446	-0.002515	-0.002981	-0.002372	-0.002323	-0.002413
$NH_3 \cdots SeF_2$	-0.018373	-0.016667	-0.01769	-0.002712	-0.003617	-0.002738	-0.002702	-0.002784
$Cl^- \cdots SCF_2$	-0.014568	-0.01158	-0.013887	-0.000908	-0.002452	-0.00232	-0.002343	-0.002368
$Br^- \cdots SCF_2$	-0.011905	-0.008957	-0.01132	-0.001209	-0.002738	-0.002656	-0.002668	-0.002708
$Cl^- \cdots SeCF_2$	-0.020956	-0.018326	-0.020298	-0.000725	-0.002656	-0.002591	-0.002667	-0.002632
$Br^- \cdots SeCF_2$	-0.017342	-0.014636	-0.016798	-0.000985	-0.002968	-0.003019	-0.003084	-0.003063
$NH_3 \cdots SCF_2$	-0.001009	-0.00081	-0.000812	-0.001322	-0.00144	-0.001342	-0.001286	-0.00137
$NH_3 \cdots SeCF_2$	-0.002418	-0.002078	-0.002167	-0.00159	-0.00189	-0.001721	-0.001668	-0.001752
$Cl^- \cdots SPF_3$	-0.011924	-0.00959	-0.011038	-0.000974	-0.002319	-0.002065	-0.002127	-0.002113
$Br^- \cdots SPF_3$	-0.009125	-0.007065	-0.008364	-0.001307	-0.002564	-0.002329	-0.002388	-0.002381
$Cl^- \cdots SePF_3$	-0.024338	-0.021033	-0.023522	-0.00072	-0.002711	-0.00258	-0.00265	-0.002634
$Br^- \cdots SePF_3$	-0.019443	-0.016329	-0.018735	-0.000999	-0.003029	-0.002984	-0.003055	-0.00304
$NH_3 \cdots SPF_3$	-0.000821	-0.000455	-0.000585	-0.001393	-0.001517	-0.001389	-0.001326	-0.00142
$NH_3 \cdots SePF_3$	-0.00288	-0.002255	-0.002544	-0.001687	-0.002065	-0.001842	-0.001782	-0.001879
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.030314	-0.028927	-0.029654	-0.001376	-0.003398	-0.002892	-0.002923	-0.002958
$Br^- \cdots PF_3$	-0.022359	-0.020798	-0.021794	-0.00172	-0.003712	-0.003254	-0.003266	-0.003331
$Cl^- \cdots AsF_3$	-0.04918	-0.048454	-0.04858	-0.001318	-0.003585	-0.003154	-0.003193	-0.003218
$Br^- \cdots AsF_3$	-0.039777	-0.038779	-0.03926	-0.001596	-0.004016	-0.003692	-0.003666	-0.00378
$NH_3 \cdots PF_3$	-0.00521	-0.004617	-0.00464	-0.002497	-0.003052	-0.002581	-0.002474	-0.002645
$NH_3 \cdots AsF_3$	-0.011208	-0.010612	-0.010587	-0.002889	-0.003819	-0.003097	-0.003007	-0.003163

Table S12: PBE0, PBE0[HF], PBE0[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	PBE0	PBE0[HF]	PBE0[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.080249	-0.07421	-0.079451	-0.000147	-0.001012	-0.001128	-0.001089	-0.00118
$Br^- \cdots ClF$	-0.079074	-0.073255	-0.07836	-0.000174	-0.001169	-0.001397	-0.001355	-0.001452
$Cl^- \cdots BrF$	-0.081445	-0.076724	-0.080581	-0.000139	-0.001134	-0.001363	-0.001328	-0.001415
$Br^- \cdots BrF$	-0.077717	-0.073104	-0.076934	-0.000172	-0.001297	-0.0017	-0.001665	-0.001756
$NH_3 \cdots ClF$	-0.02409	-0.019431	-0.023084	-0.001148	-0.001209	-0.000764	-0.000749	-0.000789
$NH_3 \cdots BrF$	-0.029986	-0.026051	-0.029077	-0.00124	-0.001429	-0.000953	-0.000937	-0.000981
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.054273	-0.051277	-0.053727	-0.000445	-0.001378	-0.001498	-0.001448	-0.001567
$Br^- \cdots SF_2$	-0.045489	-0.042234	-0.044936	-0.00055	-0.001569	-0.001854	-0.001804	-0.001929
$Cl^- \cdots SeF_2$	-0.06828	-0.066037	-0.067731	-0.000443	-0.001466	-0.001699	-0.001651	-0.001769
$Br^- \cdots SeF_2$	-0.060195	-0.057832	-0.059682	-0.000536	-0.001667	-0.002122	-0.002073	-0.002196
$NH_3 \cdots SF_2$	-0.013716	-0.011753	-0.0131	-0.001481	-0.001556	-0.001036	-0.001005	-0.001077
$NH_3 \cdots SeF_2$	-0.022268	-0.020377	-0.021728	-0.00157	-0.001812	-0.001219	-0.001187	-0.001261
$Cl^- \cdots SCF_2$	-0.01626	-0.013639	-0.015435	-0.000562	-0.001254	-0.001597	-0.001559	-0.001667
$Br^- \cdots SCF_2$	-0.013403	-0.010935	-0.012596	-0.000731	-0.001399	-0.001908	-0.001879	-0.001978
$Cl^- \cdots SeCF_2$	-0.023439	-0.021148	-0.02267	-0.000459	-0.001305	-0.001794	-0.001768	-0.001863
$Br^- \cdots SeCF_2$	-0.019561	-0.017313	-0.01883	-0.000604	-0.001454	-0.002163	-0.002148	-0.002229
$NH_3 \cdots SCF_2$	-0.001734	-0.001517	-0.001502	-0.000838	-0.000877	-0.000756	-0.000744	-0.00079
$NH_3 \cdots SeCF_2$	-0.003326	-0.002963	-0.003053	-0.000961	-0.001084	-0.000963	-0.000954	-0.000998
$Cl^- \cdots SPF_3$	-0.013453	-0.011427	-0.012312	-0.0006	-0.001204	-0.001496	-0.001457	-0.001571
$Br^- \cdots SPF_3$	-0.010552	-0.00884	-0.009488	-0.000787	-0.001333	-0.001754	-0.001725	-0.001828
$Cl^- \cdots SePF_3$	-0.026881	-0.023894	-0.025903	-0.00046	-0.001344	-0.0018	-0.00177	-0.001874
$Br^- \cdots SePF_3$	-0.021714	-0.019011	-0.020763	-0.000617	-0.001498	-0.002153	-0.002135	-0.002224
$NH_3 \cdots SPF_3$	-0.001556	-0.001212	-0.001251	-0.000894	-0.000937	-0.000795	-0.000777	-0.000832
$NH_3 \cdots SePF_3$	-0.003834	-0.003236	-0.003439	-0.001026	-0.001186	-0.001027	-0.001011	-0.001068
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.034985	-0.033424	-0.034462	-0.000786	-0.001643	-0.001766	-0.001704	-0.001848
$Br^- \cdots PF_3$	-0.025969	-0.024357	-0.025445	-0.000977	-0.001808	-0.002147	-0.002083	-0.002235
$Cl^- \cdots AsF_3$	-0.054787	-0.053866	-0.054326	-0.000754	-0.00171	-0.001916	-0.001858	-0.001995
$Br^- \cdots AsF_3$	-0.04466	-0.043566	-0.044179	-0.000908	-0.001914	-0.002384	-0.002311	-0.00247
$NH_3 \cdots PF_3$	-0.00711	-0.006353	-0.006624	-0.001524	-0.00168	-0.001194	-0.001148	-0.001247
$NH_3 \cdots AsF_3$	-0.014203	-0.013382	-0.01371	-0.001721	-0.001983	-0.001378	-0.001331	-0.001429

Table S13: M06, M06[HF], M06[LDA], Disp3 interaction energy results (in hartree) for the B30 dataset.

	M06	M06[HF]	M06[LDA]	Disp3
Halogen Bonds				
$Cl^- \cdots ClF$	-0.076903	-0.072609	-0.075268	-0.000061
$Br^- \cdots ClF$	-0.077429	-0.073214	-0.076066	-0.000063
$Cl^- \cdots BrF$	-0.078758	-0.076569	-0.076236	-0.000056
$Br^- \cdots BrF$	-0.07568	-0.073698	-0.073499	-0.000059
$NH_3 \cdots ClF$	-0.021764	-0.018377	-0.01957	-0.000126
$NH_3 \cdots BrF$	-0.028034	-0.025832	-0.025479	-0.000101
Chalcogen Bonds				
$Cl^- \cdots SF_2$	-0.052459	-0.050484	-0.051283	-0.000069
$Br^- \cdots SF_2$	-0.0445	-0.042327	-0.043351	-0.000072
$Cl^- \cdots SeF_2$	-0.067088	-0.066147	-0.065419	-0.000067
$Br^- \cdots SeF_2$	-0.059492	-0.058622	-0.057906	-0.000071
$NH_3 \cdots SF_2$	-0.013881	-0.012537	-0.012418	-0.000245
$NH_3 \cdots SeF_2$	-0.02187	-0.020744	-0.020279	-0.000206
$Cl^- \cdots SCF_2$	-0.017185	-0.014534	-0.015704	-0.000146
$Br^- \cdots SCF_2$	-0.014518	-0.012023	-0.01323	-0.000156
$Cl^- \cdots SeCF_2$	-0.025822	-0.024198	-0.023861	-0.000136
$Br^- \cdots SeCF_2$	-0.021881	-0.020202	-0.020167	-0.000145
$NH_3 \cdots SCF_2$	-0.002016	-0.001827	-0.001726	-0.000253
$NH_3 \cdots SeCF_2$	-0.004295	-0.004051	-0.003957	-0.000207
$Cl^- \cdots SPF_3$	-0.015243	-0.013291	-0.013495	-0.000149
$Br^- \cdots SPF_3$	-0.01242	-0.010717	-0.010683	-0.00016
$Cl^- \cdots SePF_3$	-0.029498	-0.02703	-0.027324	-0.000144
$Br^- \cdots SePF_3$	-0.024443	-0.022085	-0.022327	-0.000156
$NH_3 \cdots SPF_3$	-0.001898	-0.001625	-0.001525	-0.00029
$NH_3 \cdots SePF_3$	-0.004982	-0.004477	-0.004427	-0.000235
Pnictogen Bonds				
$Cl^- \cdots PF_3$	-0.035355	-0.034117	-0.034123	-0.000081
$Br^- \cdots PF_3$	-0.027122	-0.025849	-0.025649	-0.000089
$Cl^- \cdots AsF_3$	-0.055068	-0.054732	-0.053879	-0.00008
$Br^- \cdots AsF_3$	-0.045865	-0.045587	-0.044249	-0.000086
$NH_3 \cdots PF_3$	-0.008724	-0.008156	-0.007875	-0.000359
$NH_3 \cdots AsF_3$	-0.015573	-0.015048	-0.014451	-0.000323

Table S14: HH, HH[HF], HH[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	HH	HH[HF]	HH[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.071777	-0.069285	-0.068668	-0.00017	-0.001852	-0.001487	-0.001464	-0.001531
$Br^- \cdots ClF$	-0.069959	-0.067472	-0.067186	-0.000208	-0.002269	-0.001787	-0.001761	-0.001833
$Cl^- \cdots BrF$	-0.074168	-0.072237	-0.071128	-0.000171	-0.002232	-0.001745	-0.001729	-0.00178
$Br^- \cdots BrF$	-0.06972	-0.06776	-0.066972	-0.000218	-0.002714	-0.002117	-0.002099	-0.002153
$NH_3 \cdots ClF$	-0.019201	-0.017466	-0.015573	-0.001654	-0.001854	-0.001181	-0.001169	-0.001203
$NH_3 \cdots BrF$	-0.025163	-0.023687	-0.022002	-0.001826	-0.002332	-0.001419	-0.001406	-0.001445
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.048183	-0.046978	-0.046367	-0.000619	-0.002473	-0.00193	-0.001907	-0.001981
$Br^- \cdots SF_2$	-0.039227	-0.03787	-0.037366	-0.000777	-0.002953	-0.002311	-0.002282	-0.002366
$Cl^- \cdots SeF_2$	-0.062918	-0.062012	-0.061283	-0.000622	-0.002795	-0.002148	-0.00213	-0.00219
$Br^- \cdots SeF_2$	-0.054264	-0.05326	-0.052727	-0.000762	-0.003355	-0.002605	-0.002582	-0.002652
$NH_3 \cdots SF_2$	-0.011862	-0.011199	-0.009851	-0.002022	-0.002307	-0.001581	-0.001555	-0.001631
$NH_3 \cdots SeF_2$	-0.019652	-0.018991	-0.017948	-0.002212	-0.002879	-0.001829	-0.001804	-0.001878
$Cl^- \cdots SCF_2$	-0.012615	-0.011599	-0.009926	-0.000731	-0.002054	-0.001862	-0.001848	-0.001916
$Br^- \cdots SCF_2$	-0.009886	-0.008897	-0.007313	-0.000983	-0.002354	-0.002169	-0.002156	-0.002224
$Cl^- \cdots SeCF_2$	-0.018941	-0.018038	-0.016507	-0.000591	-0.002352	-0.00208	-0.00208	-0.002115
$Br^- \cdots SeCF_2$	-0.015117	-0.014193	-0.01283	-0.000809	-0.002726	-0.002452	-0.002454	-0.002487
$NH_3 \cdots SCF_2$	-0.001567	-0.00149	-0.0011	-0.001032	-0.001122	-0.001016	-0.001	-0.00106
$NH_3 \cdots SeCF_2$	-0.002967	-0.002844	-0.002313	-0.001252	-0.00149	-0.001293	-0.001279	-0.001337
$Cl^- \cdots SPF_3$	-0.010658	-0.009869	-0.00735	-0.000797	-0.001928	-0.001688	-0.001682	-0.001733
$Br^- \cdots SPF_3$	-0.008014	-0.007326	-0.005029	-0.001077	-0.00218	-0.001939	-0.001935	-0.001982
$Cl^- \cdots SePF_3$	-0.02181	-0.020609	-0.018762	-0.000585	-0.0024	-0.002055	-0.002051	-0.002095
$Br^- \cdots SePF_3$	-0.017038	-0.015926	-0.014144	-0.00082	-0.002776	-0.002413	-0.002413	-0.00245
$NH_3 \cdots SPF_3$	-0.001142	-0.001009	-0.000493	-0.001092	-0.001184	-0.001058	-0.001037	-0.001105
$NH_3 \cdots SePF_3$	-0.003107	-0.00289	-0.002116	-0.001338	-0.001633	-0.001377	-0.001357	-0.001427
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.03152	-0.030916	-0.030036	-0.001133	-0.002867	-0.002205	-0.00218	-0.002266
$Br^- \cdots PF_3$	-0.022886	-0.022254	-0.021335	-0.001418	-0.003229	-0.002567	-0.002536	-0.002634
$Cl^- \cdots AsF_3$	-0.051762	-0.051354	-0.050742	-0.001085	-0.003156	-0.002399	-0.002378	-0.002455
$Br^- \cdots AsF_3$	-0.04119	-0.040718	-0.040099	-0.001316	-0.003687	-0.002864	-0.002825	-0.002949
$NH_3 \cdots PF_3$	-0.006879	-0.006626	-0.005671	-0.00199	-0.002357	-0.001778	-0.001735	-0.001858
$NH_3 \cdots AsF_3$	-0.01364	-0.013364	-0.012452	-0.00235	-0.003014	-0.002082	-0.002043	-0.00216

Table S15: M06-2X, M06-2X[HF], M06-2X[LDA], Disp3 interaction energy results (in hartree) for the B30 dataset.

	M06-2X	M06-2X[HF]	M06-2X[LDA]	Disp3
Halogen Bonds				
$Cl^- \cdots ClF$	-0.07501	-0.071274	-0.072363	-0.000009
$Br^- \cdots ClF$	-0.072877	-0.069328	-0.070029	-0.000009
$Cl^- \cdots BrF$	-0.077112	-0.073861	-0.074838	-0.000012
$Br^- \cdots BrF$	-0.072614	-0.069349	-0.070325	-0.000011
$NH_3 \cdots ClF$	-0.019742	-0.017401	-0.016625	-0.000047
$NH_3 \cdots BrF$	-0.025837	-0.023859	-0.023183	-0.000043
Chalcogen Bonds				
$Cl^- \cdots SF_2$	-0.053052	-0.051136	-0.051547	-0.000009
$Br^- \cdots SF_2$	-0.04386	-0.041799	-0.042181	-0.00001
$Cl^- \cdots SeF_2$	-0.066623	-0.064857	-0.065397	-0.000012
$Br^- \cdots SeF_2$	-0.057916	-0.056073	-0.056648	-0.000012
$NH_3 \cdots SF_2$	-0.014085	-0.013239	-0.012224	-0.000066
$NH_3 \cdots SeF_2$	-0.021889	-0.0209	-0.020433	-0.000062
$Cl^- \cdots SCF_2$	-0.015899	-0.015099	-0.012887	-0.000042
$Br^- \cdots SCF_2$	-0.013175	-0.012418	-0.010074	-0.000043
$Cl^- \cdots SeCF_2$	-0.021829	-0.020866	-0.019171	-0.000045
$Br^- \cdots SeCF_2$	-0.018141	-0.017227	-0.01543	-0.000047
$NH_3 \cdots SCF_2$	-0.00243	-0.002265	-0.002013	-0.000074
$NH_3 \cdots SeCF_2$	-0.00393	-0.003679	-0.003268	-0.000065
$Cl^- \cdots SPF_3$	-0.013992	-0.013144	-0.010423	-0.00005
$Br^- \cdots SPF_3$	-0.011271	-0.0105	-0.008021	-0.000053
$Cl^- \cdots SePF_3$	-0.024993	-0.023611	-0.021698	-0.000049
$Br^- \cdots SePF_3$	-0.02029	-0.01905	-0.016987	-0.000052
$NH_3 \cdots SPF_3$	-0.0021	-0.001863	-0.001467	-0.000087
$NH_3 \cdots SePF_3$	-0.004275	-0.003908	-0.003175	-0.000079
Pnictogen Bonds				
$Cl^- \cdots PF_3$	-0.036722	-0.035699	-0.035388	-0.000012
$Br^- \cdots PF_3$	-0.027634	-0.026657	-0.026214	-0.000014
$Cl^- \cdots AsF_3$	-0.056395	-0.05544	-0.0555	-0.000013
$Br^- \cdots AsF_3$	-0.046065	-0.04502	-0.045191	-0.000014
$NH_3 \cdots PF_3$	-0.009692	-0.009208	-0.008493	-0.000101
$NH_3 \cdots AsF_3$	-0.017019	-0.016412	-0.015909	-0.000093

Table S16: CAM-B3LYP, CAM-B3LYP[HF], CAM-B3LYP[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	CAM-B3LYP	CAM-B3LYP[HF]	CAM-B3LYP[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.073345	-0.069482	-0.071329	-0.000149	-0.001007	-0.0015	-0.001388	-0.001535
$Br^- \cdots ClF$	-0.07171	-0.067947	-0.069896	-0.000181	-0.001223	-0.001885	-0.001764	-0.001921
$Cl^- \cdots BrF$	-0.074831	-0.071887	-0.07277	-0.00015	-0.001182	-0.001862	-0.001744	-0.001896
$Br^- \cdots BrF$	-0.070618	-0.067707	-0.068735	-0.00019	-0.001425	-0.002357	-0.002231	-0.00239
$NH_3 \cdots ClF$	-0.020998	-0.018094	-0.018831	-0.001409	-0.001103	-0.000915	-0.000871	-0.00093
$NH_3 \cdots BrF$	-0.026515	-0.02407	-0.024562	-0.001552	-0.001353	-0.001179	-0.001127	-0.001195
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.049006	-0.047438	-0.047512	-0.000528	-0.001373	-0.002028	-0.001878	-0.002082
$Br^- \cdots SF_2$	-0.040222	-0.038508	-0.038676	-0.000662	-0.00165	-0.002548	-0.002389	-0.002602
$Cl^- \cdots SeF_2$	-0.063016	-0.061892	-0.061602	-0.000532	-0.001517	-0.002338	-0.002179	-0.002392
$Br^- \cdots SeF_2$	-0.05465	-0.053458	-0.053263	-0.00065	-0.001819	-0.002956	-0.002787	-0.00301
$NH_3 \cdots SF_2$	-0.012361	-0.011335	-0.011047	-0.001729	-0.001442	-0.001242	-0.001169	-0.001272
$NH_3 \cdots SeF_2$	-0.020126	-0.019137	-0.018962	-0.001887	-0.001711	-0.001495	-0.001417	-0.001527
$Cl^- \cdots SCF_2$	-0.013221	-0.012255	-0.01066	-0.000632	-0.001317	-0.002178	-0.002039	-0.002222
$Br^- \cdots SCF_2$	-0.010426	-0.009537	-0.007861	-0.000845	-0.001547	-0.002612	-0.002483	-0.002646
$Cl^- \cdots SeCF_2$	-0.019475	-0.018753	-0.017042	-0.000513	-0.00141	-0.002499	-0.002369	-0.002545
$Br^- \cdots SeCF_2$	-0.01563	-0.014934	-0.013212	-0.000698	-0.001653	-0.003027	-0.002912	-0.00306
$NH_3 \cdots SCF_2$	-0.001592	-0.001479	-0.001318	-0.000894	-0.000904	-0.000881	-0.000844	-0.0009
$NH_3 \cdots SeCF_2$	-0.003068	-0.002879	-0.002663	-0.001076	-0.001131	-0.001153	-0.001117	-0.001172
$Cl^- \cdots SPF_3$	-0.011227	-0.010255	-0.008471	-0.000688	-0.00129	-0.002062	-0.001922	-0.002124
$Br^- \cdots SPF_3$	-0.008532	-0.007711	-0.005968	-0.000926	-0.001499	-0.00242	-0.002294	-0.002476
$Cl^- \cdots SePF_3$	-0.022794	-0.021335	-0.020199	-0.00051	-0.001467	-0.002534	-0.002398	-0.002588
$Br^- \cdots SePF_3$	-0.017952	-0.016642	-0.015413	-0.000709	-0.001719	-0.003041	-0.002922	-0.003085
$NH_3 \cdots SPF_3$	-0.00127	-0.00106	-0.000862	-0.00095	-0.000975	-0.000923	-0.000879	-0.000947
$NH_3 \cdots SePF_3$	-0.003376	-0.003036	-0.002715	-0.001152	-0.001237	-0.001233	-0.001185	-0.001259
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.031643	-0.030979	-0.030457	-0.000963	-0.001645	-0.002434	-0.002243	-0.002499
$Br^- \cdots PF_3$	-0.023124	-0.022423	-0.021863	-0.001205	-0.001922	-0.002994	-0.002788	-0.003059
$Cl^- \cdots AsF_3$	-0.05124	-0.050923	-0.050286	-0.000923	-0.001758	-0.002643	-0.002455	-0.002701
$Br^- \cdots AsF_3$	-0.040992	-0.040619	-0.039951	-0.001118	-0.002083	-0.003325	-0.003113	-0.003383
$NH_3 \cdots PF_3$	-0.006779	-0.006392	-0.006023	-0.001715	-0.001602	-0.001416	-0.00132	-0.001453
$NH_3 \cdots AsF_3$	-0.013436	-0.013073	-0.012643	-0.002017	-0.00189	-0.001655	-0.001554	-0.00169

Table S17: LC-ωPBE, LC-ωPBE[HF], LC-ωPBE[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the B30 dataset.

	LC-ωPBE	LC-ωPBE[HF]	LC-ωPBE[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Halogen Bonds								
$Cl^- \cdots ClF$	-0.071807	-0.069447	-0.068858	-0.00016	-0.001169	-0.000805	-0.000834	-0.000788
$Br^- \cdots ClF$	-0.069792	-0.067728	-0.067011	-0.000194	-0.00139	-0.000911	-0.000926	-0.00089
$Cl^- \cdots BrF$	-0.074902	-0.073264	-0.071697	-0.000159	-0.001348	-0.000858	-0.000891	-0.000831
$Br^- \cdots BrF$	-0.070349	-0.068925	-0.067248	-0.000202	-0.001588	-0.000987	-0.001007	-0.000956
$NH_3 \cdots ClF$	-0.018508	-0.016434	-0.015254	-0.001485	-0.001321	-0.001025	-0.001046	-0.001007
$NH_3 \cdots BrF$	-0.025404	-0.023674	-0.022427	-0.001634	-0.0016	-0.00108	-0.001086	-0.001061
Chalcogen Bonds								
$Cl^- \cdots SF_2$	-0.048576	-0.047763	-0.046162	-0.00056	-0.001593	-0.000992	-0.001016	-0.00093
$Br^- \cdots SF_2$	-0.039315	-0.038569	-0.036568	-0.000701	-0.00187	-0.001112	-0.001106	-0.001045
$Cl^- \cdots SeF_2$	-0.063646	-0.063197	-0.061352	-0.000562	-0.001733	-0.00105	-0.001078	-0.000979
$Br^- \cdots SeF_2$	-0.054892	-0.05456	-0.052387	-0.000687	-0.00203	-0.0012	-0.001206	-0.001127
$NH_3 \cdots SF_2$	-0.01105	-0.010212	-0.009146	-0.00183	-0.001709	-0.001411	-0.001418	-0.001394
$NH_3 \cdots SeF_2$	-0.019578	-0.018759	-0.017881	-0.001993	-0.002021	-0.001508	-0.00151	-0.001486
$Cl^- \cdots SCF_2$	-0.011255	-0.011424	-0.006231	-0.00067	-0.001475	-0.000791	-0.000822	-0.000737
$Br^- \cdots SCF_2$	-0.008698	-0.008967	-0.003431	-0.000895	-0.001693	-0.000907	-0.000914	-0.000854
$Cl^- \cdots SeCF_2$	-0.017961	-0.018374	-0.013146	-0.000543	-0.001566	-0.000845	-0.000879	-0.000757
$Br^- \cdots SeCF_2$	-0.014242	-0.014727	-0.009203	-0.000738	-0.001795	-0.000981	-0.000995	-0.000898
$NH_3 \cdots SCF_2$	-0.000935	-0.000893	-0.000407	-0.000954	-0.000997	-0.000875	-0.000853	-0.000894
$NH_3 \cdots SeCF_2$	-0.002397	-0.002279	-0.001693	-0.001143	-0.001253	-0.001021	-0.000984	-0.00103
$Cl^- \cdots SPF_3$	-0.009265	-0.009089	-0.004157	-0.000728	-0.001425	-0.000661	-0.000695	-0.000572
$Br^- \cdots SPF_3$	-0.006953	-0.006892	-0.002032	-0.000979	-0.001621	-0.000763	-0.000774	-0.00067
$Cl^- \cdots SePF_3$	-0.020737	-0.020351	-0.015891	-0.00054	-0.001617	-0.000787	-0.00081	-0.000692
$Br^- \cdots SePF_3$	-0.016236	-0.016003	-0.011275	-0.00075	-0.001853	-0.000923	-0.000928	-0.000826
$NH_3 \cdots SPF_3$	-0.000547	-0.000458	0.000233	-0.001012	-0.001067	-0.000912	-0.000887	-0.000933
$NH_3 \cdots SePF_3$	-0.002555	-0.002365	-0.001408	-0.001222	-0.001368	-0.001083	-0.001043	-0.001093
Pnictogen Bonds								
$Cl^- \cdots PF_3$	-0.031743	-0.031474	-0.029899	-0.001017	-0.001902	-0.001094	-0.001091	-0.000992
$Br^- \cdots PF_3$	-0.02294	-0.022721	-0.020765	-0.001271	-0.002161	-0.001173	-0.001134	-0.001065
$Cl^- \cdots AsF_3$	-0.051902	-0.051979	-0.050447	-0.000975	-0.002011	-0.001193	-0.001194	-0.001103
$Br^- \cdots AsF_3$	-0.041353	-0.041477	-0.03953	-0.00118	-0.002323	-0.001331	-0.001266	-0.001249
$NH_3 \cdots PF_3$	-0.005978	-0.005613	-0.004949	-0.001818	-0.001861	-0.00166	-0.001645	-0.00168
$NH_3 \cdots AsF_3$	-0.012855	-0.01251	-0.011792	-0.002131	-0.002214	-0.001893	-0.001893	-0.001911

Table S18: M11, M11[HF], M11[LDA] interaction energy results (in hartree) for the B30 dataset.

	M11	M11[HF]	M11[LDA]
Halogen Bonds			
$Cl^- \cdots ClF$	-0.072763	-0.067573	-0.069949
$Br^- \cdots ClF$	-0.06988	-0.065413	-0.066813
$Cl^- \cdots BrF$	-0.074099	-0.069824	-0.072203
$Br^- \cdots BrF$	-0.069429	-0.06575	-0.06747
$NH_3 \cdots ClF$	-0.017613	-0.015042	-0.014906
$NH_3 \cdots BrF$	-0.022849	-0.020461	-0.021128
Chalcogen Bonds			
$Cl^- \cdots SF_2$	-0.050346	-0.047752	-0.048043
$Br^- \cdots SF_2$	-0.04089	-0.038817	-0.038326
$Cl^- \cdots SeF_2$	-0.064057	-0.062023	-0.062255
$Br^- \cdots SeF_2$	-0.05538	-0.053782	-0.053501
$NH_3 \cdots SF_2$	-0.012747	-0.01192	-0.010616
$NH_3 \cdots SeF_2$	-0.019987	-0.019162	-0.01854
$Cl^- \cdots SCF_2$	-0.013787	-0.013139	-0.009262
$Br^- \cdots SCF_2$	-0.011043	-0.010715	-0.006348
$Cl^- \cdots SeCF_2$	-0.018249	-0.017347	-0.014395
$Br^- \cdots SeCF_2$	-0.014778	-0.014323	-0.010712
$NH_3 \cdots SCF_2$	-0.001917	-0.001784	-0.001037
$NH_3 \cdots SeCF_2$	-0.003206	-0.003024	-0.002087
$Cl^- \cdots SPF_3$	-0.012695	-0.011602	-0.007525
$Br^- \cdots SPF_3$	-0.009914	-0.009173	-0.005099
$Cl^- \cdots SePF_3$	-0.022366	-0.020979	-0.01785
$Br^- \cdots SePF_3$	-0.017915	-0.017055	-0.013362
$NH_3 \cdots SPF_3$	-0.001553	-0.001296	-0.000429
$NH_3 \cdots SePF_3$	-0.00348	-0.00313	-0.001915
Pnictogen Bonds			
$Cl^- \cdots PF_3$	-0.034808	-0.033477	-0.032379
$Br^- \cdots PF_3$	-0.025771	-0.024999	-0.02328
$Cl^- \cdots AsF_3$	-0.054588	-0.053662	-0.052534
$Br^- \cdots AsF_3$	-0.043621	-0.04334	-0.041727
$NH_3 \cdots PF_3$	-0.008921	-0.008614	-0.007242
$NH_3 \cdots AsF_3$	-0.016	-0.015818	-0.01441

Table S19: MN15, MN15[HF], MN15[LDA] interaction energy results (in hartree) for the B30 dataset.

	MN15	MN15[HF]	MN15[LDA]
Halogen Bonds			
$Cl^- \cdots ClF$	-0.072523	-0.069216	-0.070773
$Br^- \cdots ClF$	-0.070911	-0.067701	-0.069815
$Cl^- \cdots BrF$	-0.07653	-0.073893	-0.074553
$Br^- \cdots BrF$	-0.072221	-0.069593	-0.070797
$NH_3 \cdots ClF$	-0.019529	-0.016995	-0.017325
$NH_3 \cdots BrF$	-0.026747	-0.024315	-0.024787
Chalcogen Bonds			
$Cl^- \cdots SF_2$	-0.050726	-0.048964	-0.049342
$Br^- \cdots SF_2$	-0.042054	-0.040052	-0.040938
$Cl^- \cdots SeF_2$	-0.06629	-0.064761	-0.065036
$Br^- \cdots SeF_2$	-0.057802	-0.056118	-0.056921
$NH_3 \cdots SF_2$	-0.01343	-0.011889	-0.012225
$NH_3 \cdots SeF_2$	-0.021987	-0.020324	-0.020972
$Cl^- \cdots SCF_2$	-0.015795	-0.014297	-0.013868
$Br^- \cdots SCF_2$	-0.013244	-0.011681	-0.01154
$Cl^- \cdots SeCF_2$	-0.023035	-0.021796	-0.0212
$Br^- \cdots SeCF_2$	-0.019377	-0.017982	-0.017791
$NH_3 \cdots SCF_2$	-0.002366	-0.001981	-0.002136
$NH_3 \cdots SeCF_2$	-0.004232	-0.003668	-0.003958
$Cl^- \cdots SPF_3$	-0.012287	-0.010815	-0.009752
$Br^- \cdots SPF_3$	-0.009888	-0.008469	-0.007614
$Cl^- \cdots SePF_3$	-0.025038	-0.023086	-0.022747
$Br^- \cdots SePF_3$	-0.020432	-0.018465	-0.018319
$NH_3 \cdots SPF_3$	-0.002041	-0.001492	-0.001658
$NH_3 \cdots SePF_3$	-0.004537	-0.003722	-0.004012
Pnictogen Bonds			
$Cl^- \cdots PF_3$	-0.035203	-0.033738	-0.03382
$Br^- \cdots PF_3$	-0.026573	-0.024915	-0.025354
$Cl^- \cdots AsF_3$	-0.055105	-0.05381	-0.054212
$Br^- \cdots AsF_3$	-0.045286	-0.043406	-0.044179
$NH_3 \cdots PF_3$	-0.00907	-0.007904	-0.008435
$NH_3 \cdots AsF_3$	-0.01593	-0.014743	-0.015363

Table S20: PBE, PBE[HF], PBE[LDA], Disp, and CCSD(T) result (in kcal/mol) with respect to $H_3N\cdots ClF$ distance (r, Å) dissociation curve in Figure. 4 (b).

r	CCSD(T)	PBE	PBE[HF]	PBE[LDA]	Disp3
1.32	167.06	161.41	166.35	161.61	-0.28
1.42	100.12	95.96	100.38	96.14	-0.28
1.52	58.06	54.31	58.53	54.47	-0.29
1.62	31.2	27.19	31.45	27.34	-0.31
1.72	13.83	9.3	13.73	9.44	-0.35
1.82	2.61	-2.41	2.25	-2.28	-0.4
1.92	-4.45	-9.82	-4.92	-9.7	-0.46
2.02	-8.68	-14.19	-9.07	-14.07	-0.53
2.12	-10.95	-16.43	-11.15	-16.32	-0.58
2.22	-11.92	-17.21	-11.86	-17.1	-0.62
2.32	-12.05	-17.03	-11.73	-16.92	-0.63
2.42	-11.67	-16.25	-11.1	-16.14	-0.62
2.52	-11	-15.13	-10.23	-15.02	-0.61
2.62	-10.17	-13.83	-9.27	-13.72	-0.59
2.72	-9.3	-12.48	-8.3	-12.37	-0.58
2.82	-8.42	-11.15	-7.38	-11.05	-0.58
2.92	-7.58	-9.89	-6.54	-9.79	-0.57
3.02	-6.8	-8.73	-5.78	-8.63	-0.56
3.12	-6.08	-7.67	-5.1	-7.58	-0.54
3.22	-5.43	-6.72	-4.5	-6.64	-0.51
3.32	-4.85	-5.88	-3.98	-5.81	-0.47
3.42	-4.34	-5.15	-3.52	-5.08	-0.43
3.52	-3.88	-4.5	-3.13	-4.44	-0.39
3.62	-3.47	-3.94	-2.78	-3.89	-0.35
3.72	-3.11	-3.45	-2.48	-3.41	-0.32
3.82	-2.79	-3.03	-2.21	-2.99	-0.29
3.92	-2.51	-2.67	-1.98	-2.63	-0.26
4.02	-2.26	-2.35	-1.78	-2.32	-0.23
4.12	-2.04	-2.08	-1.6	-2.05	-0.21
4.22	-1.84	-1.84	-1.44	-1.82	-0.19
4.32	-1.67	-1.63	-1.3	-1.62	-0.17
4.42	-1.51	-1.45	-1.18	-1.44	-0.15
4.52	-1.37	-1.29	-1.06	-1.29	-0.13
4.62	-1.25	-1.16	-0.97	-1.15	-0.12
4.72	-1.15	-1.04	-0.88	-1.04	-0.1
4.82	-1.05	-0.94	-0.8	-0.93	-0.09
4.92	-0.97	-0.85	-0.74	-0.85	-0.08
5.02	-0.89	-0.77	-0.68	-0.77	-0.07

3. S22 Dataset

Here, we elucidate the effect of density error on more classic examples of weak non-covalent interactions. The S22 dataset includes 7 hydrogen bonds (HB), 8 van der Waals dominant complexes (vdW), and 7 mixed complexes (Mix).[3] In Table S21 SC-DFT shows a relatively large error yet small functional dependency. The dispersion correction is suitable for substantially improving SC-DFT interaction energy. This is because the silico-empirical parameters of the DFT-D(D3, D3(BJ), XDM) correction are determined, in reference to CCSD(T)/CBS,[3,4] for their fitting datasets including the S22.[5–8]

The density correction with HF density alone does not show any noticeable improvement over SC-DFT. Based on the classification in the main text, weak non-covalent interactions in the S22 dataset are *normal*. However, HF-DFT-D statistics (whether it is D3, or D3(BJ), or XDM) is as accurate as its SC-DFT-D. SCAN has been reported to perform better than other approximations for weak non-covalent interactions, because it can capture the long-distance portion of the van der Waals interaction relatively well.[9] SCAN and HF-SCAN result in same energies for the S22 dataset and SCAN functional is normal for the overall S22 dataset. In the S22 dataset, the formic acid dimer is the only abnormal case for some GGAs in Table S22.

Computational Details

All HF, DFT (SVWN,[10,11] BP86,[12,13] PBE,[14] PW86PBE,[15] PBE0,[16] M06,[17] M11,[18] MN15,[19] CAM-B3LYP,[20] LC-ωPBE,[21] BLYP,[13,22] B3LYP,[23] BHandHLYP[24]) HF-DFT, results are performed with Gaussian16 package[25] and for SCAN,[9] CCSD(T) are performed in TURBOMOLE 7.2.1 package.[26] In addition, dispersion correction D3 and D3(BJ) calculations are performed with the latest version of dftd3 program,[5,6] and XDM calculations are performed with postg program.[7,8] Dunning's augmented correlation-consistent quadruple zeta basis set (aug-cc-pVQZ)[27] is used for the calculations in Fig. S1, and Table S1. For

Table S21 and Table S22, aug-cc-pVTZ basis set[28,29] was used for almost all calculation. Especially, for SCAN results in Table S21, Ahlrichs' newer redefinition quadruple zeta (def2-QZVP) basis set[30] is used. To perform every calculation at their given orientation, molecular symmetry within the calculation was not considered. For the energy convergence criteria, SCF=tight option for the Gaussian16 while scfconv=7 and denconv=1.0d-6 are used for TURBOMOLE.

Table S21: DFT, HF-DFT with Disp3, Disp3BJ, XDM dispersion correction results (in kcal/mol) for the S22 dataset (HB denotes hydrogen bond, vdW denotes systems with pre dominant dispersion contribution, and mix denotes the mixed complexes). all calculated in aug-cc-pVTZ level (except SCAN which is calculated in def2-QZVP), which is used to fit XDM correction. Structures and reference CCSD(T)/CBS energies are from Ref.[3,4]

	MAE								ME							
	HB		vdW		Mix		S22		HB		vdW		Mix		S22	
DFT	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
SVWN	5.67	3.75	0.78	0.74	1.32	1.32	2.51	1.88	-5.67	-3.75	-0.78	-0.52	-1.32	-1.32	-2.51	-1.81
BP86	2.15	2.85	6.15	6.15	3.08	3.08	3.9	4.12	2.15	2.85	6.15	6.15	3.08	3.08	3.9	4.12
PBE	0.99	1.32	4.36	4.36	1.86	1.86	2.49	2.6	0.99	1.32	4.36	4.36	1.86	1.86	2.49	2.6
PW86PBE	1.41	2.05	4.5	4.5	2.07	2.07	2.74	2.95	1.41	2.05	4.5	4.5	2.07	2.07	2.74	2.95
BLYP	3.09	3.09	7.1	7.1	3.6	3.6	4.71	4.71	3.09	3.09	7.1	7.1	3.6	3.6	4.71	4.71
TPSS	1.78	2.1	5.59	5.59	2.57	2.57	3.42	3.52	1.78	2.1	5.59	5.59	2.57	2.57	3.42	3.52
revTPSS	1.84	2.15	4.75	4.75	2.21	2.21	3.02	3.11	1.84	2.15	4.75	4.75	2.21	2.21	3.02	3.11
SCAN	0.61	0.61	1.41	1.41	0.7	0.7	0.93	0.93	-0.38	-0.38	1.41	1.41	0.64	0.64	0.59	0.59
B3LYP	1.89	1.89	5.93	5.93	2.79	2.79	3.65	3.65	1.89	1.89	5.93	5.93	2.79	2.79	3.65	3.65
PBE0	0.8	0.8	4.16	4.16	1.65	1.65	2.29	2.29	0.68	0.68	4.16	4.16	1.65	1.65	2.25	2.25
M06	0.6	0.6	0.75	0.75	0.57	0.57	0.64	0.64	0.54	0.54	0.75	0.75	0.57	0.57	0.63	0.63
HH	0.98	0.98	4.93	4.93	2.04	2.04	2.75	2.75	0.85	0.85	4.93	4.93	2.04	2.04	2.71	2.71
M06-2X	0.53	0.53	0.22	0.22	0.28	0.28	0.34	0.34	0.25	0.25	-0.17	-0.17	-0.03	-0.03	0.01	0.01
CAM-B3LYP	0.82	0.82	4.36	4.36	1.82	1.82	2.42	2.42	0.52	0.52	4.36	4.36	1.82	1.82	2.33	2.33
LC-wPBE	1.86	1.86	4.27	4.27	1.85	1.85	2.73	2.73	1.86	1.86	4.27	4.27	1.85	1.85	2.73	2.73
M11	0.69	0.69	0.29	0.29	0.33	0.33	0.43	0.43	0.45	0.45	0.21	0.21	-0.01	-0.01	0.22	0.22
MN15	0.74	0.74	0.63	0.63	0.33	0.33	0.57	0.57	0.7	0.7	-0.63	-0.63	-0.3	-0.3	-0.1	-0.1
	HB		vdW		Mix		S22		HB		vdW		Mix		S22	
DFT-D3	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
BP86	0.91	0.81	0.95	0.95	0.45	0.45	0.78	0.75	-0.84	-0.14	-0.91	-0.91	-0.45	-0.45	-0.74	-0.52
PBE	0.67	0.7	0.5	0.5	0.22	0.22	0.46	0.48	-0.67	-0.34	0.32	0.32	-0.18	-0.18	-0.15	-0.05
PW86PBE	0.42	0.76	0.27	0.27	0.17	0.17	0.28	0.39	-0.42	0.23	0.1	0.1	-0.15	-0.15	-0.15	0.06
BLYP	0.23	0.23	0.44	0.44	0.15	0.15	0.28	0.28	-0.11	-0.11	-0.44	-0.44	-0.15	-0.15	-0.24	-0.24
TPSS	0.5	0.49	0.29	0.29	0.19	0.19	0.32	0.32	-0.47	-0.16	0.16	0.16	-0.13	-0.13	-0.13	-0.03
revTPSS	0.42	0.44	0.68	0.68	0.5	0.5	0.54	0.54	-0.42	-0.11	-0.68	-0.68	-0.5	-0.5	-0.54	-0.44
B3LYP	0.68	0.68	0.22	0.22	0.27	0.27	0.38	0.38	-0.68	-0.68	-0.04	-0.04	-0.27	-0.27	-0.32	-0.32
PBE0	0.99	0.99	0.36	0.36	0.4	0.4	0.57	0.57	-0.99	-0.99	0.2	0.2	-0.4	-0.4	-0.37	-0.37
M06	0.19	0.19	0.78	0.78	0.27	0.27	0.43	0.43	-0.04	-0.04	-0.78	-0.78	-0.26	-0.26	-0.38	-0.38
HH	1.19	1.19	0.5	0.5	0.39	0.39	0.68	0.68	-1.19	-1.19	0.28	0.28	-0.39	-0.39	-0.4	-0.4
M06-2X	0.36	0.36	0.61	0.61	0.33	0.33	0.44	0.44	0.02	0.02	-0.6	-0.6	-0.33	-0.33	-0.31	-0.31
CAM-B3LYP	1.27	1.27	0.44	0.44	0.32	0.32	0.67	0.67	-1.27	-1.27	0.27	0.27	-0.32	-0.32	-0.41	-0.41
LC-wPBE	0.25	0.25	0.13	0.13	0.42	0.42	0.26	0.26	-0.04	-0.04	-0.08	-0.08	-0.42	-0.42	-0.18	-0.18
	HB		vdW		Mix		S22		HB		vdW		Mix		S22	
DFT-D3(BJ)	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
BP86	0.69	0.83	0.91	0.91	0.21	0.21	0.62	0.66	-0.5	0.21	-0.75	-0.75	-0.14	-0.14	-0.48	-0.25
PBE	0.72	0.71	0.4	0.4	0.23	0.23	0.45	0.44	-0.72	-0.39	0.22	0.22	-0.15	-0.15	-0.2	-0.09
PW86PBE	0.41	0.74	0.28	0.28	0.17	0.17	0.29	0.39	-0.41	0.24	-0.04	-0.04	-0.11	-0.11	-0.18	0.02
BLYP	0.25	0.25	0.45	0.45	0.11	0.11	0.28	0.28	-0.04	-0.04	-0.39	-0.39	0.02	0.02	-0.15	-0.15
TPSS	0.43	0.43	0.31	0.31	0.15	0.15	0.3	0.3	-0.38	-0.07	0.17	0.17	-0.01	-0.01	-0.06	0.04
revTPSS	0.33	0.37	0.67	0.67	0.38	0.38	0.47	0.48	-0.32	-0.02	-0.67	-0.67	-0.38	-0.38	-0.47	-0.37
B3LYP	0.72	0.72	0.37	0.37	0.22	0.22	0.43	0.43	-0.7	-0.7	-0.36	-0.36	-0.22	-0.22	-0.43	-0.43
PBE0	0.92	0.92	0.23	0.23	0.32	0.32	0.48	0.48	-0.92	-0.92	0.07	0.07	-0.31	-0.31	-0.37	-0.37
HH	1.13	1.13	0.23	0.23	0.29	0.29	0.54	0.54	-1.13	-1.13	0.06	0.06	-0.29	-0.29	-0.43	-0.43
CAM-B3LYP	1.03	1.03	0.2	0.2	0.17	0.17	0.45	0.45	-1.03	-1.03	0.16	0.16	-0.16	-0.16	-0.32	-0.32
LC-wPBE	0.33	0.33	0.33	0.33	0.36	0.36	0.34	0.34	0.11	0.11	-0.32	-0.32	-0.32	-0.32	-0.18	-0.18
	HB		vdW		Mix		S22		HB		vdW		Mix		S22	
DFT-XDM	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF	SC	HF
PBE	0.3	0.44	0.86	0.86	0.31	0.31	0.51	0.55	-0.26	0.08	0.84	0.84	0.22	0.22	0.29	0.4
PW86PBE	0.26	0.75	0.45	0.45	0.22	0.22	0.32	0.47	-0.22	0.45	0.38	0.38	0.14	0.14	0.11	0.33
BLYP	0.32	0.32	0.18	0.18	0.13	0.13	0.21	0.21	-0.32	-0.32	-0.12	-0.12	0.07	0.07	-0.12	-0.12
B3LYP	0.46	0.46	0.17	0.17	0.15	0.15	0.26	0.26	-0.45	-0.45	0.15	0.15	0.08	0.08	-0.06	-0.06
PBE0	0.55	0.55	0.67	0.67	0.19	0.19	0.48	0.48	-0.55	-0.55	0.66	0.66	0.01	0.01	0.07	0.07
HH	0.89	0.89	0.3	0.3	0.17	0.17	0.45	0.45	-0.89	-0.89	0.27	0.27	-0.13	-0.13	-0.22	-0.22
CAM-B3LYP	0.85	0.85	0.41	0.41	0.13	0.13	0.46	0.46	-0.85	-0.85	0.41	0.41	0	0	-0.12	-0.12
LC-wPBE	0.39	0.39	0.23	0.23	0.21	0.21	0.28	0.28	0.12	0.12	0.14	0.14	-0.1	-0.1	0.06	0.06

Table S22: Density sensitivity (kcal/mol) of DFT calculations for the S22 dataset: ${}^{a}S^{PBE}$ was used to determine normal (N) and abnormal (A) classes shown here; above 2.0 kcal/mol for abnormal systems.

complex	^{a}	Density Sensitivity, S				
		PBE	PW86PBE	BLYP	B3LYP	PBE0
Hydrogen bonds (HB)						
Formic acid dimer (C_{2h})	A	2.2	2.4	1.2	1.6	0.4
Adenine thymine WC (C_1)	N	1.9	2.2	1.2	1.5	0.3
2-pyridoxine 2-aminopyridine (C_1)	N	1.8	2.0	1.1	1.3	0.3
Uracil dimer (C_{2h})	N	1.5	1.7	0.9	1.1	0.3
Formamide dimer (C_{2h})	N	1.4	1.6	0.9	1.1	0.2
$(H_2O)_2$ (C_s)	N	0.6	0.7	0.3	0.5	0.1
$(NH_3)_2$ (C_{2h})	N	0.4	0.5	0.2	0.3	0.1
Mixed complexes (Mix)						
Phenol dimer (C_1)	N	0.4	0.7	0.2	0.4	0.3
Benzene H_2O (C_s)	N	0.2	0.3	0.1	0.2	0.2
Indole benzene T-shape (C_1)	N	0.2	0.3	0.1	0.2	0.2
Benzene HCN (C_s)	N	0.1	0.2	0.1	0.1	0.1
Benzene NH_3 (C_s)	N	0.1	0.2	0.1	0.2	0.2
Benzene dimer (C_{2v})	N	0.1	0.2	0.1	0.2	0.2
Ethene ethine (C_{2v})	N	0.1	0.1	0.1	0.1	0.1
van der Waals dispersion (vdW)						
Adenine thymine stack (C_1)	N	0.7	1.2	0.4	0.8	0.6
Uracil dimer (C_2)	N	0.5	0.9	0.3	0.6	0.5
$(C_2H_4)_2$ (D_{2d})	N	0.1	0.3	0.1	0.2	0.2
Pyrazine dimer (C_s)	N	0.1	0.2	0.2	0.3	0.3
$(CH_4)_2$ (D_{3d})	N	0.1	0.2	0.2	0.2	0.1
Benzene dimer (C_{2h})	N	0.1	0.1	0.1	0.2	0.3
Benzene CH_4 (C_3)	N	0.1	0.1	0.1	0.1	0.1
Indole benzene (C_1)	N	0.0	0.2	0.2	0.3	0.4

Table S23: Reference CCSD(T)/CBS value (in kcal/mol) for the S22 dataset from Ref.[4]

	CCSD(T)/CBS
Hydrogen bonds	
$(NH_3)_2$ (C_{2h})	-3.133
$(H_2O)_2$ (C_s)	-4.989
Formic acid dimer (C_{2h})	-18.753
Formamide dimer (C_{2h})	-16.062
Uracil dimer (C_{2h})	-20.641
2-pyridoxine 2-aminopyridine (C_1)	-16.934
Adenine thymine WC (C_1)	-16.66
Mixed complexes	
Ethene ethine (C_{2v})	-1.496
Benzene H_2O (C_s)	-3.275
Benzene NH_3 (C_s)	-2.312
Benzene HCN (C_s)	-4.541
Benzene dimer (C_{2v})	-2.717
Indole benzene T-shape (C_1)	-5.627
Phenol dimer (C_1)	-7.097
van der Waals dispersion	
$(CH_4)_2$ (D_{3d})	-0.527
$(C_2H_4)_2$ (D_{2d})	-1.472
Benzene CH_4 (C_3)	-1.448
Benzene dimer (C_{2h})	-2.654
Pyrazine dimer (C_s)	-4.255
Uracil dimer (C_2)	-9.805
Indole benzene (C_1)	-4.524
Adenine thymine stack (C_1)	-11.73

Table S24: LDA, LDA[HF] interaction energy results (in hartree) for the S22 dataset.

	LDA	LDA[HF]
Hydrogen bonds		
$(NH_3)_2$ (C_{2h})	-0.008334	-0.007059
$(H_2O)_2$ (C_s)	-0.012811	-0.011093
Formic acid dimer (C_{2h})	-0.044222	-0.039161
Formamide dimer (C_{2h})	-0.035893	-0.032145
Uracil dimer (C_{2h})	-0.042953	-0.039195
2-pyridoxine 2-aminopyridine (C_1)	-0.037554	-0.03334
Adenine thymine WC (C_1)	-0.036377	-0.031745
Mixed complexes		
Ethene ethine (C_{2v})	-0.003891	-0.003582
Benzene H_2O (C_s)	-0.007509	-0.006655
Benzene NH_3 (C_s)	-0.005225	-0.004618
Benzene HCN (C_s)	-0.00986	-0.00923
Benzene dimer (C_{2v})	-0.00542	-0.004837
Indole benzene T-shape (C_1)	-0.010781	-0.009806
Phenol dimer (C_1)	-0.015205	-0.013246
van der Waals dispersion		
$(CH_4)_2$ (D_{3d})	-0.001423	-0.000882
$(C_2H_4)_2$ (D_{2d})	-0.004235	-0.003316
Benzene CH_4 (C_3)	-0.003542	-0.003103
Benzene dimer (C_{2h})	-0.004877	-0.004598
Pyrazine dimer (C_s)	-0.007889	-0.00747
Uracil dimer (C_2)	-0.017457	-0.014917
Indole benzene (C_1)	-0.007952	-0.007312
Adenine thymine stack (C_1)	-0.020622	-0.017308

Table S25: BP86, BP86[HF], BP86[LDA], Disp3, Disp3BJ interaction energy results (in hartree) for the S22 dataset.

	BP86	BP86[HF]	BP86[LDA]	Disp3	Disp3BJ
Hydrogen bonds					
$(NH_3)_2$ (C_{2h})	-0.003012	-0.002259	-0.002886	-0.001663	-0.001359
$(H_2O)_2$ (C_s)	-0.00658	-0.005446	-0.006461	-0.001338	-0.000941
Formic acid dimer (C_{2h})	-0.0277	-0.023623	-0.027514	-0.004413	-0.003791
Formamide dimer (C_{2h})	-0.021945	-0.019062	-0.021695	-0.004799	-0.004071
Uracil dimer (C_{2h})	-0.028058	-0.02506	-0.027769	-0.006092	-0.005534
2-pyridoxine 2-aminopyridine (C_1)	-0.022697	-0.019273	-0.022435	-0.007182	-0.006645
Adenine thymine WC (C_1)	-0.020932	-0.017175	-0.020608	-0.007856	-0.007136
Mixed complexes					
Ethene ethine (C_{2v})	-0.000808	-0.000552	-0.000689	-0.001983	-0.00174
Benzene H_2O (C_s)	-0.0016	-0.001056	-0.001431	-0.004339	-0.003553
Benzene NH_3 (C_s)	0.000126	0.000522	0.000302	-0.004357	-0.003749
Benzene HCN (C_s)	-0.002961	-0.002402	-0.002726	-0.005014	-0.004737
Benzene dimer (C_{2v})	0.001619	0.002127	0.001879	-0.006694	-0.006528
Indole benzene T-shape (C_1)	-0.001036	-0.000268	-0.000718	-0.009017	-0.008689
Phenol dimer (C_1)	-0.004156	-0.002911	-0.003863	-0.007918	-0.006919
van der Waals dispersion					
$(CH_4)_2$ (D_{3d})	0.001189	0.001402	0.001333	-0.001792	-0.001472
$(C_2H_4)_2$ (D_{2d})	0.001406	0.001898	0.0016	-0.004196	-0.003321
Benzene CH_4 (C_3)	0.001492	0.001817	0.001678	-0.004178	-0.003764
Benzene dimer (C_{2h})	0.005459	0.005734	0.005788	-0.01128	-0.011988
Pyrazine dimer (C_s)	0.00369	0.003961	0.004056	-0.011893	-0.011951
Uracil dimer (C_2)	-0.001006	0.000591	-0.000479	-0.017225	-0.016101
Indole benzene (C_1)	0.006447	0.006977	0.006885	-0.016	-0.016871
Adenine thymine stack (C_1)	0.001695	0.003904	0.002418	-0.023463	-0.022544

Table S26: PBE, PBE[HF], PBE[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	PBE	PBE[HF]	PBE[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.00451	-0.003797	-0.004382	-0.000912	-0.000933	-0.000669	-0.000618	-0.000683
$(H_2O)_2$ (C_s)	-0.007904	-0.006838	-0.007793	-0.000705	-0.00066	-0.000451	-0.000405	-0.000458
Formic acid dimer (C_{2h})	-0.029321	-0.025624	-0.029138	-0.002203	-0.00245	-0.001693	-0.001627	-0.001719
Formamide dimer (C_{2h})	-0.023742	-0.021282	-0.023476	-0.002508	-0.002619	-0.001891	-0.001831	-0.001923
Uracil dimer (C_{2h})	-0.03002	-0.02735	-0.029734	-0.003471	-0.003563	-0.002633	-0.002582	-0.002682
2-pyridoxine 2-aminopyridine (C_1)	-0.024889	-0.021821	-0.024624	-0.004163	-0.004267	-0.003178	-0.003169	-0.00324
Adenine thymine WC (C_1)	-0.02341	-0.020049	-0.023082	-0.004538	-0.004575	-0.003448	-0.003401	-0.003522
Mixed complexes								
Ethene ethine (C_{2v})	-0.001994	-0.001768	-0.001892	-0.001132	-0.001094	-0.000919	-0.000921	-0.00093
Benzene H_2O (C_s)	-0.003358	-0.002916	-0.003196	-0.002485	-0.002257	-0.001702	-0.001597	-0.001735
Benzene NH_3 (C_s)	-0.001611	-0.001292	-0.001442	-0.002549	-0.002373	-0.001938	-0.001863	-0.001981
Benzene HCN (C_s)	-0.004774	-0.004337	-0.004537	-0.002622	-0.002903	-0.002173	-0.002169	-0.002206
Benzene dimer (C_{2v})	-0.000466	-0.000061	-0.000209	-0.004	-0.004046	-0.003499	-0.003557	-0.003575
Indole benzene T-shape (C_1)	-0.003659	-0.003067	-0.00334	-0.005401	-0.005434	-0.004529	-0.004582	-0.004631
Phenol dimer (C_1)	-0.00651	-0.005503	-0.006182	-0.004553	-0.00438	-0.003589	-0.003564	-0.003661
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	-0.000196	0.000034	-0.000093	-0.001132	-0.000956	-0.000799	-0.000763	-0.000823
$(C_2H_4)_2$ (D_{2d})	-0.000604	-0.000176	-0.000391	-0.002094	-0.002099	-0.001634	-0.001635	-0.001671
Benzene CH_4 (C_3)	-0.000202	0.000058	-0.00002	-0.002422	-0.002362	-0.002049	-0.00201	-0.002101
Benzene dimer (C_{2h})	0.002668	0.002908	0.003027	-0.006706	-0.007088	-0.006299	-0.006354	-0.00644
Pyrazine dimer (C_s)	0.000801	0.00106	0.001214	-0.006727	-0.00708	-0.005958	-0.005928	-0.006082
Uracil dimer (C_2)	-0.005	-0.003599	-0.004437	-0.009863	-0.009662	-0.007956	-0.007741	-0.00813
Indole benzene (C_1)	0.003058	0.003494	0.003546	-0.009316	-0.009959	-0.008812	-0.008862	-0.009016
Adenine thymine stack (C_1)	-0.00299	-0.001054	-0.002197	-0.01327	-0.013527	-0.011386	-0.011136	-0.011658

Table S27: PW86PBE, PW86PBE[HF], PW86PBE[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	PW86PBE	PW86PBE[HF]	PW86PBE[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.004274	-0.003474	-0.004165	-0.001014	-0.00097	-0.000898	-0.000856	-0.000915
$(H_2O)_2$ (C_s)	-0.007665	-0.006497	-0.007569	-0.000792	-0.000676	-0.000665	-0.000626	-0.000675
Formic acid dimer (C_{2h})	-0.028152	-0.024499	-0.027927	-0.002479	-0.002559	-0.002379	-0.002304	-0.002414
Formamide dimer (C_{2h})	-0.023157	-0.020538	-0.022875	-0.002801	-0.002767	-0.002506	-0.002413	-0.002543
Uracil dimer (C_{2h})	-0.029318	-0.026492	-0.028997	-0.003809	-0.003806	-0.003315	-0.003188	-0.00335
2-pyridoxine 2-aminopyridine (C_1)	-0.024017	-0.020781	-0.023714	-0.004544	-0.004576	-0.003983	-0.003854	-0.004032
Adenine thymine WC (C_1)	-0.022593	-0.019014	-0.022247	-0.004946	-0.004911	-0.004361	-0.004186	-0.004413
Mixed complexes								
Ethene ethine (C_{2v})	-0.00176	-0.001465	-0.001663	-0.001235	-0.001185	-0.001082	-0.001093	-0.001089
Benzene H_2O (C_s)	-0.003025	-0.002439	-0.002878	-0.002712	-0.00242	-0.002125	-0.002124	-0.002141
Benzene NH_3 (C_s)	-0.00133	-0.000904	-0.001179	-0.002772	-0.002566	-0.002314	-0.002325	-0.002337
Benzene HCN (C_s)	-0.004317	-0.003736	-0.004049	-0.002943	-0.003129	-0.002613	-0.00266	-0.002634
Benzene dimer (C_{2v})	-0.000167	0.000367	0.000096	-0.004348	-0.004425	-0.003962	-0.004038	-0.004007
Indole benzene T-shape (C_1)	-0.00313	-0.002341	-0.002801	-0.005855	-0.005915	-0.005227	-0.005283	-0.005289
Phenol dimer (C_1)	-0.006276	-0.005041	-0.005996	-0.004965	-0.004739	-0.004267	-0.004203	-0.00431
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	0.000102	0.000353	0.000194	-0.001197	-0.001032	-0.000999	-0.00096	-0.001026
$(C_2H_4)_2$ (D_{2d})	-0.000316	0.000207	-0.000148	-0.002328	-0.002249	-0.001961	-0.001956	-0.001996
Benzene CH_4 (C_3)	0.000015	0.000353	0.000182	-0.002635	-0.002568	-0.002459	-0.002464	-0.00249
Benzene dimer (C_{2h})	0.002792	0.003201	0.003078	-0.007247	-0.007845	-0.007219	-0.007337	-0.007309
Pyrazine dimer (C_s)	0.00099	0.001417	0.001306	-0.007332	-0.007782	-0.006916	-0.006938	-0.007
Uracil dimer (C_2)	-0.00465	-0.002938	-0.004226	-0.010742	-0.010583	-0.009371	-0.009147	-0.009481
Indole benzene (C_1)	0.003121	0.003811	0.003539	-0.010114	-0.011003	-0.010145	-0.010259	-0.010279
Adenine thymine stack (C_1)	-0.00277	-0.000429	-0.002077	-0.014492	-0.014796	-0.013353	-0.013117	-0.01356

Table S28: BLYP, BLYP[HF], BLYP[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	BLYP	BLYP[HF]	BLYP[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.002861	-0.002278	-0.002769	-0.00178	-0.001714	-0.002161	-0.002005	-0.00219
$(H_2O)_2$ (C_s)	-0.006417	-0.005548	-0.006356	-0.001441	-0.001247	-0.001679	-0.001537	-0.0017
Formic acid dimer (C_{2h})	-0.025141	-0.022141	-0.02497	-0.004767	-0.004781	-0.005745	-0.005419	-0.005801
Formamide dimer (C_{2h})	-0.020175	-0.018148	-0.019968	-0.005171	-0.004948	-0.005629	-0.005245	-0.005676
Uracil dimer (C_{2h})	-0.026454	-0.024214	-0.02627	-0.00648	-0.006415	-0.006569	-0.006121	-0.006579
2-pyridoxine 2-aminopyridine (C_1)	-0.020497	-0.017835	-0.0203	-0.007635	-0.007612	-0.00777	-0.00721	-0.007776
Adenine thymine WC (C_1)	-0.018846	-0.015952	-0.018624	-0.008363	-0.008142	-0.008472	-0.007808	-0.008475
Mixed complexes								
Ethene ethine (C_{2v})	-0.000655	-0.00042	-0.000603	-0.00212	-0.001952	-0.002027	-0.002006	-0.001961
Benzene H_2O (C_s)	-0.000943	-0.000568	-0.000839	-0.004612	-0.004114	-0.004176	-0.004219	-0.004079
Benzene NH_3 (C_s)	0.000664	0.000955	0.000786	-0.004638	-0.0042	-0.004252	-0.004291	-0.004156
Benzene HCN (C_s)	-0.001904	-0.00139	-0.001672	-0.005419	-0.005444	-0.005312	-0.005359	-0.005207
Benzene dimer (C_{2v})	0.002548	0.003019	0.002777	-0.0071	-0.007038	-0.006746	-0.006796	-0.006615
Indole benzene T-shape (C_1)	0.000533	0.00118	0.000808	-0.00953	-0.00951	-0.009026	-0.009019	-0.008928
Phenol dimer (C_1)	-0.003193	-0.002359	-0.002926	-0.008471	-0.007713	-0.00784	-0.007507	-0.007752
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	0.000991	0.001108	0.001073	-0.001881	-0.001646	-0.001677	-0.0015	-0.001693
$(C_2H_4)_2$ (D_{2d})	0.001615	0.001956	0.00179	-0.004622	-0.003881	-0.004023	-0.00393	-0.004007
Benzene CH_4 (C_3)	0.001942	0.002219	0.002105	-0.004477	-0.004136	-0.004386	-0.004334	-0.004286
Benzene dimer (C_{2h})	0.007198	0.007764	0.007476	-0.011969	-0.01265	-0.012076	-0.012235	-0.01191
Pyrazine dimer (C_s)	0.005437	0.005948	0.005717	-0.012711	-0.012964	-0.012113	-0.011957	-0.012034
Uracil dimer (C_2)	0.000943	0.002103	0.001323	-0.018351	-0.017616	-0.016415	-0.015607	-0.016382
Indole benzene (C_1)	0.009141	0.009947	0.009581	-0.017035	-0.017952	-0.017407	-0.017531	-0.01726
Adenine thymine stack (C_1)	0.005263	0.007024	0.006001	-0.02508	-0.024749	-0.023969	-0.023084	-0.02412

Table S29: TPSS, TPSS[HF], TPSS[LDA], Disp3, Disp3BJ interaction energy results (in hartree) for the S22 dataset.

	TPSS	TPSS[HF]	TPSS[LDA]	Disp3	Disp3BJ
Hydrogen bonds					
$(NH_3)_2$ (C_{2h})	-0.003583	-0.003063	-0.003345	-0.001243	-0.001155
$(H_2O)_2$ (C_s)	-0.007136	-0.006226	-0.00696	-0.000981	-0.000812
Formic acid dimer (C_{2h})	-0.0285	-0.024987	-0.028364	-0.0032	-0.003111
Formamide dimer (C_{2h})	-0.022509	-0.020278	-0.022242	-0.003534	-0.003332
Uracil dimer (C_{2h})	-0.028625	-0.026302	-0.028368	-0.004646	-0.004515
2-pyridoxine 2-aminopyridine (C_1)	-0.023156	-0.020497	-0.022873	-0.005525	-0.005416
Adenine thymine WC (C_1)	-0.021464	-0.018638	-0.021061	-0.006047	-0.005809
Mixed complexes					
Ethene ethine (C_{2v})	-0.001448	-0.001321	-0.001271	-0.00152	-0.001405
Benzene H_2O (C_s)	-0.002345	-0.002079	-0.002089	-0.00333	-0.002888
Benzene NH_3 (C_s)	-0.000644	-0.00047	-0.00036	-0.003369	-0.003036
Benzene HCN (C_s)	-0.00377	-0.003516	-0.00352	-0.003674	-0.003767
Benzene dimer (C_{2v})	0.000742	0.000979	0.001115	-0.005205	-0.005209
Indole benzene T-shape (C_1)	-0.002011	-0.001643	-0.001556	-0.007038	-0.006972
Phenol dimer (C_1)	-0.004943	-0.004188	-0.004523	-0.006079	-0.005592
van der Waals dispersion					
$(CH_4)_2$ (D_{3d})	0.000204	0.000357	0.000535	-0.001454	-0.001213
$(C_2H_4)_2$ (D_{2d})	0.000519	0.000775	0.000999	-0.003063	-0.002696
Benzene CH_4 (C_3)	0.000713	0.000857	0.001021	-0.003219	-0.003029
Benzene dimer (C_{2h})	0.004618	0.004523	0.005152	-0.008809	-0.009334
Pyrazine dimer (C_s)	0.00287	0.002782	0.003472	-0.009107	-0.009326
Uracil dimer (C_2)	-0.002109	-0.001158	-0.001235	-0.013238	-0.012658
Indole benzene (C_1)	0.005706	0.005657	0.006347	-0.012377	-0.013126
Adenine thymine stack (C_1)	0.00071	0.001912	0.001725	-0.017928	-0.017712

Table S30: revTPSS, revTPSS[HF], revTPSS[LDA] interaction energy results (in hartree) for the S22 dataset.

	revTPSS	revTPSS[HF]	revTPSS[LDA]
Hydrogen bonds			
$(NH_3)_2$ (C_{2h})	-0.003776	-0.003247	-0.003572
$(H_2O)_2$ (C_s)	-0.00719	-0.006277	-0.007045
Formic acid dimer (C_{2h})	-0.028263	-0.024839	-0.02814
Formamide dimer (C_{2h})	-0.022562	-0.020395	-0.022309
Uracil dimer (C_{2h})	-0.028407	-0.026176	-0.028145
2-pyridoxine 2-aminopyridine (C_1)	-0.022864	-0.020343	-0.022582
Adenine thymine WC (C_1)	-0.021246	-0.018511	-0.020891
Mixed complexes			
Ethene ethine (C_{2v})	-0.001508	-0.001388	-0.001362
Benzene H_2O (C_s)	-0.002846	-0.00253	-0.002678
Benzene NH_3 (C_s)	-0.001099	-0.000918	-0.000903
Benzene HCN (C_s)	-0.004379	-0.004138	-0.004202
Benzene dimer (C_{2v})	0.000096	0.000287	0.000363
Indole benzene T-shape (C_1)	-0.003017	-0.002672	-0.002713
Phenol dimer (C_1)	-0.005712	-0.004916	-0.005428
van der Waals dispersion			
$(CH_4)_2$ (D_{3d})	0.000181	0.000317	0.00046
$(C_2H_4)_2$ (D_{2d})	0.000183	0.000417	0.000527
Benzene CH_4 (C_3)	0.000294	0.000404	0.000512
Benzene dimer (C_{2h})	0.003331	0.003082	0.003689
Pyrazine dimer (C_s)	0.001446	0.001219	0.001855
Uracil dimer (C_2)	-0.004097	-0.003042	-0.003568
Indole benzene (C_1)	0.003701	0.003506	0.004116
Adenine thymine stack (C_1)	-0.002521	-0.001235	-0.001903

Table S31: SCAN, SCAN[HF], SCAN[LDA] interaction energy results (in hartree) for the S22 dataset.

	SCAN	SCAN[HF]	SCAN[LDA]
Hydrogen bonds			
$(NH_3)_2$ (C_{2h})	-0.005128	0.004568	-0.004858
$(H_2O)_2$ (C_s)	-0.008934	0.008034	-0.00873
Formic acid dimer (C_{2h})	-0.033354	0.030167	-0.033188
Formamide dimer (C_{2h})	-0.026515	0.024263	-0.026292
Uracil dimer (C_{2h})	-0.032698	0.030503	-0.0325
2-pyridoxine 2-aminopyridine (C_1)	-0.026918	0.024435	-0.026764
Adenine thymine WC (C_1)	-0.025516	0.022732	-0.025294
Mixed complexes			
Ethene ethine (C_{2v})	-0.002186	0.002056	-0.002096
Benzene H_2O (C_s)	-0.005534	0.005053	-0.005428
Benzene NH_3 (C_s)	-0.003275	0.003016	-0.003174
Benzene HCN (C_s)	-0.006492	0.006285	-0.006336
Benzene dimer (C_{2v})	-0.002461	0.002368	-0.002325
Indole benzene T-shape (C_1)	-0.00647	0.006162	-0.006293
Phenol dimer (C_1)	-0.009572	0.008764	-0.009307
van der Waals dispersion			
$(CH_4)_2$ (D_{3d})	-0.000567	0.000396	-0.000448
$(C_2H_4)_2$ (D_{2d})	-0.001643	0.001357	-0.001445
Benzene CH_4 (C_3)	-0.001404	0.001269	-0.001301
Benzene dimer (C_{2h})	-0.0018	0.002013	-0.001601
Pyrazine dimer (C_s)	-0.004312	0.004573	-0.004075
Uracil dimer (C_2)	-0.01296	0.011726	-0.012695
Indole benzene (C_1)	-0.003366	0.003477	-0.003081
Adenine thymine stack (C_1)	-0.014066	0.012646	-0.013612

Table S32: B3LYP, B3LYP[HF], B3LYP[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	B3LYP	B3LYP[HF]	B3LYP[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.003508	-0.003117	-0.003218	-0.001461	-0.001414	-0.001412	-0.001336	-0.001462
$(H_2O)_2$ (C_s)	-0.007208	-0.006615	-0.00689	-0.001179	-0.001018	-0.001053	-0.00098	-0.001089
Formic acid dimer (C_{2h})	-0.028016	-0.025908	-0.027331	-0.003707	-0.003913	-0.003695	-0.003569	-0.00378
Formamide dimer (C_{2h})	-0.022579	-0.021106	-0.021975	-0.0041	-0.004081	-0.00378	-0.003653	-0.003879
Uracil dimer (C_{2h})	-0.02905	-0.027499	-0.028476	-0.005301	-0.005359	-0.004659	-0.004527	-0.004772
2-pyridoxine 2-aminopyridine (C_1)	-0.022367	-0.020543	-0.021743	-0.006225	-0.006373	-0.005537	-0.005414	-0.005671
Adenine thymine WC (C_1)	-0.021001	-0.01902	-0.020306	-0.006741	-0.006823	-0.006006	-0.005828	-0.006164
Mixed complexes								
Ethene ethine (C_{2v})	-0.001179	-0.001045	-0.001078	-0.001687	-0.001636	-0.001543	-0.001548	-0.001548
Benzene H_2O (C_s)	-0.00207	-0.001828	-0.001793	-0.003706	-0.003428	-0.003086	-0.00304	-0.003128
Benzene NH_3 (C_s)	-0.000317	-0.000136	-0.000079	-0.003755	-0.003528	-0.003263	-0.003246	-0.00331
Benzene HCN (C_s)	-0.003428	-0.003151	-0.003146	-0.004374	-0.004522	-0.003881	-0.003914	-0.003904
Benzene dimer (C_{2v})	0.001279	0.001543	0.001569	-0.005887	-0.00595	-0.005407	-0.0055	-0.005467
Indole benzene T-shape (C_1)	-0.001274	-0.000888	-0.000872	-0.007854	-0.008021	-0.007138	-0.007215	-0.007243
Phenol dimer (C_1)	-0.005054	-0.004473	-0.004503	-0.006788	-0.006486	-0.005921	-0.005846	-0.006029
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	0.000575	0.000681	0.00075	-0.001468	-0.001388	-0.001386	-0.001323	-0.001446
$(C_2H_4)_2$ (D_{2d})	0.000695	0.000936	0.001006	-0.003376	-0.003219	-0.002994	-0.002985	-0.003051
Benzene CH_4 (C_3)	0.001083	0.001242	0.0013	-0.003579	-0.003486	-0.00337	-0.003362	-0.003427
Benzene dimer (C_{2h})	0.005587	0.005838	0.005895	-0.009618	-0.010674	-0.009941	-0.010085	-0.01007
Pyrazine dimer (C_s)	0.00357	0.003789	0.003954	-0.00999	-0.01087	-0.009819	-0.009808	-0.00999
Uracil dimer (C_2)	-0.002135	-0.001314	-0.001404	-0.0146	-0.014762	-0.01309	-0.012781	-0.013414
Indole benzene (C_1)	0.00691	0.007291	0.007412	-0.013625	-0.015115	-0.014124	-0.014278	-0.014347
Adenine thymine stack (C_1)	0.001313	0.002446	0.002426	-0.01988	-0.020733	-0.018964	-0.018637	-0.01948

Table S33: PBE0, PBE0[HF], PBE0[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	PBE0	PBE0[HF]	PBE0[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.004396	-0.004023	-0.004051	-0.000938	-0.000833	-0.000637	-0.000609	-0.000675
$(H_2O)_2$ (C_s)	-0.007919	-0.007329	-0.007536	-0.000738	-0.00057	-0.000422	-0.000394	-0.000448
Formic acid dimer (C_{2h})	-0.030553	-0.028291	-0.029938	-0.002233	-0.002199	-0.001632	-0.001596	-0.001689
Formamide dimer (C_{2h})	-0.024655	-0.023135	-0.024045	-0.002555	-0.002408	-0.001838	-0.001812	-0.001904
Uracil dimer (C_{2h})	-0.031106	-0.029523	-0.030476	-0.003508	-0.003385	-0.0026	-0.002585	-0.002682
2-pyridoxine 2-aminopyridine (C_1)	-0.024973	-0.02317	-0.024303	-0.004162	-0.00408	-0.003154	-0.00318	-0.003244
Adenine thymine WC (C_1)	-0.023693	-0.021719	-0.02292	-0.004501	-0.004387	-0.003414	-0.003408	-0.003524
Mixed complexes								
Ethene ethine (C_{2v})	-0.002009	-0.001934	-0.001857	-0.001117	-0.001058	-0.000909	-0.000926	-0.000936
Benzene H_2O (C_s)	-0.00364	-0.00346	-0.003311	-0.002438	-0.002134	-0.001647	-0.001584	-0.001733
Benzene NH_3 (C_s)	-0.001774	-0.001662	-0.001495	-0.002529	-0.002293	-0.001899	-0.001863	-0.001992
Benzene HCN (C_s)	-0.005476	-0.005337	-0.005177	-0.002753	-0.002776	-0.002146	-0.002166	-0.002209
Benzene dimer (C_{2v})	-0.000711	-0.000588	-0.000399	-0.004039	-0.00402	-0.003516	-0.003598	-0.003621
Indole benzene T-shape (C_1)	-0.004139	-0.003924	-0.003696	-0.005371	-0.005348	-0.004543	-0.004626	-0.004679
Phenol dimer (C_1)	-0.006999	-0.006462	-0.006405	-0.004548	-0.004261	-0.00357	-0.003591	-0.00369
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	-0.000097	0.000035	0.000106	-0.001026	-0.000916	-0.000779	-0.000762	-0.000822
$(C_2H_4)_2$ (D_{2d})	-0.000621	-0.000407	-0.000272	-0.002066	-0.001975	-0.001614	-0.001636	-0.001673
Benzene CH_4 (C_3)	-0.000273	-0.000193	-0.00004	-0.002421	-0.002313	-0.002027	-0.002017	-0.002115
Benzene dimer (C_{2h})	0.002612	0.002456	0.002984	-0.006539	-0.007139	-0.006306	-0.006398	-0.006494
Pyrazine dimer (C_s)	0.000566	0.000413	0.00106	-0.006563	-0.007014	-0.005916	-0.005944	-0.006108
Uracil dimer (C_2)	-0.005893	-0.005174	-0.005054	-0.009652	-0.009515	-0.007863	-0.00776	-0.00816
Indole benzene (C_1)	0.002858	0.002745	0.003381	-0.009146	-0.009989	-0.00882	-0.008915	-0.009081
Adenine thymine stack (C_1)	-0.004121	-0.003226	-0.003019	-0.013074	-0.013301	-0.011288	-0.011163	-0.011701

Table S34: M06, M06[HF], M06[LDA], Disp3 interaction energy results (in hartree) for the S22 dataset.

	M06	M06[HF]	M06[LDA]	Disp3
Hydrogen bonds				
$(NH_3)_2$ (C_{2h})	-0.004486	-0.004091	-0.004039	-0.000304
$(H_2O)_2$ (C_s)	-0.007633	-0.00717	-0.007045	-0.000205
Formic acid dimer (C_{2h})	-0.030181	-0.029064	-0.028599	-0.00047
Formamide dimer (C_{2h})	-0.025124	-0.023806	-0.024258	-0.000698
Uracil dimer (C_{2h})	-0.031116	-0.029908	-0.029964	-0.001349
2-pyridoxine 2-aminopyridine (C_1)	-0.025589	-0.024128	-0.024388	-0.001672
Adenine thymine WC (C_1)	-0.02468	-0.022834	-0.023459	-0.001802
Mixed complexes				
Ethene ethine (C_{2v})	-0.001986	-0.001826	-0.001718	-0.000428
Benzene H_2O (C_s)	-0.004997	-0.004716	-0.004442	-0.000902
Benzene NH_3 (C_s)	-0.003071	-0.002897	-0.002598	-0.001045
Benzene HCN (C_s)	-0.006347	-0.006022	-0.006025	-0.000808
Benzene dimer (C_{2v})	-0.003157	-0.002865	-0.002656	-0.001802
Indole benzene T-shape (C_1)	-0.007082	-0.006522	-0.006375	-0.002365
Phenol dimer (C_1)	-0.010164	-0.009395	-0.009344	-0.001852
van der Waals dispersion				
$(CH_4)_2$ (D_{3d})	-0.000376	-0.00025	0.000084	-0.000483
$(C_2H_4)_2$ (D_{2d})	-0.002329	-0.001885	-0.001702	-0.000507
Benzene CH_4 (C_3)	-0.001678	-0.001558	-0.001301	-0.001028
Benzene dimer (C_{2h})	-0.003452	-0.00364	-0.002612	-0.002807
Pyrazine dimer (C_s)	-0.005022	-0.005424	-0.004188	-0.002426
Uracil dimer (C_2)	-0.013886	-0.013001	-0.012545	-0.003667
Indole benzene (C_1)	-0.005633	-0.005668	-0.004554	-0.003727
Adenine thymine stack (C_1)	-0.016099	-0.014947	-0.014359	-0.004857

Table S35: HH, HH[HF], HH[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	HH	HH[HF]	HH[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.004084	-0.003928	-0.003405	-0.001154	-0.001059	-0.00097	-0.00094	-0.00103
$(H_2O)_2$ (C_s)	-0.007953	-0.007704	-0.007107	-0.000935	-0.00075	-0.000685	-0.000656	-0.000731
Formic acid dimer (C_{2h})	-0.030577	-0.029723	-0.028706	-0.002897	-0.002927	-0.002533	-0.002484	-0.002622
Formamide dimer (C_{2h})	-0.02472	-0.024112	-0.023283	-0.003233	-0.00308	-0.002713	-0.002667	-0.002811
Uracil dimer (C_{2h})	-0.031569	-0.030939	-0.030118	-0.004256	-0.004126	-0.003561	-0.003517	-0.003676
2-pyridoxine 2-aminopyridine (C_1)	-0.023692	-0.022958	-0.022058	-0.004952	-0.004911	-0.004289	-0.004265	-0.004409
Adenine thymine WC (C_1)	-0.022758	-0.021963	-0.020966	-0.005352	-0.005268	-0.004636	-0.004585	-0.004792
Mixed complexes								
Ethene ethine (C_{2v})	-0.001634	-0.001594	-0.001442	-0.001321	-0.001258	-0.001226	-0.001233	-0.001241
Benzene H_2O (C_s)	-0.003097	-0.003016	-0.002537	-0.002855	-0.002617	-0.002335	-0.0023	-0.002428
Benzene NH_3 (C_s)	-0.00118	-0.001127	-0.000759	-0.002962	-0.002724	-0.002576	-0.00256	-0.002665
Benzene HCN (C_s)	-0.004967	-0.004898	-0.004512	-0.003542	-0.003456	-0.00298	-0.002997	-0.003019
Benzene dimer (C_{2v})	0.00017	0.000239	0.000595	-0.004756	-0.004649	-0.004512	-0.00457	-0.004573
Indole benzene T-shape (C_1)	-0.002854	-0.002735	-0.002207	-0.006253	-0.006245	-0.005887	-0.005939	-0.005987
Phenol dimer (C_1)	-0.00679	-0.00655	-0.00572	-0.005441	-0.005027	-0.00471	-0.0047	-0.004836
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	0.000208	0.000263	0.0005	-0.001063	-0.00107	-0.001091	-0.001069	-0.001155
$(C_2H_4)_2$ (D_{2d})	-0.000141	-0.000044	0.00038	-0.002643	-0.002435	-0.002275	-0.00228	-0.00233
Benzene CH_4 (C_3)	0.000345	0.000382	0.00066	-0.002886	-0.002708	-0.002707	-0.002703	-0.00279
Benzene dimer (C_{2h})	0.00444	0.004461	0.004794	-0.007495	-0.008323	-0.008247	-0.008325	-0.008384
Pyrazine dimer (C_s)	0.00209	0.0021	0.002634	-0.007732	-0.008413	-0.007918	-0.00793	-0.008101
Uracil dimer (C_2)	-0.005037	-0.004707	-0.003817	-0.011306	-0.011402	-0.010472	-0.010349	-0.010847
Indole benzene (C_1)	0.005263	0.005314	0.00589	-0.010656	-0.011761	-0.011587	-0.011673	-0.01181
Adenine thymine stack (C_1)	-0.002348	-0.001946	-0.000534	-0.015508	-0.016028	-0.015071	-0.014944	-0.015608

Table S36: M06-2X, M06-2X[HF], M06-2X[LDA], Disp3 interaction energy results (in hartree) for the S22 dataset.

	M06-2X	M06-2X[HF]	M06-2X[LDA]	Disp3
Hydrogen bonds				
$(NH_3)_2$ (C_{2h})	-0.005046	-0.004718	-0.004503	-0.000067
$(H_2O)_2$ (C_s)	-0.008213	-0.00785	-0.00735	-0.000035
Formic acid dimer (C_{2h})	-0.031101	-0.029493	-0.029878	-0.000111
Formamide dimer (C_{2h})	-0.025512	-0.02439	-0.024298	-0.000192
Uracil dimer (C_{2h})	-0.031975	-0.030751	-0.030756	-0.000616
2-pyridoxine 2-aminopyridine (C_1)	-0.025464	-0.024031	-0.024125	-0.000693
Adenine thymine WC (C_1)	-0.024741	-0.023025	-0.023392	-0.00081
Mixed complexes				
Ethene ethine (C_{2v})	-0.002252	-0.002193	-0.00204	-0.000122
Benzene H_2O (C_s)	-0.005953	-0.005581	-0.005548	-0.000219
Benzene NH_3 (C_s)	-0.003918	-0.003612	-0.003622	-0.000304
Benzene HCN (C_s)	-0.008003	-0.007751	-0.007603	-0.000239
Benzene dimer (C_{2v})	-0.003912	-0.003667	-0.003522	-0.000719
Indole benzene T-shape (C_1)	-0.00845	-0.007974	-0.007835	-0.000905
Phenol dimer (C_1)	-0.010984	-0.01011	-0.01012	-0.000807
van der Waals dispersion				
$(CH_4)_2$ (D_{3d})	-0.000667	-0.000555	-0.00046	-0.000107
$(C_2H_4)_2$ (D_{2d})	-0.002498	-0.002058	-0.002201	-0.000179
Benzene CH_4 (C_3)	-0.002284	-0.002068	-0.002053	-0.000389
Benzene dimer (C_{2h})	-0.004223	-0.004071	-0.003677	-0.000829
Pyrazine dimer (C_s)	-0.006672	-0.006545	-0.006027	-0.000603
Uracil dimer (C_2)	-0.016366	-0.014238	-0.015701	-0.000954
Indole benzene (C_1)	-0.007395	-0.006907	-0.006603	-0.00108
Adenine thymine stack (C_1)	-0.020084	-0.017637	-0.018875	-0.001353

Table S37: CAM-B3LYP, CAM-B3LYP[HF], CAM-B3LYP[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	CAM-B3LYP	CAM-B3LYP[HF]	CAM-B3LYP[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.00444	-0.004138	-0.004106	-0.001003	-0.000749	-0.00073	-0.000674	-0.000757
$(H_2O)_2$ (C_s)	-0.008319	-0.007821	-0.007922	-0.000808	-0.000492	-0.000482	-0.000432	-0.000499
Formic acid dimer (C_{2h})	-0.031192	-0.029465	-0.030363	-0.002484	-0.002019	-0.00186	-0.001768	-0.001877
Formamide dimer (C_{2h})	-0.025122	-0.02391	-0.024503	-0.002796	-0.002271	-0.00209	-0.002008	-0.00211
Uracil dimer (C_{2h})	-0.031754	-0.030506	-0.031132	-0.003747	-0.003336	-0.002868	-0.002802	-0.002899
2-pyridoxine 2-aminopyridine (C_1)	-0.024671	-0.023286	-0.023902	-0.004367	-0.004046	-0.003459	-0.003439	-0.003485
Adenine thymine WC (C_1)	-0.023592	-0.022076	-0.02274	-0.004721	-0.004362	-0.00372	-0.003663	-0.003768
Mixed complexes								
Ethene ethine (C_{2v})	-0.001685	-0.001617	-0.001555	-0.00116	-0.001056	-0.00103	-0.001019	-0.001035
Benzene H_2O (C_s)	-0.003361	-0.003195	-0.00304	-0.002496	-0.00206	-0.001851	-0.001704	-0.001923
Benzene NH_3 (C_s)	-0.001498	-0.00139	-0.001241	-0.002612	-0.002278	-0.002124	-0.00201	-0.002197
Benzene HCN (C_s)	-0.005055	-0.004926	-0.004727	-0.003079	-0.002753	-0.002437	-0.002392	-0.002466
Benzene dimer (C_{2v})	-0.000301	-0.000159	-0.000023	-0.004225	-0.00417	-0.003906	-0.003915	-0.00396
Indole benzene T-shape (C_1)	-0.003449	-0.003216	-0.00303	-0.005545	-0.005485	-0.005022	-0.005018	-0.005098
Phenol dimer (C_1)	-0.00748	-0.006968	-0.006943	-0.004807	-0.00431	-0.003955	-0.0039	-0.004018
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	0.000058	0.000171	0.000206	-0.00094	-0.000884	-0.000883	-0.000836	-0.00091
$(C_2H_4)_2$ (D_{2d})	-0.00048	-0.000284	-0.000204	-0.00228	-0.001903	-0.001873	-0.001853	-0.001896
Benzene CH_4 (C_3)	-0.000004	0.00008	0.000185	-0.002557	-0.002342	-0.002233	-0.002159	-0.002298
Benzene dimer (C_{2h})	0.003352	0.003389	0.00362	-0.006621	-0.007479	-0.007075	-0.007045	-0.007196
Pyrazine dimer (C_s)	0.000966	0.000997	0.001315	-0.006765	-0.007196	-0.006742	-0.006621	-0.00685
Uracil dimer (C_2)	-0.006062	-0.005372	-0.005476	-0.009906	-0.009706	-0.008882	-0.008576	-0.009075
Indole benzene (C_1)	0.003741	0.003829	0.004209	-0.009383	-0.010424	-0.009894	-0.009846	-0.010087
Adenine thymine stack (C_1)	-0.004075	-0.00329	-0.003026	-0.013582	-0.013544	-0.012755	-0.012397	-0.013069

Table S38: LC-ωPBE, LC-ωPBE[HF], LC-ωPBE[LDA], Disp3, Disp3BJ, XDM, XDM(HF), XDM(LDA) interaction energy results (in hartree) for the S22 dataset.

	LC-ωPBE	LC-ωPBE[HF]	LC-ωPBE[LDA]	Disp3	Disp3BJ	XDM	XDM(HF)	XDM(LDA)
Hydrogen bonds								
$(NH_3)_2$ (C_{2h})	-0.003645	-0.003448	-0.003068	-0.001069	-0.000881	-0.000962	-0.000949	-0.000984
$(H_2O)_2$ (C_s)	-0.007005	-0.006603	-0.00645	-0.000861	-0.000595	-0.000751	-0.000741	-0.000768
Formic acid dimer (C_{2h})	-0.028734	-0.026814	-0.028214	-0.002643	-0.002372	-0.002646	-0.002608	-0.002709
Formamide dimer (C_{2h})	-0.022527	-0.02128	-0.022079	-0.002972	-0.002613	-0.002673	-0.002614	-0.002759
Uracil dimer (C_{2h})	-0.028486	-0.027236	-0.02785	-0.003961	-0.003701	-0.003487	-0.003398	-0.003594
2-pyridoxine 2-aminopyridine (C_1)	-0.022449	-0.021127	-0.021575	-0.004628	-0.004468	-0.004184	-0.004075	-0.004327
Adenine thymine WC (C_1)	-0.021303	-0.019853	-0.020258	-0.004999	-0.004808	-0.004626	-0.004478	-0.00477
Mixed complexes								
Ethene ethine (C_{2v})	-0.001462	-0.00149	-0.001073	-0.001234	-0.001165	-0.001089	-0.001136	-0.001118
Benzene H_2O (C_s)	-0.003412	-0.003422	-0.002799	-0.002669	-0.002331	-0.002177	-0.002309	-0.002214
Benzene NH_3 (C_s)	-0.001558	-0.001613	-0.001019	-0.002778	-0.00252	-0.002344	-0.00247	-0.002388
Benzene HCN (C_s)	-0.005329	-0.005383	-0.004651	-0.003256	-0.003077	-0.00264	-0.002765	-0.002687
Benzene dimer (C_{2v})	-0.000481	-0.000529	0.000119	-0.004467	-0.004478	-0.003951	-0.00411	-0.004039
Indole benzene T-shape (C_1)	-0.00384	-0.003868	-0.00298	-0.005879	-0.005931	-0.00527	-0.005429	-0.005397
Phenol dimer (C_1)	-0.00637	-0.005965	-0.005591	-0.005082	-0.004699	-0.004365	-0.004379	-0.004477
van der Waals dispersion								
$(CH_4)_2$ (D_{3d})	0.000215	0.00029	0.000529	-0.001018	-0.000994	-0.00103	-0.001016	-0.001076
$(C_2H_4)_2$ (D_{2d})	-0.000184	-0.00009	0.000378	-0.002419	-0.002159	-0.001958	-0.001972	-0.002008
Benzene CH_4 (C_3)	-0.000011	-0.000055	0.000405	-0.0027	-0.002557	-0.002509	-0.002604	-0.002578
Benzene dimer (C_{2h})	0.002696	0.002051	0.003488	-0.007057	-0.008059	-0.007216	-0.00747	-0.007349
Pyrazine dimer (C_s)	0.000644	0.000002	0.00156	-0.00722	-0.007883	-0.006925	-0.007061	-0.007017
Uracil dimer (C_2)	-0.005521	-0.005199	-0.00446	-0.010576	-0.010649	-0.009393	-0.009401	-0.009618
Indole benzene (C_1)	0.002846	0.002115	0.003961	-0.009995	-0.011272	-0.010134	-0.010429	-0.010331
Adenine thymine stack (C_1)	-0.004332	-0.0041	-0.002565	-0.014473	-0.01488	-0.013404	-0.01341	-0.013694

Table S39: M11, M11[HF], M11[LDA] interaction energy results (in hartree) for the S22 dataset.

	M11	M11[HF]	M11[LDA]
Hydrogen bonds			
$(NH_3)_2$ (C_{2h})	-0.004603	-0.00432	-0.00367
$(H_2O)_2$ (C_s)	-0.007844	-0.007353	-0.006827
Formic acid dimer (C_{2h})	-0.031218	-0.029076	-0.030566
Formamide dimer (C_{2h})	-0.025299	-0.024009	-0.024608
Uracil dimer (C_{2h})	-0.031674	-0.030396	-0.030668
2-pyridoxine 2-aminopyridine (C_1)	-0.024879	-0.023447	-0.023931
Adenine thymine WC (C_1)	-0.024268	-0.0226	-0.023075
Mixed complexes			
Ethene ethine (C_{2v})	-0.00227	-0.002225	-0.001558
Benzene H_2O (C_s)	-0.00588	-0.005761	-0.004606
Benzene NH_3 (C_s)	-0.00379	-0.003724	-0.002722
Benzene HCN (C_s)	-0.008366	-0.008141	-0.006949
Benzene dimer (C_{2v})	-0.003692	-0.003635	-0.002477
Indole benzene T-shape (C_1)	-0.008303	-0.00821	-0.006655
Phenol dimer (C_1)	-0.010932	-0.010129	-0.00936
van der Waals dispersion			
$(CH_4)_2$ (D_{3d})	-0.000378	-0.000319	0.000037
$(C_2H_4)_2$ (D_{2d})	-0.002381	-0.002252	-0.001504
Benzene CH_4 (C_3)	-0.002127	-0.002022	-0.001211
Benzene dimer (C_{2h})	-0.00345	-0.003712	-0.001654
Pyrazine dimer (C_s)	-0.005975	-0.006264	-0.004156
Uracil dimer (C_2)	-0.01564	-0.014369	-0.013565
Indole benzene (C_1)	-0.006256	-0.006333	-0.003742
Adenine thymine stack (C_1)	-0.019128	-0.017639	-0.015706

Table S40: MN15, MN15[HF], MN15[LDA] interaction energy results (in hartree) for the S22 dataset.

	MN15	MN15[HF]	MN15[LDA]
Hydrogen bonds			
$(NH_3)_2$ (C_{2h})	-0.004962	-0.004298	-0.004783
$(H_2O)_2$ (C_s)	-0.007879	-0.007129	-0.007564
Formic acid dimer (C_{2h})	-0.030096	-0.027274	-0.0296
Formamide dimer (C_{2h})	-0.024471	-0.022169	-0.024211
Uracil dimer (C_{2h})	-0.030974	-0.028338	-0.030325
2-pyridoxine 2-aminopyridine (C_1)	-0.024645	-0.021805	-0.023879
Adenine thymine WC (C_1)	-0.02404	-0.020808	-0.023112
Mixed complexes			
Ethene ethine (C_{2v})	-0.002518	-0.002101	-0.002332
Benzene H_2O (C_s)	-0.006262	-0.005414	-0.006051
Benzene NH_3 (C_s)	-0.00446	-0.003721	-0.004238
Benzene HCN (C_s)	-0.008317	-0.007505	-0.007971
Benzene dimer (C_{2v})	-0.004627	-0.003596	-0.00415
Indole benzene T-shape (C_1)	-0.009182	-0.007612	-0.008568
Phenol dimer (C_1)	-0.011159	-0.009446	-0.010649
van der Waals dispersion			
$(CH_4)_2$ (D_{3d})	-0.001358	-0.000866	-0.001162
$(C_2H_4)_2$ (D_{2d})	-0.003686	-0.002708	-0.003401
Benzene CH_4 (C_3)	-0.003098	-0.002431	-0.002821
Benzene dimer (C_{2h})	-0.005382	-0.004185	-0.00476
Pyrazine dimer (C_s)	-0.007162	-0.006071	-0.006572
Uracil dimer (C_2)	-0.016175	-0.013034	-0.015481
Indole benzene (C_1)	-0.0086	-0.006767	-0.007672
Adenine thymine stack (C_1)	-0.020619	-0.016544	-0.019304

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