

Supporting Information

for

‘Beyond Born-Mayer: Improved models for short-range repulsion in ab initio force fields’

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Contents

S1 Waldman-Hagler Analysis of B_{ij} Combination Rule	2
S2 Force Field Fit Quality: Exact Overlap Model vs. Slater-ISA FF	5
S3 Extrapolation Algorithm for ISA Exponents	6
S4 Non-polarizable, point-charge Lennard-Jones Force Fields	8
S5 Born-Mayer-sISA: Scale Factor Tests	8
S5.1 Comparison to S_{ij}	8
S5.2 Comparison to V_{FF}	9
S6 Slater-OPT and Born-Mayer-OPT Force Fields	11
S7 Monomer Geometries	12
S8 Homomonomeric Parameters	15
S8.1 Multipole Moments	15
S8.2 Slater-ISA FF Parameters	18
S8.3 Born-Mayer-IP FF Parameters	21
S8.4 Born-Mayer-sISA FF Parameters	24
S9 Force Field Fits for Homomonomeric Systems	26
S10 Force Field Accuracy for LJ FF	34

S1 Parameter Robustness for Argon	39
S12 Parameter Robustness for Ethane; LJ FF results	41

S1 Waldman-Hagler Analysis of B_{ij} Combination Rule

The exact expressions for the overlap of two Slater densities $\rho_i = D_i \exp(-B_i r)$ and $\rho_j = D_j \exp(-B_j r)$ are shown here, first in the limiting case where the two exponents are equal ($B_i = B_j = B_{ij}$):

$$\begin{aligned} S_{B_i=B_j}^{ij} &= D_{ij} P(B_{ij}, r_{ij}) \exp(-B_{ij} r_{ij}) \\ D_{ij} &= \pi D_i D_j B_{ij}^{-3} \\ P(B_{ij}, r_{ij}) &= \frac{1}{3} (B_{ij} r_{ij})^2 + B_{ij} r_{ij} + 1, \end{aligned} \tag{1}$$

and second in the case where $B_i \neq B_j$:

$$\begin{aligned} S_{B_i \neq B_j}^{ij} &= \frac{16\pi D_i D_j \exp(-\{B_i + B_j\} r_{ij}/2)}{(B_i^2 - B_j^2)^3 r_{ij}} \times \\ &\left[\left(\frac{B_i - B_j}{2} \right)^2 \left(\exp \left(\{B_i - B_j\} \frac{r_{ij}}{2} \right) - \exp \left(-\{B_i - B_j\} \frac{r_{ij}}{2} \right) \right) \right. \\ &\quad \times \left(\left(\frac{B_i + B_j}{2} \right)^2 r_{ij}^2 + (B_i + B_j) r_{ij} + 2 \right) \\ &\quad - \left(\frac{B_i + B_j}{2} \right)^2 \exp \left(\{B_i - B_j\} \frac{r_{ij}}{2} \right) \times \left(\left(\frac{B_i - B_j}{2} \right)^2 r_{ij}^2 - (B_i - B_j) r_{ij} + 2 \right) \\ &\quad \left. + \left(\frac{B_i + B_j}{2} \right)^2 \exp \left(-\{B_i - B_j\} \frac{r_{ij}}{2} \right) \times \left(\left(\frac{B_i - B_j}{2} \right)^2 r_{ij}^2 + (B_i - B_j) r_{ij} + 2 \right) \right]. \end{aligned} \tag{2}$$

Each overlap formula has been given a subscript to indicate limits on B_i and B_j .

Our goal is to ascertain the extent to which $S_{B_i \neq B_j}^{ij}$ can be accurately modeled by the functional form and variables of $S_{B_i=B_j}^{ij}$. D_i and D_j are pre-factors appearing in both equations, and we set these variables to unity without loss of generality. To find values of B_{ij} such that $S_{B_i \neq B_j}^{ij}(B_i, B_j, r_{ij}) \approx S_{B_i=B_j}^{ij}(B_{ij}, r_{ij})$, we first treat B_{ij} as a completely adjustable

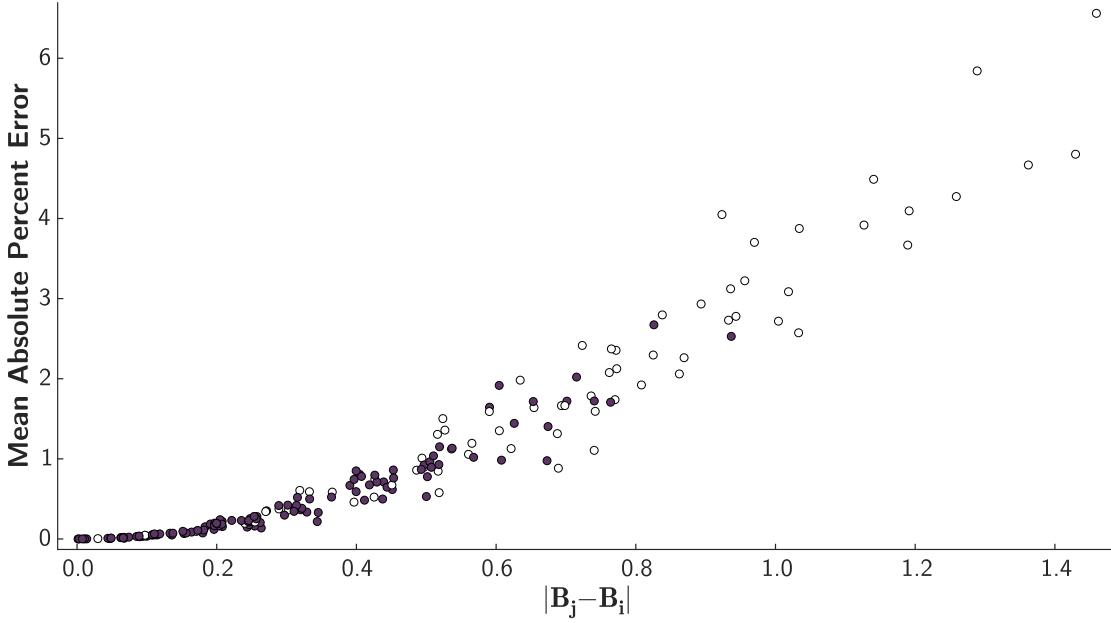


Figure S1. Mean absolute percent error of fitted overlap values as a function of the absolute difference between B_i and B_j values. Element pairs containing He, Li, Ne and/or Na are shown as empty circles. Deviations below 1% are seen for most element pairs, with noble gases and alkali metals posing a more significant challenge. Scatter in the plot is due to small variations in the absolute values of r_{ij} fit for each pair. As expected, $S_{B_i \neq B_j}^{ij}$ and $S_{B_i = B_j}^{ij}$ closely agree for $|B_i - B_j| \approx 0$.

parameter, and later test for the existence of some simple combining function f such that $B_{ij} = f(B_i, B_j)$.

To optimize B_{ij} , we first require a training set of relevant $S_{B_i \neq B_j}^{ij}$ values. B_i , B_j , and r_{ij} are the only variables appearing in $S_{B_i \neq B_j}^{ij}$, and we could in principle fit B_{ij} values over a grid of B_i , B_j and r_{ij} combinations. However, we are only interested in the subset of points which are chemically relevant. Consequently, we developed a library of B_i values by deriving exponents from the ionization potentials of the first three rows of the periodic table (plus bromine and iodine). For each pair of elements, $B = 2\sqrt{2\text{IP}}$,¹ and a range of r_{ij} values corresponding to 0.8-1.2 times the sum of the van der Waals radii of the two atoms was selected. B_{ij} values in $S_{B_i = B_j}^{ij}$ were then optimized (in a least-squares sense) for each element pair separately; Mean absolute percent errors (MAPE) for fitted overlaps are shown in Figure S1 and in Table S11.

Relative errors for fitting are acceptably small for all element pairs. Excluding certain noble gases and alkali metals (He, Li, Ne, Na) from consideration, these being the elements

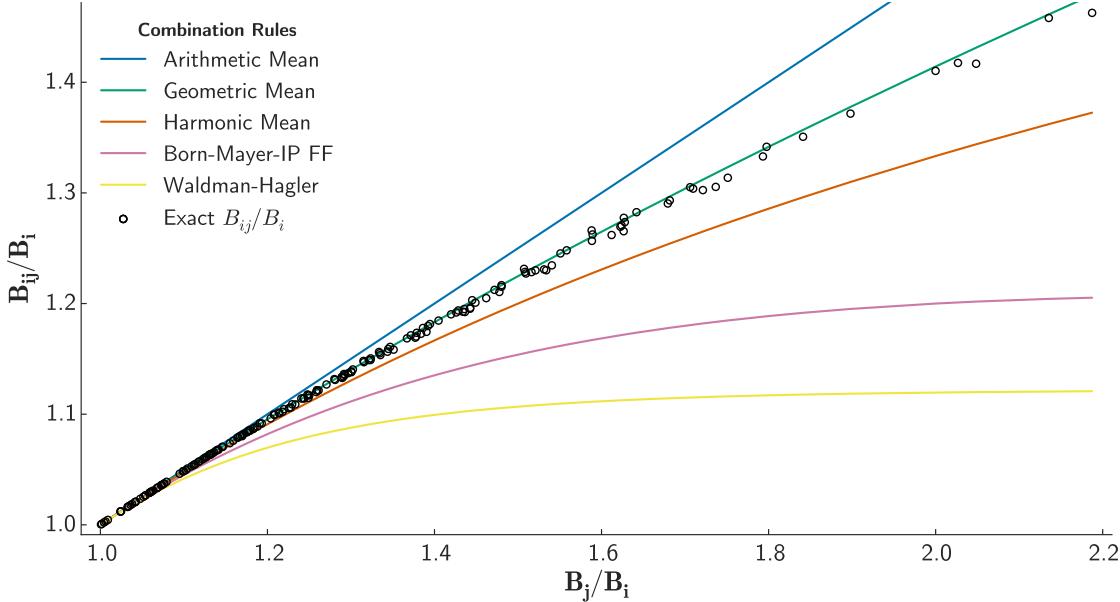


Figure S2. Waldman-Hagler-style analysis of possible B_{ij} combination rules. Exact B_{ij} values are derived from fitting an approximate overlap density of the form $S_{ij} = A_{ij}K_2(r_{ij})\exp(-B_{ij}r_{ij})$ to the exact overlap density (as given by Rosen and by Tai^{3,4}) of two distinct Slater orbitals whose exponents correspond to atomic exponents for the elements H-Ar, Cl, Br, and I. For each overlap pair, a range of r_{ij} values was used from 0.8 to 1.2 times the sum of the pair's van der Waals radii. The geometric mean combination rule $B_{ij} = \sqrt{B_i B_j}$ models the exact B_{ij} values with near-perfect agreement, justifying our choice of combination rule.

with the most disparate B_i values compared to other elements, MAPE drops below 3% for all pairs, with the vast majority of MAPE below 1%. Our focus in this work is primarily on organic compounds where $|B_i - B_j|$ is small; empirically, these errors always translate to very small errors in the exchange energy itself. Use of an effective B_{ij} may require further testing in cases with extremely disparate B_i and B_j values.

We next tested whether the optimized B_{ij} could instead be modeled by a combination rule $B_{ij} = f(B_i, B_j)$. On the basis of symmetry and scaling considerations, Waldman and Hagler demonstrate that if a combination rule $f(B_i, B_j)$ exists, a plot of B_{ij}/B_i vs. B_j/B_i should lie on a single curve.² Remarkably (see Figure S2), a geometric mean combination rule $B_{ij} = \sqrt{B_i B_j}$ models the fitted B_{ij} values with nearly quantitatively. This result allows the computation of Slater overlaps using the much simpler form of $S_{B_i=B_j}^{ij}$ (1) from individual atoms-in-molecule exponents B_i and B_j .

S2 Force Field Fit Quality: Exact Overlap Model vs. Slater-ISA FF

A direct test of the approximate overlap model (Equation 1 with B_i values extracted from ISA calculations, synonymous with the Slater-ISA FF in the main text) is made by directly comparing the accuracy of force fields fit by the exact and approximate overlap models. Table S1 shows average RMS errors for each energy component that uses an explicit short-range term. Differences in RMS errors between models are negligible, with use of the more approximate overlap model introducing (at most) an additional 2% extra error compared to the exact overlap model. Use of $S_{B_i=B_j}^{ij}$ to compute all overlaps is thus well justified.

Table S1. Comparison of geometric mean RMS errors over the 91 dimer test set for the Approximate Overlap Model (that is, the Slater-ISA FF) and the Exact Overlap Model. ‘Attractive’ RMS errors, representing the average RMS error for the subset of points whose energies are net attractive ($E_{\text{int}} < 0$), are shown in parentheses to the right of the total average RMS errors. The average ratio of RMS errors (Slater-ISA FF/ Exact Overlap Model) for each pair in the 91 dimer test set, α (dimensionless), is also shown. α values greater than 1 indicate that on average the Exact Overlap Model is more accurate compared to the Slater-ISA FF.

Component	Slater-ISA FF (kJ mol ⁻¹)	Exact Overlap Model (kJ mol ⁻¹)	α
Exchange	2.641 (0.686)	2.581 (0.679)	1.023 (1.010)
Electrostatics	1.087 (0.351)	1.083 (0.350)	1.004 (1.003)
Induction	0.251 (0.095)	0.252 (0.095)	0.998 (0.999)
δ^{HF}	0.246 (0.068)	0.245 (0.068)	1.004 (1.007)

S3 Extrapolation Algorithm for ISA Exponents

Unphysical asymptotic charge density decays occasionally arise in the ISA procedure due to basis set incompleteness and numerical instabilities. These unphysical decays can skew optimization of B_i^{ISA} parameters, and need to be corrected. Generally speaking, there exists some range of distances in the valence region that *does* exhibit the expected exponential decay; we extrapolate the decay from this intermediate region to describe the asymptotic region using the following algorithm:

1. Take the log of each atomic density (henceforth logdens) to linearize the asymptotic density.
2. Compute the 2nd derivative of logdens. This can be done analytically, as the BS-ISA procedure outputs an analytical expression (in terms of Gaussian basis functions) for the atomic density.
3. Determine the ‘intermediate region’ of exponential decay by locating the largest range where the 2nd derivative of logdens is zero to within a fixed tolerance. Here we utilize a tolerance of 0.3 a.u. (absolute cutoff) or 190% of the smallest exponent in the Gaussian basis set (relative cutoff), whichever is smaller. The latter cutoff accounts for the eventual asymptotic Gaussian-type decay dictated by the smallest ζ in the ISA basis. The endpoints of this intermediate region are denoted $r1$ and $r2$, respectively.
4. Calculate the slope m and intercept b for the line defined by $r1$, $r2$, and their respective values of logdens.
5. Replace all values of logdens after $r2$ with $mr + b$. The resulting atomic density is labeled in the main text as ‘Asymptotically-corrected ISA densities’.

A visual of these steps is shown in Figure S3.

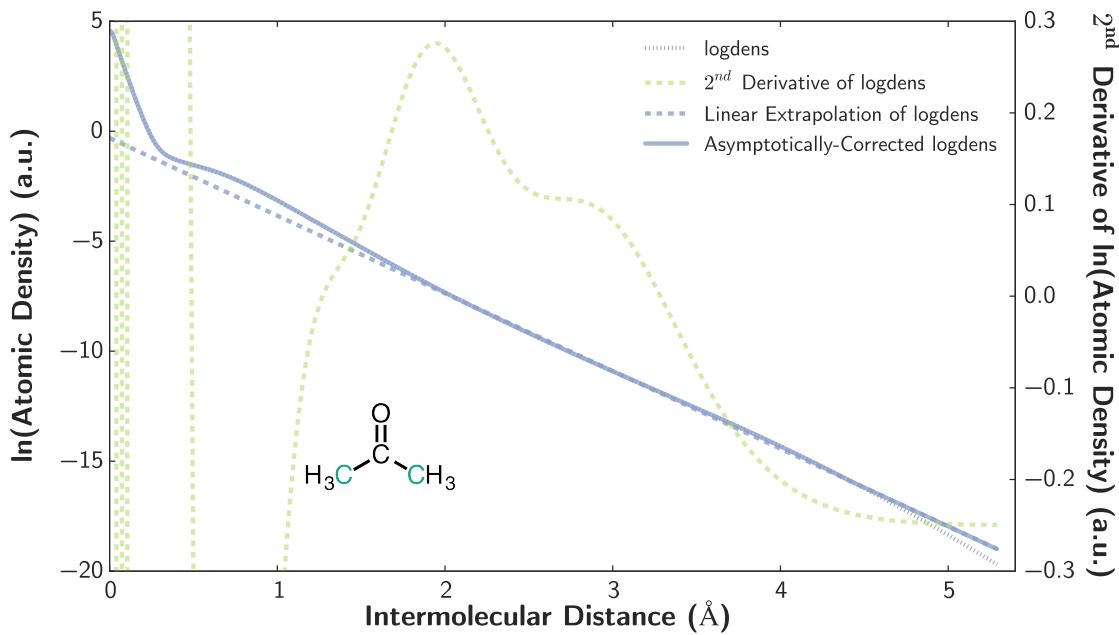


Figure S3. Linear extrapolation algorithm for the methyl carbon in acetone. Depicted are (in legend order) Steps 1, 2, 4, and 5 in the extrapolation algorithm. Note that some portions of the 2^{nd} derivative extend off the graph; also note that most of logdens is located underneath the asymptotically-corrected curve.

S4 Non-polarizable, point-charge Lennard-Jones Force Fields

As described in the main text, a non-polarizable, rank 0 multipole version of LJ FF was fit in order to produce force fields most in line with popular standard force fields. Results for this LJ FF are shown in Table Table S2; unsurprisingly, these force fields are less accurate and less transferable compared to LJ FF in the main text, which includes polarizability and higher-order multipole moments.

Table S2. Comparison of characteristic RMSE and $\|MSE\|$ over the 91 dimer test set for the non-polarizable, rank 0 multipole Lennard-Jones model. The LJ models are not parameterized on a component-by-component basis, thus $RMSE/\|MSE\|$ values for only the total FF energy is shown. ‘Attractive’ errors, representing the average $RMSE/\|MSE\|$ for the subset of points whose energies are net attractive ($E_{int} < 0$), are shown in parentheses to the right of the total average RMS errors. ‘Dimer-Specific Fits’ and ‘Transferable Fits’ are as in the main text.

	Dimer-Specific Fits (kJ mol ⁻¹)	Transferable Fits (kJ mol ⁻¹)
$RMSE$	5.116 (0.560)	4.513 (0.658)
$\ MSE\ $	0.803 (0.038)	0.562 (0.079)

S5 Born-Mayer-sISA: Scale Factor Tests

S5.1 Comparison to S_{ij}

Exact S_{ij} (eq. (1) and eq. (2)) values were computed for various element pairs as in Section S1. Born-Mayer overlaps of the form

$$S_{ij} \approx K_{ij} \exp(-\xi B_{ij} r_{ij})$$

where

$$K_{ij} = \frac{K}{B_{ij}^3}$$

$$B_{ij} = \sqrt{B_i B_j}$$

were fit to these exact overlaps; K and ξ were optimized as universal parameters by performing a log-weighted fit over the entire set of S_{ij} values.

Table S3. Optimized Born-Mayer parameters, ξ and K , for fits to $S_{ij} \approx \frac{K}{(B_i B_j)^{3/2}} \exp(-\xi \sqrt{B_i B_j} r_{ij})$. B_i and B_j values have been chosen as in S1. Tabulated r_{ij} ranges are expressed as a fraction of the sum of van der Waals radii for atoms i and j .

Range of r_{ij}	ξ	K
[0.8, 1.2]	0.738	12.2
[1.0, 2.0]	0.812	20.9
[1.0, 4.0]	0.878	42.6

Optimized parameters are shown in Table S3 for various ranges of r_{ij} . As shown in Table S3, the scale factor ξ is highly sensitive to the values of r_{ij} included in the fits, with larger values of r_{ij} tending to increase ξ . On the other hand, ξ is fairly insensitive to the values of B_i and B_j : setting $\xi = \xi_0 + \xi_1 B_{ij}$ does not significantly improve fit quality. On the grounds of our overlap tests, it is difficult to establish a precise value for ξ , though our results do suggest that $\xi \sim 0.80$ and is largely independent of the atomic exponents themselves.

S5.2 Comparison to V_{FF}

Alternatively, we optimized the Born-Mayer-sISA FF scale factor by minimizing errors in the force field itself. Average RMS errors for a variety of scale factors are shown in Table S4. Regardless of whether we consider each energy component separately, or focus on the overall energy, setting $\xi = 0.84$ is optimal; RMS errors for this choice are comparable to the Slater-ISA FF itself.

Table S4. Average RMS errors over the 91 dimer test set for Born-Mayer-sISA FF using different exponential scale factors. All quantities are in kJ mol^{-1} except for scale factors, which are unitless. ‘Attractive’ RMS errors, representing the average RMS error for the subset of points whose energies are net attractive (i.e., where $E_{tot} < 0$), are shown in parentheses to the right of the total average RMS errors. Geometric (rather than arithmetic) averages are used in all cases.

Component	Born-Mayer-sISA Scale Factor					
	$\xi = 0.80$	$\xi = 0.82$	$\xi = 0.84$	$\xi = 0.86$	$\xi = 0.88$	$\xi = 0.90$
Exchange	3.078 (0.697)	2.690 (0.668)	2.677 (0.686)	2.841 (0.702)	3.225 (0.742)	3.798 (0.791)
Electrostatics	1.144 (0.418)	1.105 (0.378)	1.083 (0.352)	1.077 (0.342)	1.104 (0.354)	1.105 (0.373)
Induction	0.258 (0.099)	0.253 (0.097)	0.250 (0.096)	0.246 (0.095)	0.243 (0.094)	0.240 (0.094)
δ^{HF}	0.241 (0.072)	0.244 (0.069)	0.248 (0.068)	0.255 (0.070)	0.263 (0.075)	0.272 (0.082)
Dispersion	0.934 (0.383)	0.803 (0.337)	0.856 (0.336)	1.078 (0.370)	1.388 (0.426)	1.740 (0.496)
Total Energy	1.970 (0.503)	1.775 (0.455)	1.751 (0.453)	1.818 (0.465)	2.084 (0.516)	2.451 (0.577)

S6 Slater-OPT and Born-Mayer-OPT Force Fields

We developed a Slater-OPT force field, identical to the Slater-ISA FF except that B_{ij} parameters were optimized to reproduce the DFT-SAPT exchange-repulsion energy. Analogously, we developed Born-Mayer-OPT as an extension of the Born-Mayer-sISA FF. Treating B_{ij} as a completely unconstrained parameter led to poor dispersion energies and overall transferability, and was not considered further. Instead, exponents were optimized using a harmonic penalty function of the form $k(B - B_0)^2$, with $k = 10^{-5}$ a.u. For Slater-OPT, B_0 values were taken from the Slater-ISA FF; for Born-Mayer-OPT, the Born-Mayer-IP FF values were used. RMS errors for Slater-OPT and Born-Mayer-OPT are shown in Table S5. For both Dimer-Specific and Transferable fits, Slater-OPT and Born-Mayer-OPT are of comparable quality. Both force fields are only slight improvements to either the Slater-ISA FF or the Born-Mayer-sISA FF; considering the extra number of free parameters required to optimize atomic exponents, we consider these results further confirmation of the inherent quality of the ISA exponents.

Table S5. Comparison of geometric mean RMS errors over the 91 dimer test set for the Slater-OPT and Born-Mayer-OPT methods. ‘Attractive’ RMS errors, representing the average RMS error for the subset of points whose energies are net attractive ($E_{\text{int}} < 0$), are shown in parentheses to the right of the total average RMS errors.

Component	Dimer-Specific Fits		Transferable Fits	
	Slater-OPT (kJ mol ⁻¹)	Born-Mayer-OPT (kJ mol ⁻¹)	Slater-OPT (kJ mol ⁻¹)	Born-Mayer-OPT (kJ mol ⁻¹)
Exchange	2.513 (0.636)	2.433 (0.639)	2.507 (0.665)	2.459 (0.671)
Electrostatics	1.087 (0.362)	1.068 (0.352)	1.129 (0.359)	1.113 (0.352)
Induction	0.256 (0.097)	0.252 (0.096)	0.282 (0.102)	0.280 (0.102)
δ^{HF}	0.241 (0.068)	0.244 (0.067)	0.272 (0.077)	0.276 (0.077)
Dispersion	0.836 (0.330)	0.822 (0.349)	0.823 (0.331)	0.820 (0.350)
Total Energy				
<i>RMSE</i>	1.549 (0.448)	1.597 (0.450)	1.482 (0.454)	1.532 (0.458)
$\ MSE\ $	0.160 (0.065)	0.160 (0.084)	0.149 (0.057)	0.204 (0.130)

S7 Monomer Geometries

Geometries for each molecule in the 91 dimer test set are listed below, in alphabetical order. Also listed are the relevant energies (highest occupied molecular orbital and ionization potential) for the asymptotic correction required in DFT-SAPT calculations of each molecule. All asymptotic corrections were performed at a PBE0/aug-cc-pVTZ level of theory. Distances and energies are in a.u.

Table S6. Cartesian coordinates for each molecule in the 91 dimer test set. HOMO and I.P. values, necessary for DFT-SAPT calculations, are also shown. All units are in a.u.

Acetone			
C	0.000000	0.000000	-2.280333
O	0.000000	0.000000	0.000000
C	0.000000	2.435101	-3.793814
C	0.000000	-2.435101	-3.793814
H	0.000000	4.050439	-2.525430
H	0.000000	-4.050439	-2.525430
H	1.657668	2.514281	-5.019869
H	-1.657668	2.514281	-5.019869
H	-1.657668	-2.514281	-5.019869
H	1.657668	-2.514281	-5.019869
HOMO:		-0.266741	
I.P.:		0.35386979	
Ar			
Ar	0.000000	0.000000	0.000000
HOMO:		-0.440599	
I.P.:		0.58049447	
Chloromethane			
C	0.000000	0.000000	-3.365602
Cl	0.000000	0.000000	0.000000
H	1.969851	0.000000	-4.102784
H	-0.984925	1.705856	-4.102784
H	-0.984925	-1.705856	-4.102784
HOMO:		-0.313074	
I.P.:		0.41507894	
CO ₂			
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.196051
O	0.000000	0.000000	-2.196051

Table S6 – continued from previous page

HOMO:	-0.394037		
I.P.:	0.51235857		
Dimethyl Ether			
O	0.000000	0.000000	0.000000
C	0.000000	2.205121	-1.495718
C	0.000000	-2.205121	-1.495718
H	0.000000	3.871860	-0.266451
H	0.000000	-3.871860	-0.266451
H	1.691305	2.227420	-2.690781
H	-1.691305	2.227420	-2.690781
H	-1.691305	-2.227420	-2.690781
H	1.691305	-2.227420	-2.690781
HOMO: -0.272835			
I.P.:	0.36469012		
Ethane			
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.902619
H	-1.926009	0.000000	0.735670
H	0.963004	1.667872	0.735670
H	0.963004	-1.667872	0.735670
H	1.926009	0.000000	-3.638290
H	-0.963004	-1.667872	-3.638290
H	-0.963004	1.667872	-3.638290
HOMO: -0.353672			
I.P.:	0.45125450		
Ethanol			
C	4.487344	-0.256436	0.000000
C	2.242538	1.511403	0.000000
O	0.000000	0.000000	0.000000
H	-1.392728	1.194685	0.000000
H	6.208128	0.902911	0.000000
H	4.356008	-1.440160	1.675998
H	4.356008	-1.440160	-1.675998
H	2.199641	2.699285	1.672786
H	2.199641	2.699285	-1.672786
HOMO: -0.287342			
I.P.:	0.38582676		
Ethene			

Table S6 – continued from previous page

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.530343
H	0.000000	1.755367	1.063160
H	0.000000	-1.755367	1.063160
H	0.000000	1.755367	-3.593503
H	0.000000	-1.755367	-3.593503
HOMO:		-0.288580	
I.P.:		0.38518748	
H₂O			
O	0.000000	0.000000	0.000000
H	0.000000	1.430901	-1.108324
H	0.000000	-1.430901	-1.108324
HOMO:		-0.333820	
I.P.:		0.46592291	
Methane			
C	0.000000	0.000000	0.000000
H	1.185992	1.185992	1.185992
H	1.185992	-1.185992	-1.185992
H	-1.185992	1.185992	-1.185992
H	-1.185992	-1.185992	1.185992
HOMO:		-0.403996	
I.P.:		0.51955025	
Methanol			
C	0.000000	2.696639	0.000000
O	0.000000	0.000000	0.000000
H	-1.947174	3.401885	0.000000
H	0.973776	3.401885	1.686392
H	0.973776	3.401885	-1.686392
H	1.709635	-0.584303	0.000000
HOMO:		-0.292049	
I.P.:		0.39901686	
Methyl Amine			
C	0.000000	2.779976	0.000000
N	0.000000	0.000000	0.000000
H	-1.887836	3.667203	0.000000
H	1.026877	3.452719	1.668817
H	1.026877	3.452719	-1.668817
H	-0.960170	-0.632113	-1.537670
H	-0.960170	-0.632113	1.537670

Table S6 – continued from previous page

HOMO:	-0.255840		
I.P.:	0.35552078		
NH₃			
N	0.000000	0.000000	0.000000
H	0.000000	-1.771996	-0.721119
H	1.534647	0.886093	-0.721119
H	-1.534647	0.886093	-0.721119
HOMO:	-0.284421		
I.P.:	0.39987353		

S8 Homomonomeric Parameters

Parameters for each molecule (as fit to homomonomeric dimers) are given for the Slater-ISA FF, the Born-Mayer-IP FF, and the Born-Mayer-sISA FF. Multipole moments are listed in the first subsection, as these values are identical for all force fields. The next subsections list A_i , B_i , $C_{i,n}$ parameters for each atom type in each molecule, as well as Drude oscillator charges Q_{drude} .

S8.1 Multipole Moments

Multipole moments for each atom in each molecule are listed in Table S7. Multipoles are expressed in spherical form following notation used by Stone.⁵ Note that the global coordinate system is used, with molecular geometries as in Table S6.

Table S7. Multipole moments for each molecule in the 91 dimer test set.

Atomtype	Q_{00}	Q_{10}	Q_{11c}	Q_{11s}	Q_{20}	Q_{21c}	Q_{21s}	Q_{22c}	Q_{22s}
Acetone									
C	0.822823	0.032377	-0.000000	0.000008	0.061201	0.000000	0.000010	0.069618	-0.000000
O	-0.566051	0.052408	0.000000	-0.000006	-0.010114	-0.000000	-0.000005	0.208541	0.000000
C	-0.643920	-0.019563	0.000000	0.018539	-0.032511	-0.000000	0.055572	0.026108	0.000000
C	-0.643917	-0.019574	-0.000000	-0.018565	-0.032523	-0.000000	-0.055581	0.026137	-0.000000
H	0.183107	0.008510	0.000000	0.005856	0.003477	0.000000	-0.014721	0.007936	-0.000000
H	0.183102	0.008518	0.000000	-0.005869	0.003477	0.000000	0.014719	0.007935	0.000000
H	0.166216	-0.003633	0.013504	0.002747	-0.004132	0.004151	0.000390	-0.005004	-0.001098
H	0.166216	-0.003633	-0.013504	0.002747	-0.004132	-0.004151	0.000390	-0.005004	0.001098
H	0.166211	-0.003643	-0.013515	-0.002750	-0.004130	-0.004151	-0.000390	-0.005001	-0.001097
H	0.166211	-0.003643	0.013515	-0.002750	-0.004130	0.004151	-0.000390	-0.005001	0.001097

Table S7 – continued from previous page

Atomtype	Q_{00}	Q_{10}	Q_{11c}	Q_{11s}	Q_{20}	Q_{21c}	Q_{21s}	Q_{22c}	Q_{22s}
Ar									
Ar	-0.000001	0.000000	-0.000000	-0.000000	0.000000	-0.000000	0.000000	0.000000	-0.000000
Chloromethane									
C	-0.129184	0.150325	0.000110	-0.000000	0.087465	-0.000447	-0.000000	0.001151	-0.000000
Cl	-0.210641	0.052239	0.000658	0.000000	0.877399	-0.001560	-0.000000	-0.001996	0.000000
H	0.113201	0.008115	-0.002774	0.000000	0.004064	-0.006342	-0.000000	0.042912	-0.000000
H	0.113312	0.008567	0.001173	-0.002103	0.003553	0.003107	-0.005492	-0.021408	-0.037132
H	0.113312	0.008567	0.001173	0.002103	0.003553	0.003106	0.005492	-0.021408	0.037132
CO₂									
C	0.875432	-0.000029	-0.000000	0.000000	0.099260	0.000000	-0.000000	0.000000	-0.000000
O	-0.437738	0.119374	0.000000	-0.000000	-0.114162	0.000000	0.000000	-0.000000	-0.000000
O	-0.437693	-0.119229	0.000000	-0.000000	-0.113954	-0.000000	0.000000	-0.000000	-0.000000
Dimethyl Ether									
O	-0.314909	-0.206124	-0.000000	0.000003	-0.151378	0.000000	-0.000032	-0.276448	0.000000
C	-0.008061	0.073831	0.000000	-0.137375	-0.039589	-0.000000	-0.120322	-0.187908	-0.000000
C	-0.008074	0.073826	0.000000	0.137356	-0.039615	-0.000000	0.120322	-0.187889	-0.000000
H	0.081597	0.035961	0.000000	0.027126	0.012620	-0.000000	-0.010743	-0.027848	0.000000
H	0.081596	0.035969	0.000000	-0.027141	0.012620	-0.000000	0.010745	-0.027846	-0.000000
H	0.041964	-0.011654	0.038697	-0.012289	-0.011465	-0.006417	-0.031313	-0.005419	-0.013633
H	0.041964	-0.011654	-0.038697	-0.012289	-0.011465	0.006417	-0.031313	-0.005420	0.013633
H	0.041961	-0.011665	-0.038709	0.012282	-0.011462	0.006414	0.031315	-0.005417	-0.013630
H	0.041961	-0.011665	0.038709	0.012282	-0.011462	-0.006414	0.031315	-0.005417	0.013630
Ethane									
C	-0.252064	-0.105205	0.000223	0.000000	0.017039	0.000023	0.000000	0.000263	0.000000
C	-0.252073	0.105203	-0.000223	-0.000000	0.017046	0.000023	-0.000000	0.000263	0.000000
H	0.084138	-0.002714	-0.029130	0.000000	0.010090	-0.004825	-0.000000	0.005963	0.000000
H	0.083964	-0.002670	0.014633	0.025321	0.010216	0.002349	0.004123	-0.003080	0.005170
H	0.083964	-0.002670	0.014633	-0.025321	0.010216	0.002349	-0.004123	-0.003079	-0.005170
H	0.084139	0.002714	0.029130	0.000000	0.010090	-0.004826	-0.000000	0.005963	-0.000000
H	0.083966	0.002670	-0.014633	-0.025321	0.010216	0.002349	0.004123	-0.003079	0.005170
H	0.083966	0.002670	-0.014633	0.025321	0.010216	0.002349	-0.004123	-0.003079	-0.005170
Ethanol									
C	-0.454684	-0.000000	-0.039641	0.014163	-0.008827	0.000000	0.000000	0.010209	-0.032164
C	0.358740	0.000000	-0.069875	-0.132865	-0.113067	-0.000000	-0.000000	0.068791	0.101359
O	-0.631721	0.000000	0.130683	0.011422	-0.302583	0.000000	-0.000000	0.199670	-0.056302
H	0.378043	0.000000	-0.003297	-0.006693	-0.026225	0.000000	0.000000	0.007122	0.007765
H	0.121728	0.000000	0.012449	0.016567	-0.005502	-0.000000	0.000000	0.003426	0.002573
H	0.133343	0.011880	-0.013005	-0.009345	-0.004744	0.000758	0.003331	0.003627	-0.001624
H	0.133343	-0.011880	-0.013005	-0.009345	-0.004744	-0.000758	-0.003331	0.003627	-0.001624
H	-0.019396	0.060093	-0.004406	0.012749	0.002102	-0.016691	0.024901	0.004948	0.006625
H	-0.019396	-0.060093	-0.004406	0.012749	0.002102	0.016691	-0.024901	0.004948	0.006625

Table S7 – continued from previous page

Atomtype	Q_{00}	Q_{10}	Q_{11c}	Q_{11s}	Q_{20}	Q_{21c}	Q_{21s}	Q_{22c}	Q_{22s}
Ethene									
C	-0.313293	-0.027522	-0.000000	-0.000000	-0.004502	-0.000000	-0.000000	-0.032496	-0.000000
C	-0.313300	0.027520	0.000000	0.000000	-0.004500	-0.000000	0.000000	-0.032493	0.000000
H	0.156647	0.006874	0.000000	0.030185	0.010877	0.000000	-0.012146	-0.002508	0.000000
H	0.156647	0.006874	0.000000	-0.030185	0.010877	0.000000	0.012146	-0.002508	-0.000000
H	0.156649	-0.006874	-0.000000	0.030185	0.010877	0.000000	0.012146	-0.002508	-0.000000
H	0.156649	-0.006874	-0.000000	-0.030185	0.010877	-0.000000	-0.012146	-0.002508	-0.000000
H₂O									
O	-0.824768	0.164548	-0.000000	-0.000000	0.003122	-0.000000	0.000000	-0.509003	0.000000
H	0.412384	0.015330	-0.000000	0.011691	0.007533	-0.000000	-0.005192	-0.026364	-0.000000
H	0.412384	0.015330	0.000000	-0.011691	0.007533	-0.000000	0.005192	-0.026364	-0.000000
Methane									
C	-0.671142	-0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.000000	0.000000
H	0.167785	0.009014	0.009014	0.009014	-0.000000	-0.006242	-0.006242	-0.000000	-0.006242
H	0.167785	-0.009014	0.009014	-0.009014	0.000000	0.006242	-0.006242	0.000000	0.006242
H	0.167785	-0.009014	-0.009014	0.009014	0.000000	-0.006242	0.006242	-0.000000	0.006242
H	0.167785	0.009014	-0.009014	-0.009014	-0.000000	0.006242	0.006242	0.000000	-0.006242
Methanol									
C	0.018572	0.000000	-0.008053	-0.180359	-0.134131	-0.000000	-0.000000	-0.143630	0.003983
O	-0.576407	0.000000	-0.041545	0.164405	-0.281268	0.000000	0.000000	-0.044235	-0.176494
H	0.083857	0.000000	-0.047267	0.000587	-0.034067	0.000000	-0.000000	-0.017460	0.002169
H	0.043088	0.042570	0.022329	0.000573	0.002279	0.019107	-0.006061	-0.023729	0.000122
H	0.043088	-0.042570	0.022329	0.000573	0.002279	-0.019107	0.006061	-0.023729	0.000122
H	0.387801	-0.000000	-0.004333	-0.003390	-0.025935	-0.000000	0.000000	-0.015610	-0.005664
Methyl Amine									
C	0.022408	-0.000000	-0.001858	-0.174589	-0.015557	-0.000000	-0.000000	-0.132232	0.003031
N	-0.772659	-0.000000	-0.030670	0.191476	0.224002	-0.000000	-0.000000	-0.352581	0.274836
H	0.016969	-0.000000	-0.046914	0.007332	-0.030932	-0.000000	-0.000000	0.000177	-0.005506
H	0.059643	0.038600	0.026296	-0.006486	-0.006433	0.020931	0.002691	-0.026049	-0.000003
H	0.059643	-0.038600	0.026296	-0.006486	-0.006433	-0.020931	-0.002691	-0.026049	-0.000003
H	0.306998	-0.008938	0.012951	0.001795	-0.000413	-0.010919	-0.012059	-0.028898	0.012496
H	0.306998	0.008938	0.012951	0.001795	-0.000413	0.010919	0.012059	-0.028898	0.012496
NH₃									
N	-1.050272	0.113155	0.000000	0.000637	-0.661903	0.000000	-0.001312	0.001250	-0.000000
H	0.350420	0.018866	0.000000	-0.007172	-0.023309	-0.000000	-0.004344	0.015849	0.000000
H	0.349926	0.018818	0.006316	0.003662	-0.023015	0.003834	0.002117	-0.007862	-0.013755
H	0.349926	0.018818	-0.006316	0.003662	-0.023015	-0.003834	0.002117	-0.007862	0.013755

S8.2 Slater-ISA FF Parameters

A_i , B_i , $C_{i,n}$ parameters for the Slater-ISA FF are listed in Table S8. A_{ij} , B_{ij} , and $C_{ij,n}$ parameters can be determined from the following combination rules:

$$\begin{aligned} A_{ij} &= A_i A_j \\ B_{ij} &= \sqrt{B_i B_j} \\ C_{ij,n} &= \sqrt{C_{i,n} C_{j,n}} \end{aligned}$$

Parameters are given for each unique atom type in each molecule; where multiple atom types exist for a particular element, atom types are labeled first with the element name and second by connectivity. Thus the carbonyl carbon in acetone is labeled ‘CO’, whereas the methyl carbon is labeled ‘CH’.

The total force field energy is defined by the following equations:

$$\begin{aligned} B_i &= B_i^{ISA} \\ P(B_{ij}, r_{ij}) &= \frac{1}{3}(B_{ij}r_{ij})^2 + B_{ij}r_{ij} + 1 \\ x &= B_{ij}r_{ij} - \frac{2B_{ij}^2r_{ij} + 3B_{ij}}{B_{ij}^2r_{ij}^2 + 3B_{ij}r_{ij} + 3}r_{ij} \\ f_{2n}(x) &= 1 - e^{-x} \sum_{k=0}^{2n} \frac{(x)^k}{k!} \\ V_{ij}^{\text{exch}} &= A_{ij}^{\text{exch}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) \\ V_{ij}^{\text{elst}} &= -A_{ij}^{\text{elst}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) + \sum_{tu} Q_t^i T_{tu} Q_u^j \\ V_{ij}^{\text{ind}} &= -A_{ij}^{\text{ind}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) + V_{\text{shell}}^{(2)} \\ V_{ij}^{\delta^{\text{HF}}} &= -A_{ij}^{\delta^{\text{HF}}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) + V_{\text{shell}}^{(3-\infty)} \\ V_{ij}^{\text{disp}} &= - \sum_{n=3}^6 f_{2n}(x) \frac{C_{ij,2n}}{r_{ij}^{2n}} \\ V_{\text{FF}} &= \sum_{ij} V_{ij}^{\text{elst}} + V_{ij}^{\text{exch}} + V_{ij}^{\text{ind}} + V_{ij}^{\delta^{\text{HF}}} + V_{ij}^{\text{disp}} \end{aligned}$$

The Tang-Toennies damping function f is defined in the main text; the polarization energy $V_{\text{shell}} = V_{\text{shell}}^{(2)} + V_{\text{shell}}^{(3-\infty)}$ arising from drude oscillators is defined in ref. 1.

Table S8. Slater-ISA FF parameters.

Atomtype	A_{exch}	A_{elst}	A_{ind}	$A_{\delta HF}$	B	C_6	C_8	C_{10}	C_{12}	Q_{drude}
Acetone										
CO	3.804952	2.105976	2.063011	0.491181	2.604683	13.406	145.511	6091.546	80859.461	-0.4541
OC	4.178782	2.590649	0.144518	1.137061	2.360638	22.881	353.376	10131.697	174478.272	-0.9327
CH	2.204201	1.308847	0.000000	0.029237	1.932603	23.494	353.376	4001.387	41152.121	-1.2947
HC	0.591374	0.289797	0.178630	0.223158	2.266776	2.245	42.098	1104.938	0.000	0.0000
Ar										
Ar	6.130962	3.607145	0.816138	1.255571	2.183303	71.007	1556.382	37687.507	709695.360	-1.0694
Chloromethane										
H	0.971257	0.472534	0.222683	0.447693	2.621813	2.245	42.098	1104.938	0.000	0.0000
C	6.467461	3.353818	0.506661	0.000000	2.344966	23.494	353.376	4001.387	41152.121	-1.2833
Cl	5.963451	3.862537	1.467911	1.098777	2.052787	93.240	1615.853	65715.929	1310829.439	-1.2661
CO₂										
C	2.944847	1.541728	1.090558	0.180486	2.329865	19.902	392.050	6560.549	144984.178	-0.8645
O	4.810107	2.675187	0.377269	1.109199	2.489856	15.043	264.275	6361.827	104726.425	-0.7611
Dimethyl Ether										
H	0.581181	0.286373	0.143439	0.202139	2.167921	2.245	42.098	1104.938	0.000	0.0000
C	1.767333	1.211427	0.000000	0.000000	2.023109	23.494	353.376	4001.387	41152.121	-1.3211
O	4.345253	2.836892	0.461020	1.090828	2.440026	12.235	266.573	6615.160	125669.048	-0.0001
Ethane										
H	0.631650	0.315461	0.131793	0.219936	2.230203	2.245	42.098	1104.938	0.000	0.0000
C	1.910136	1.281663	0.141830	0.053648	2.005074	23.494	353.376	4001.387	41152.121	-1.2959
Ethanol										
CO	2.913808	2.307707	0.000000	0.000000	2.238251	23.494	353.376	4001.387	41152.121	-1.2545
OH	4.405898	2.864522	0.249909	0.990766	2.364797	14.592	320.063	8074.269	154258.592	-0.8362
HC	0.567445	0.273172	0.150893	0.203159	2.206603	2.245	42.098	1104.938	0.000	0.0000
HO	0.202063	0.069581	0.160674	0.066068	2.044162	1.627	16.150	918.236	0.000	0.0000
CH	2.007588	1.232904	0.053800	0.111974	1.957305	23.494	353.376	4001.387	41152.121	-1.1875
Ethene										
C	2.776192	1.784015	0.373691	0.595405	1.917413	28.252	422.533	9835.457	152927.660	-1.2627
H	0.631922	0.201132	0.133224	0.230793	2.464030	2.245	42.098	1104.938	0.000	0.0000
H₂O										
H	0.272492	0.104357	0.179978	0.076004	2.167067	0.776	3.042	270.370	0.000	0.0000
O	3.837717	2.565879	0.049844	0.819591	2.288712	25.358	536.662	12267.338	220953.821	-0.9794
Methane										
C	2.117483	1.363604	0.080199	0.139272	1.916253	23.494	353.376	4001.387	41152.121	-1.2959
H	0.832442	0.378112	0.197234	0.275122	2.444062	2.245	42.098	1104.938	0.000	0.0000
Methanol										
CO	1.716271	1.018657	0.075645	0.000000	2.015251	23.494	353.376	4001.387	41152.121	-1.2724
OH	4.379738	2.834034	0.232433	0.972620	2.373075	14.592	320.063	8074.269	154258.592	-0.8102
HO	0.192535	0.064937	0.156032	0.067016	2.080537	1.627	16.150	918.236	0.000	0.0000
HC	0.572402	0.299836	0.151486	0.205148	2.201724	2.245	42.098	1104.938	0.000	0.0000

Table S8 – continued from previous page

Atomtype	A_{exch}	A_{elst}	A_{ind}	$A_{\delta HF}$	B	C_6	C_8	C_{10}	C_{12}	Q_{drude}
Methyl Amine										
HN	0.297883	0.075404	0.157275	0.106014	2.264301	1.627	16.150	918.236	0.000	0.0000
N	3.141193	2.168747	0.193794	0.658763	2.020158	22.664	623.023	19359.417	472166.465	-1.1026
C	2.331206	1.684778	0.103555	0.000000	2.048098	23.494	353.376	4001.387	41152.121	-1.2667
HC	0.549424	0.253325	0.141786	0.212025	2.202002	2.245	42.098	1104.938	0.000	0.0000
NH₃										
H	0.456908	0.162377	0.216086	0.153989	2.457227	1.627	16.150	918.236	0.000	-1.1928
N	2.628746	1.857589	0.105469	0.514765	1.941661	22.664	623.023	19359.417	472166.465	0.0000

S8.3 Born-Mayer-IP FF Parameters

A_i , B_i , $C_{i,n}$ parameters for the Born-Mayer-IP FF are listed in Table S9. A_{ij} , B_{ij} , and $C_{ij,n}$ parameters can be determined from the following combination rules:

$$\begin{aligned} A_{ij} &= A_i A_j \\ B_{ij} &= \frac{B_i B_j (B_i + B_j)}{B_i^2 + B_j^2} \\ C_{ij,n} &= \sqrt{C_{i,n} C_{j,n}} \end{aligned}$$

Parameters are given for each unique atom type in each molecule; where multiple atom types exist for a particular element, atom types are labeled first with the element name and second by connectivity. Thus the carbonyl carbon in acetone is labeled ‘CO’, whereas the methyl carbon is labeled ‘CH’.

The total force field energy is defined by the following equations:

$$\begin{aligned} B_i &= 2\sqrt{2IP_i} \\ P(B_{ij}, r_{ij}) &= 1 \\ x &= B_{ij}r_{ij} \\ f_{2n}(x) &= 1 - e^{-x} \sum_{k=0}^{2n} \frac{(x)^k}{k!} \\ V_{ij}^{\text{exch}} &= A_{ij}^{\text{exch}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) \\ V_{ij}^{\text{elst}} &= -A_{ij}^{\text{elst}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) + \sum_{tu} Q_t^i T_{tu} Q_u^j \\ V_{ij}^{\text{ind}} &= -A_{ij}^{\text{ind}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) + V_{\text{shell}}^{(2)} \\ V_{ij}^{\delta\text{HF}} &= -A_{ij}^{\delta\text{HF}} P(B_{ij}, r_{ij}) \exp(-B_{ij}r_{ij}) + V_{\text{shell}}^{(3-\infty)} \\ V_{ij}^{\text{disp}} &= - \sum_{n=3}^6 f_{2n}(x) \frac{C_{ij,2n}}{r_{ij}^{2n}} \\ V_{\text{FF}} &= \sum_{ij} V_{ij}^{\text{elst}} + V_{ij}^{\text{exch}} + V_{ij}^{\text{ind}} + V_{ij}^{\delta\text{HF}} + V_{ij}^{\text{disp}} \end{aligned}$$

The Tang-Toennies damping function f is defined in the main text; the polarization energy E_{pol} arising from drude oscillators is defined in ref. 1.

Table S9. Born-Mayer-IP FF parameters.

Atomtype	A_{exch}	A_{elst}	A_{ind}	$A_{\delta HF}$	B	C_6	C_8	C_{10}	C_{12}	Q_{drude}
Acetone										
CO	5.567455	2.919090	2.729352	0.705232	1.819469	13.406	145.511	6091.546	80859.461	-0.4541
OC	12.941114	8.025300	0.409461	3.556175	2.000912	22.881	353.376	10131.697	174478.272	-0.9327
CH	10.952564	6.356726	0.000000	0.230007	1.819469	23.494	353.376	4001.387	41152.121	-1.2947
HC	2.111731	1.047688	0.616407	0.767149	1.999464	2.245	42.098	1104.938	0.000	0.0000
Ar										
Ar	50.711700	26.176317	5.968585	9.099102	2.152496	71.007	1556.382	37687.507	709695.360	-1.0694
Chloromethane										
H	1.773426	0.876699	0.418998	0.906852	1.999464	2.245	42.098	1104.938	0.000	0.0000
C	12.813654	7.191403	1.079346	0.000000	1.819469	23.494	353.376	4001.387	41152.121	-1.2833
Cl	34.276817	20.817366	7.997654	5.798695	1.952538	93.240	1615.853	65715.929	1310829.439	-1.2661
CO₂										
C	5.176487	2.984618	2.277174	0.274561	1.819469	19.902	392.050	6560.549	144984.178	-0.8645
O	11.349651	6.499242	0.865006	2.716049	2.000912	15.043	264.275	6361.827	104726.425	-0.7611
Dimethyl Ether										
H	2.329781	1.183750	0.564499	0.806639	1.999464	2.245	42.098	1104.938	0.000	0.0000
C	8.563364	4.968189	0.131071	0.074779	1.819469	23.494	353.376	4001.387	41152.121	-1.3211
O	11.989376	7.808839	1.317489	3.114127	2.000912	12.235	266.573	6615.160	125669.048	-0.0001
Ethane										
H	2.250973	1.158733	0.485471	0.781917	1.999464	2.245	42.098	1104.938	0.000	0.0000
C	10.461511	5.586592	0.612844	0.406278	1.819469	23.494	353.376	4001.387	41152.121	-1.2959
Ethanol										
CO	8.222663	5.833862	0.000000	0.000000	1.819469	23.494	353.376	4001.387	41152.121	-1.2545
OH	13.923864	8.979075	0.940969	3.229934	2.000912	14.592	320.063	8074.269	154258.592	-0.8362
HC	2.149784	1.068436	0.570784	0.766874	1.999464	2.245	42.098	1104.938	0.000	0.0000
HO	1.019177	0.356079	0.751733	0.328847	1.999464	1.627	16.150	918.236	0.000	0.0000
CH	10.141256	5.806452	0.278019	0.593277	1.819469	23.494	353.376	4001.387	41152.121	-1.1875
Ethene										
C	15.765638	9.111034	1.960627	2.997793	1.819469	28.252	422.533	9835.457	152927.660	-1.2627
H	1.601044	0.584328	0.335499	0.611640	1.999464	2.245	42.098	1104.938	0.000	0.0000
H₂O										
H	1.141499	0.446043	0.697274	0.318684	1.999464	0.776	3.042	270.370	0.000	0.0000
O	13.932606	9.201940	0.282581	2.951132	2.000912	25.358	536.662	12267.338	220953.821	-0.9794
Methane										
C	11.713473	6.761088	0.527832	0.632892	1.819469	23.494	353.376	4001.387	41152.121	-1.2959
H	2.225001	1.035042	0.508080	0.739327	1.999464	2.245	42.098	1104.938	0.000	0.0000
Methanol										
CO	7.433631	4.180536	0.401704	0.000000	1.819469	23.494	353.376	4001.387	41152.121	-1.2724
OH	13.542794	8.726014	0.795157	3.058222	2.000912	14.592	320.063	8074.269	154258.592	-0.8102
HO	0.922058	0.309528	0.702616	0.306417	1.999464	1.627	16.150	918.236	0.000	0.0000
HC	2.230349	1.176985	0.567045	0.789220	1.999464	2.245	42.098	1104.938	0.000	0.0000
Methyl Amine										

Table S9 – continued from previous page

Atomtype	A_{exch}	A_{elst}	A_{ind}	$A_{\delta HF}$	B	C_6	C_8	C_{10}	C_{12}	Q_{drude}
HN	1.224682	0.421352	0.547503	0.429622	1.999464	1.627	16.150	918.236	0.000	0.0000
N	23.338368	15.290981	1.429713	4.422039	2.067111	22.664	623.023	19359.417	472166.465	-1.1026
C	10.818390	6.130391	0.375108	0.000000	1.819469	23.494	353.376	4001.387	41152.121	-1.2667
HC	2.000843	1.025883	0.546828	0.808373	1.999464	2.245	42.098	1104.938	0.000	0.0000
NH₃										
H	1.291205	0.567250	0.560466	0.444433	1.999464	1.627	16.150	918.236	0.000	-1.1928
N	23.837579	14.999330	0.902266	4.021003	2.067111	22.664	623.023	19359.417	472166.465	0.0000

S8.4 Born-Mayer-sISA FF Parameters

A_i , B_i , $C_{i,n}$ parameters for the Born-Mayer-sISA FF are listed in Table S10. A_{ij} , B_{ij} , and $C_{ij,n}$ parameters can be determined from the following combination rules:

$$\begin{aligned} A_{ij} &= A_i A_j \\ B_{ij} &= \sqrt{B_i B_j} \\ C_{ij,n} &= \sqrt{C_{i,n} C_{j,n}} \end{aligned}$$

Parameters are given for each unique atom type in each molecule; where multiple atom types exist for a particular element, atom types are labeled first with the element name and second by connectivity. Thus the carbonyl carbon in acetone is labeled ‘CO’, whereas the methyl carbon is labeled ‘CH’.

The total force field energy is defined by the following equations:

$$\begin{aligned} B_i &= 0.84 B_i^{ISA} \\ P(B_{ij}, r_{ij}) &= 1 \\ x &= B_{ij} r_{ij} \\ f_{2n}(x) &= 1 - e^{-x} \sum_{k=0}^{2n} \frac{(x)^k}{k!} \\ V_{ij}^{\text{exch}} &= A_{ij}^{\text{exch}} P(B_{ij}, r_{ij}) \exp(-B_{ij} r_{ij}) \\ V_{ij}^{\text{elst}} &= -A_{ij}^{\text{elst}} P(B_{ij}, r_{ij}) \exp(-B_{ij} r_{ij}) + \sum_{tu} Q_t^i T_{tu} Q_u^j \\ V_{ij}^{\text{ind}} &= -A_{ij}^{\text{ind}} P(B_{ij}, r_{ij}) \exp(-B_{ij} r_{ij}) + V_{\text{shell}}^{(2)} \\ V_{ij}^{\delta\text{HF}} &= -A_{ij}^{\delta\text{HF}} P(B_{ij}, r_{ij}) \exp(-B_{ij} r_{ij}) + V_{\text{shell}}^{(3-\infty)} \\ V_{ij}^{\text{disp}} &= - \sum_{n=3}^6 f_{2n}(x) \frac{C_{ij,2n}}{r_{ij}^{2n}} \\ V_{\text{FF}} &= \sum_{ij} V_{ij}^{\text{elst}} + V_{ij}^{\text{exch}} + V_{ij}^{\text{ind}} + V_{ij}^{\delta\text{HF}} + V_{ij}^{\text{disp}} \end{aligned}$$

The Tang-Toennies damping function f is defined in the main text; the polarization energy $V_{\text{shell}} = V_{\text{shell}}^{(2)} + V_{\text{shell}}^{(3-\infty)}$ arising from drude oscillators is defined in ref. 1.

Table S10. Born-Mayer-sISA FF parameters.

Atomtype	A_{exch}	A_{elst}	A_{ind}	$A_{\delta HF}$	B	C_6	C_8	C_{10}	C_{12}	Q_{drude}
Acetone										
CO	11.298138	6.260674	6.375244	1.474927	2.187934	13.406	145.511	6091.546	80859.461	-0.4541
OC	12.485402	7.747160	0.426691	3.414128	1.982936	22.881	353.376	10131.697	174478.272	-0.9327
CH	6.752770	3.978541	0.000000	0.139991	1.623387	23.494	353.376	4001.387	41152.121	-1.2947
HC	1.703654	0.836792	0.517761	0.641695	1.904091	2.245	42.098	1104.938	0.000	0.0000
Ar										
Ar	17.754951	10.759634	2.431058	3.745351	1.833974	71.007	1556.382	37687.507	709695.360	-1.0694
Chloromethane										
H	2.839538	1.357582	0.664424	1.323373	2.202323	2.245	42.098	1104.938	0.000	0.0000
C	19.308314	10.282602	1.457576	0.000000	1.969771	23.494	353.376	4001.387	41152.121	-1.2833
Cl	17.706793	11.554461	4.398795	3.296506	1.724341	93.240	1615.853	65715.929	1310829.439	-1.2661
CO₂										
C	8.367127	4.534796	3.258447	0.502437	1.957087	19.902	392.050	6560.549	144984.178	-0.8645
O	14.291097	8.007681	1.115752	3.326093	2.091479	15.043	264.275	6361.827	104726.425	-0.7611
Dimethyl Ether										
H	1.669015	0.824934	0.413473	0.583661	1.821054	2.245	42.098	1104.938	0.000	0.0000
C	5.566661	3.695046	0.009130	0.000000	1.699411	23.494	353.376	4001.387	41152.121	-1.3211
O	12.945665	8.498393	1.411434	3.323600	2.049622	12.235	266.573	6615.160	125669.048	-0.0001
Ethane										
H	1.817180	0.907864	0.387236	0.628205	1.873370	2.245	42.098	1104.938	0.000	0.0000
C	6.043273	3.920646	0.401363	0.227334	1.684262	23.494	353.376	4001.387	41152.121	-1.2959
Ethanol										
CO	9.226602	7.053649	0.000000	0.000000	1.880131	23.494	353.376	4001.387	41152.121	-1.2545
OH	13.217432	8.587995	0.791412	3.010794	1.986430	14.592	320.063	8074.269	154258.592	-0.8362
HC	1.619514	0.783441	0.436133	0.585641	1.853547	2.245	42.098	1104.938	0.000	0.0000
HO	0.577312	0.197433	0.455572	0.189697	1.717096	1.627	16.150	918.236	0.000	0.0000
CH	6.248381	3.766536	0.169208	0.364715	1.644136	23.494	353.376	4001.387	41152.121	-1.1875
Ethene										
C	8.247499	5.331602	1.119056	1.784735	1.610627	28.252	422.533	9835.457	152927.660	-1.2627
H	1.870937	0.594220	0.392884	0.678627	2.069785	2.245	42.098	1104.938	0.000	0.0000
H₂O										
H	0.788146	0.300709	0.513573	0.220782	1.820336	0.776	3.042	270.370	0.000	0.0000
O	11.526687	7.698249	0.177170	2.460372	1.922518	25.358	536.662	12267.338	220953.821	-0.9794
Methane										
C	6.266192	4.123257	0.269389	0.480514	1.609652	23.494	353.376	4001.387	41152.121	-1.2959
H	2.471370	1.103960	0.572840	0.792712	2.053012	2.245	42.098	1104.938	0.000	0.0000
Methanol										
CO	5.275558	3.097679	0.245621	0.000000	1.692810	23.494	353.376	4001.387	41152.121	-1.2724
OH	13.144521	8.507288	0.717814	2.940249	1.993383	14.592	320.063	8074.269	154258.592	-0.8102
HO	0.548765	0.182757	0.445382	0.190565	1.747651	1.627	16.150	918.236	0.000	0.0000
HC	1.656132	0.867569	0.436199	0.594834	1.849448	2.245	42.098	1104.938	0.000	0.0000
Methyl Amine										

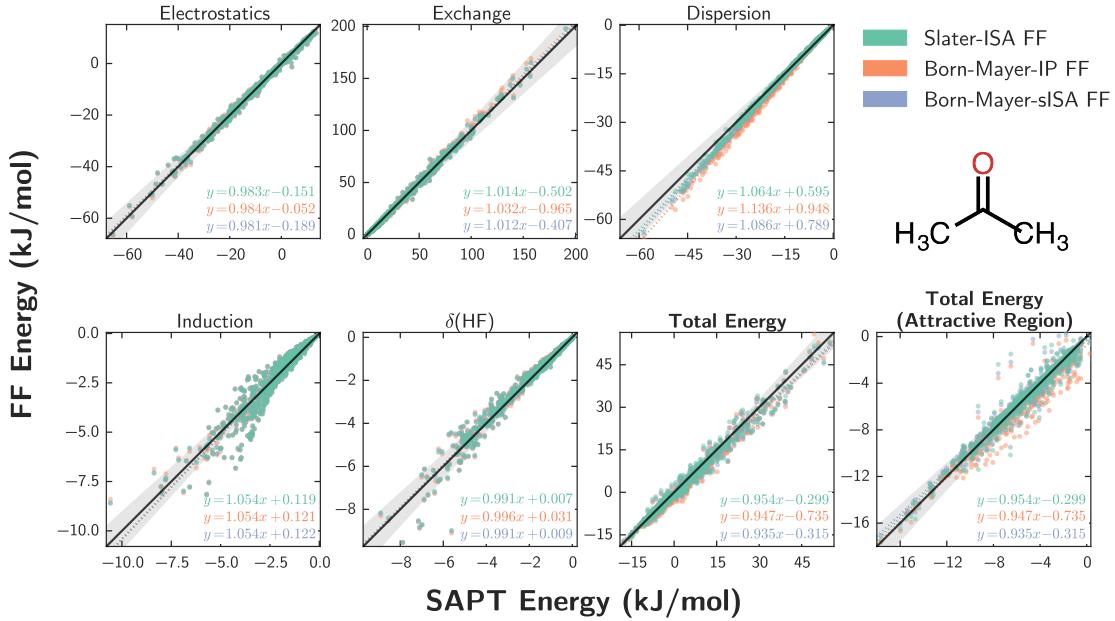
Table S10 – continued from previous page

Atomtype	A_{exch}	A_{elst}	A_{ind}	$A_{\delta HF}$	B	C_6	C_8	C_{10}	C_{12}	Q_{drude}
HN	0.868281	0.222074	0.455689	0.311158	1.902013	1.627	16.150	918.236	0.000	0.0000
N	9.399190	6.470677	0.592158	1.969396	1.696933	22.664	623.023	19359.417	472166.465	-1.1026
C	7.274600	5.119244	0.292498	0.000000	1.720403	23.494	353.376	4001.387	41152.121	-1.2667
HC	1.572214	0.728368	0.413461	0.613379	1.849682	2.245	42.098	1104.938	0.000	0.0000
NH₃										
H	1.346119	0.487459	0.631866	0.455708	2.064071	1.627	16.150	918.236	0.000	-1.1928
N	7.875825	5.515104	0.323871	1.528953	1.630995	22.664	623.023	19359.417	472166.465	0.0000

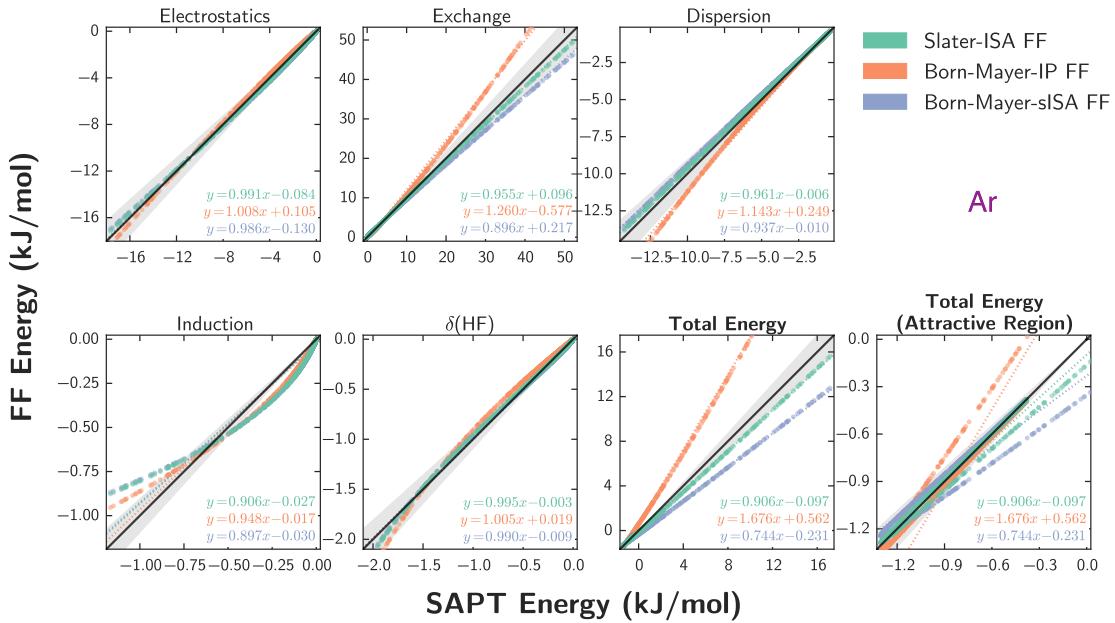
S9 Force Field Fits for Homomonomeric Systems

Scatter plots are shown for each homomonomeric system as an indication of force field quality with respect to DFT-SAPT (PBE0/AC) benchmark energies (Figure S4). As in the main text, fits for each energy component are displayed along with two views of the total interaction energy.

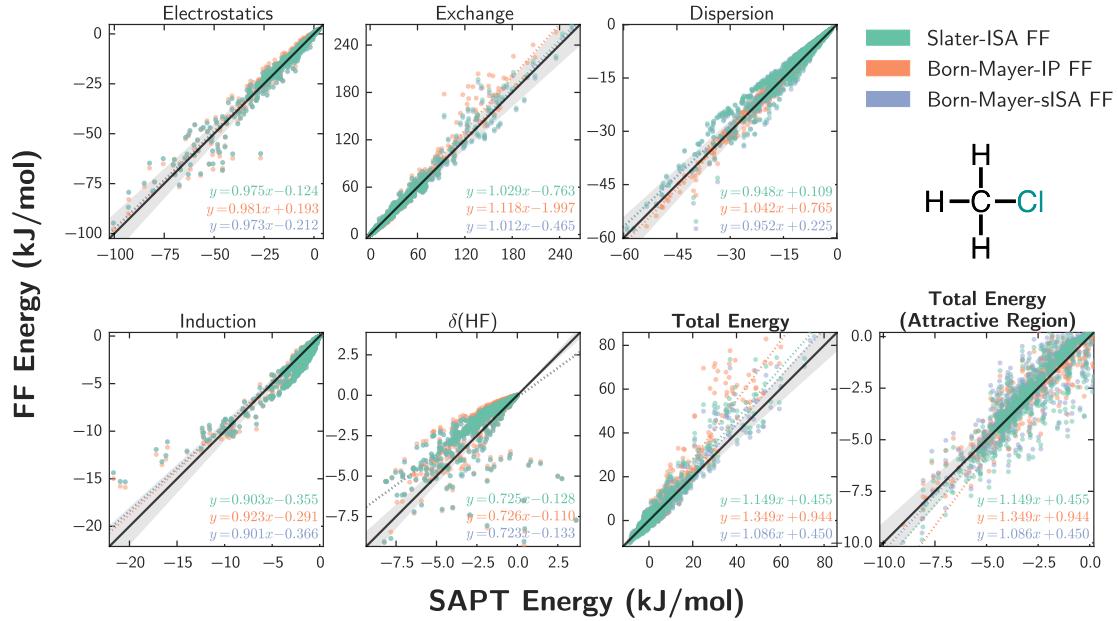
(a) Acetone Dimer



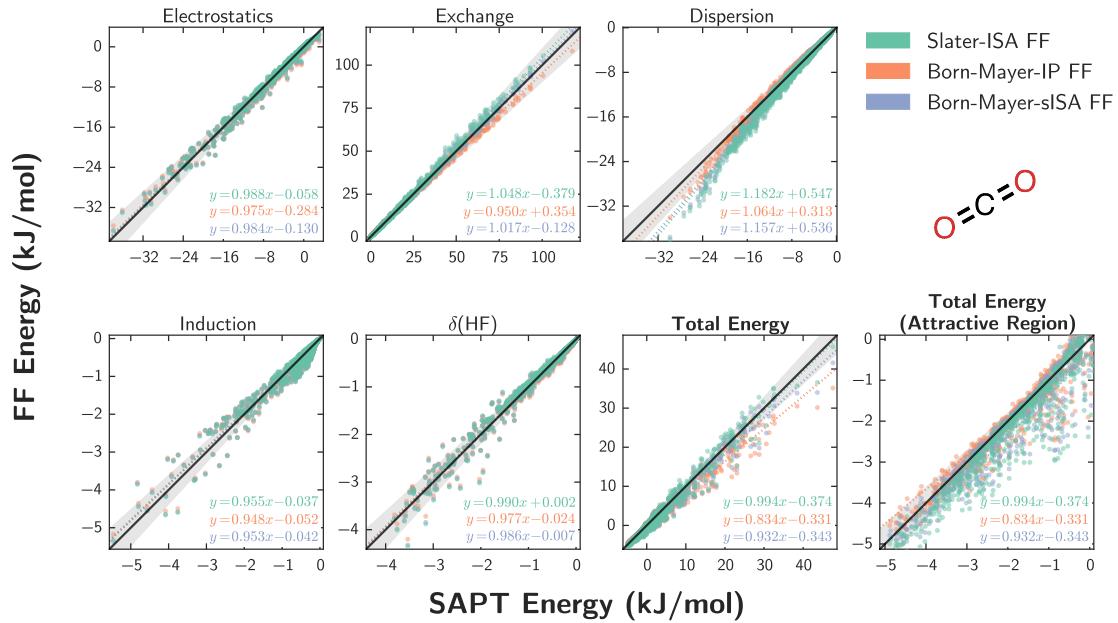
(b) Ar Dimer



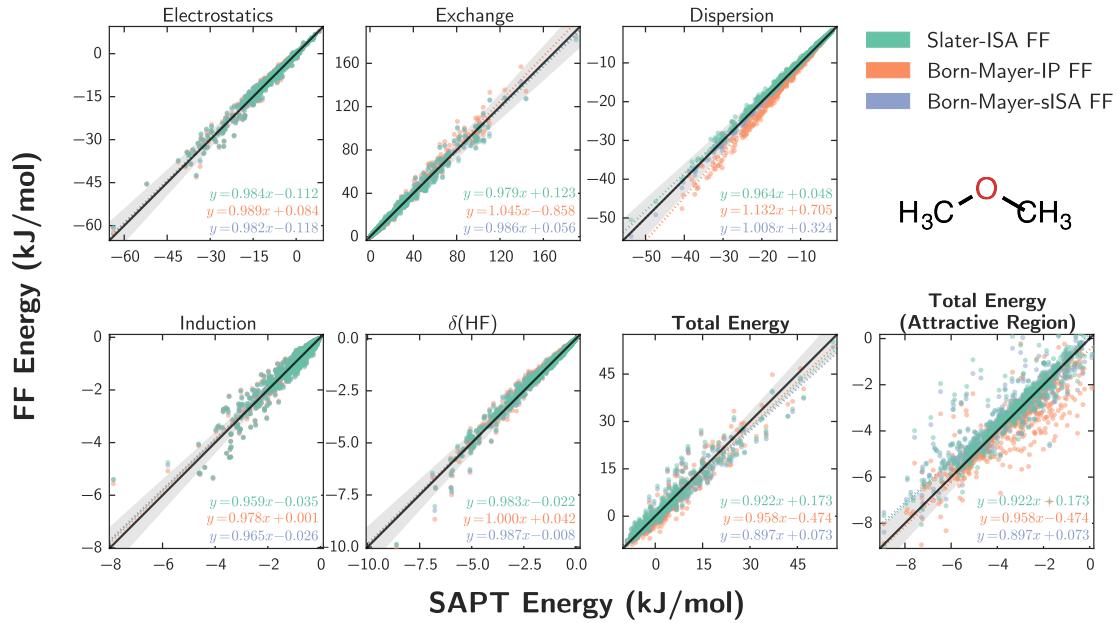
(c) Chloromethane Dimer



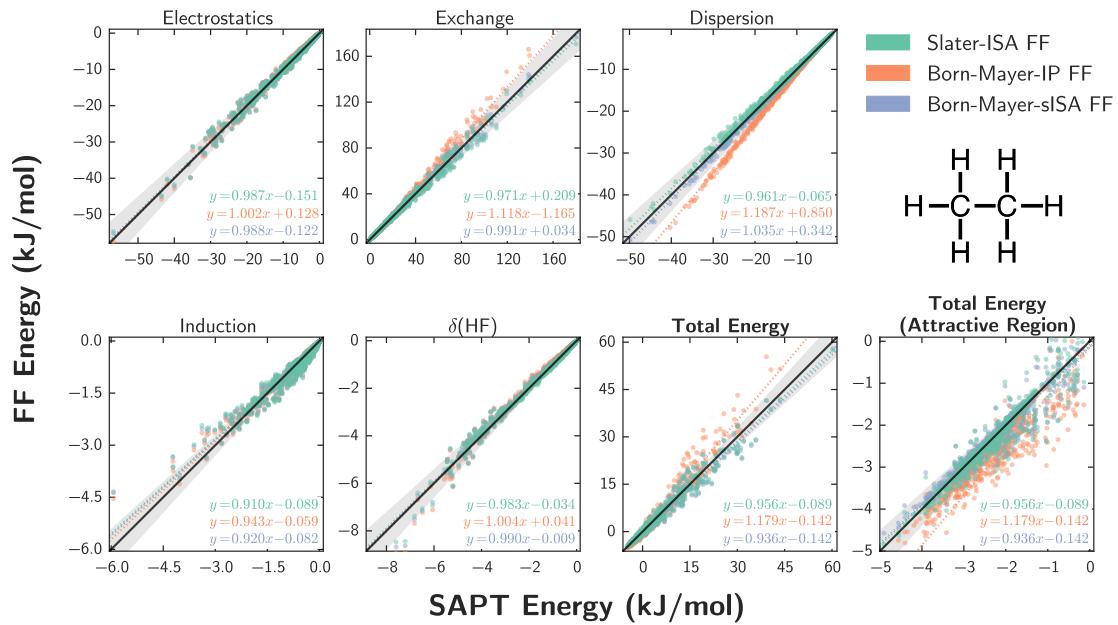
(d) CO₂ Dimer



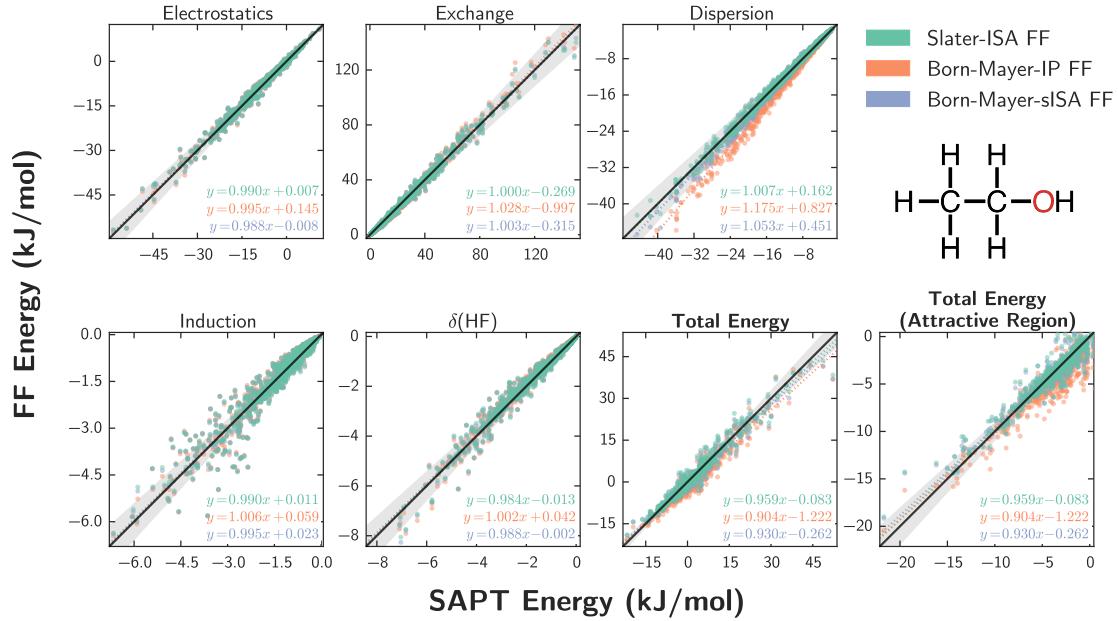
(e) Dimethyl Ether Dimer



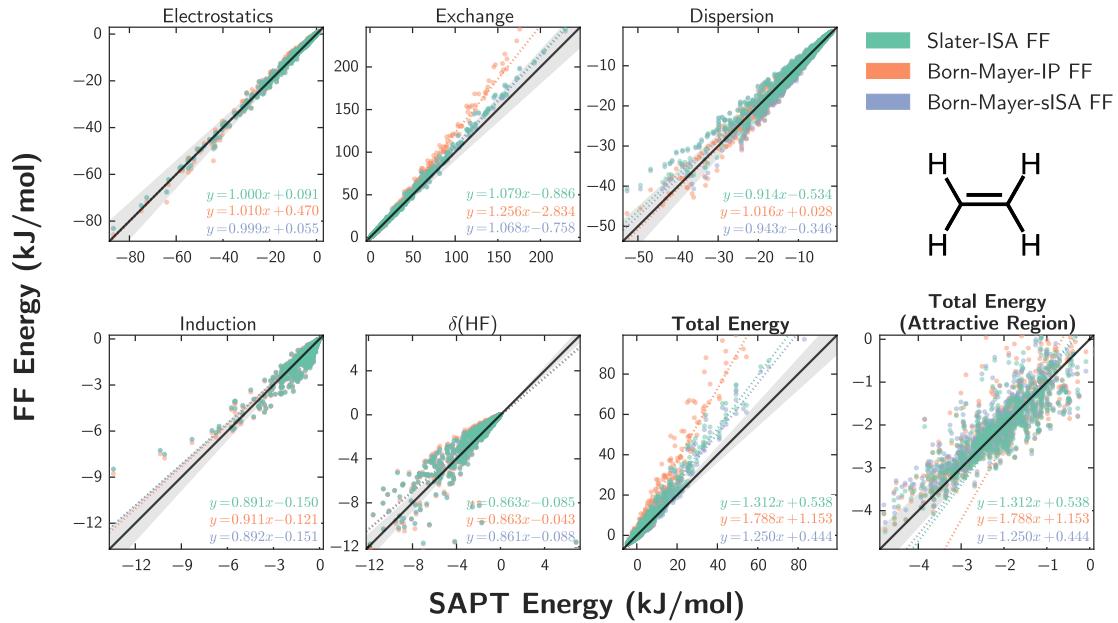
(f) Ethane Dimer



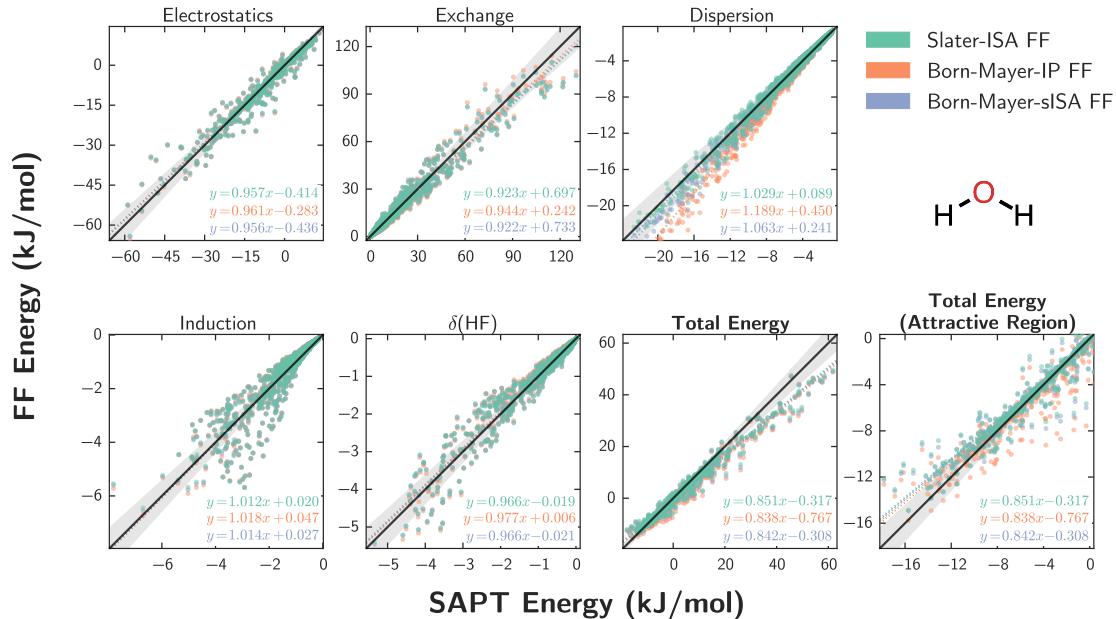
(g) Ethanol Dimer



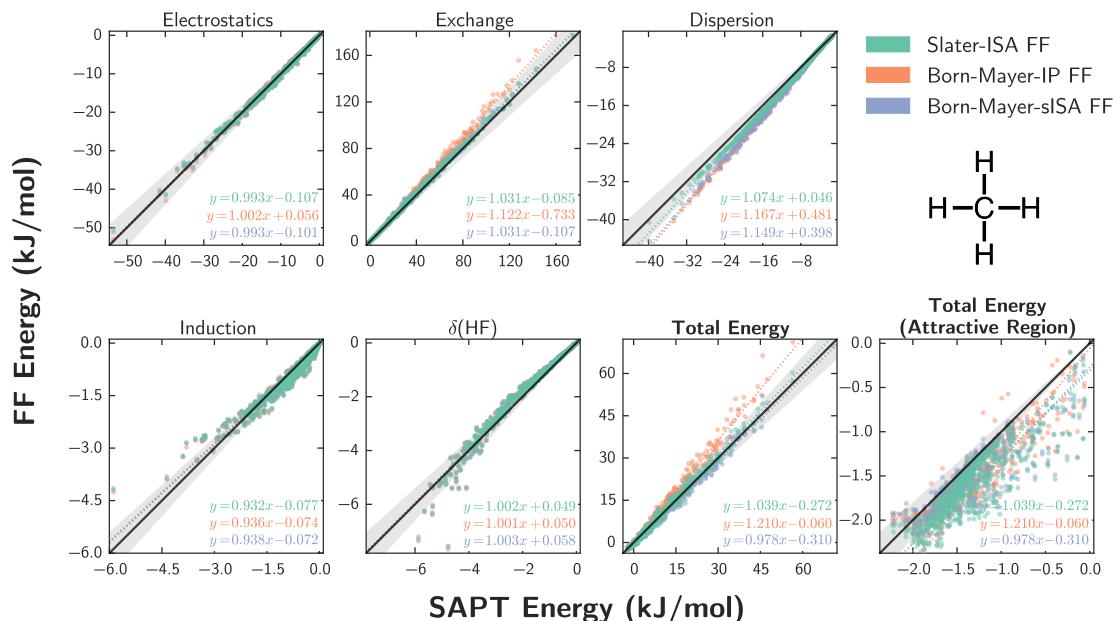
(h) Ethene Dimer



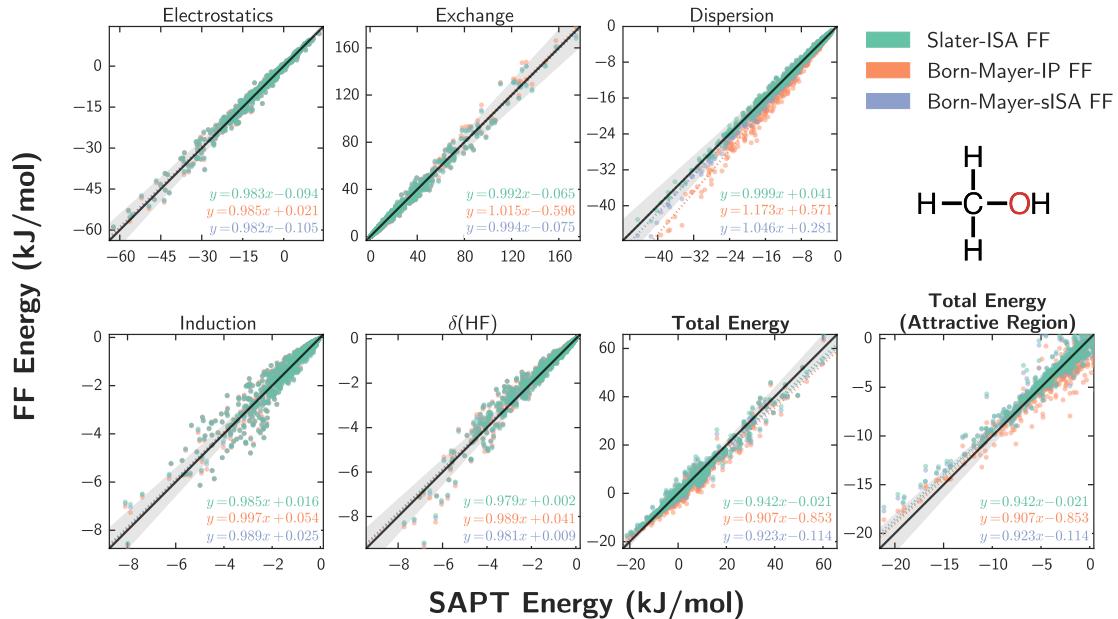
(i) H₂O Dimer



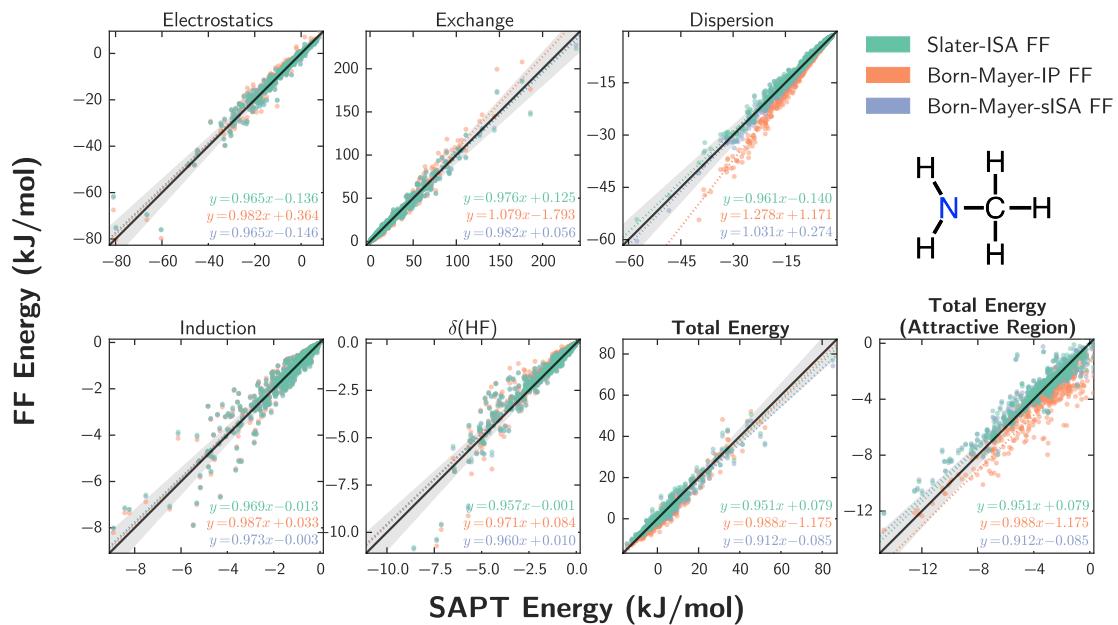
(j) Methane Dimer



(k) Methanol Dimer



(l) Methyl Amine Dimer



(m) NH₃ Dimer

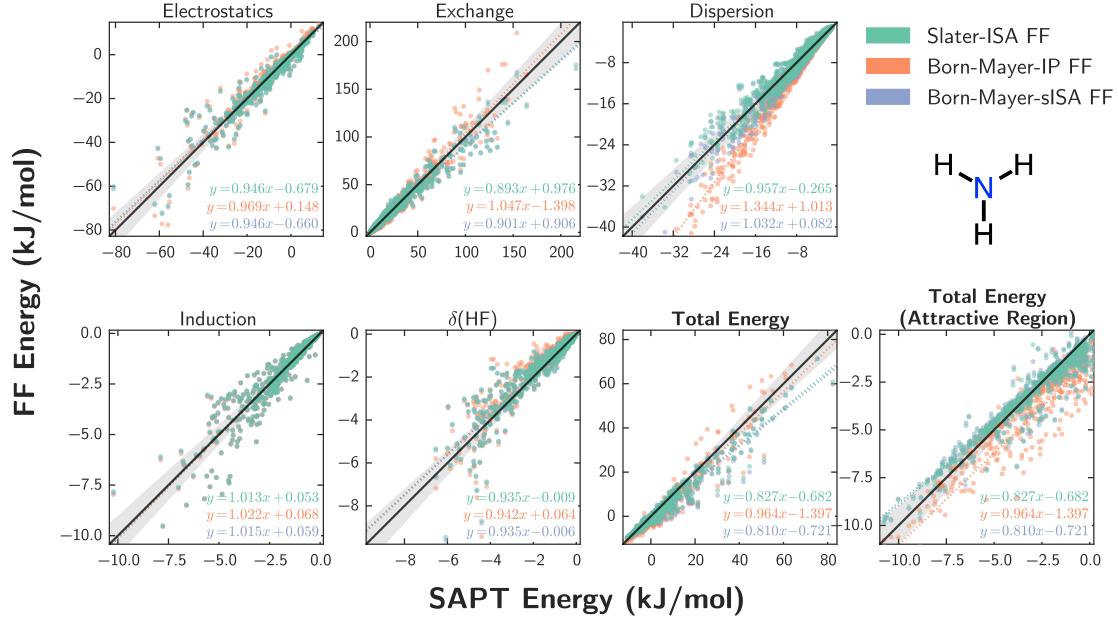


Figure S4. Force field fits for the homomeric systems using the Slater-ISA FF (green), Born-Mayer-IP FF (orange) and Born-Mayer-sISA FF (blue). Fits for each energy component are displayed along with two views of the total interaction energy. The $y = x$ line (black) indicates perfect agreement between reference energies and each force field, while shaded grey areas represent points within $\pm 10\%$ agreement of the benchmark. To guide the eye, a line of best fit (dotted line) has been computed for each force field and for each energy component.

S10 Force Field Accuracy for LJ FF

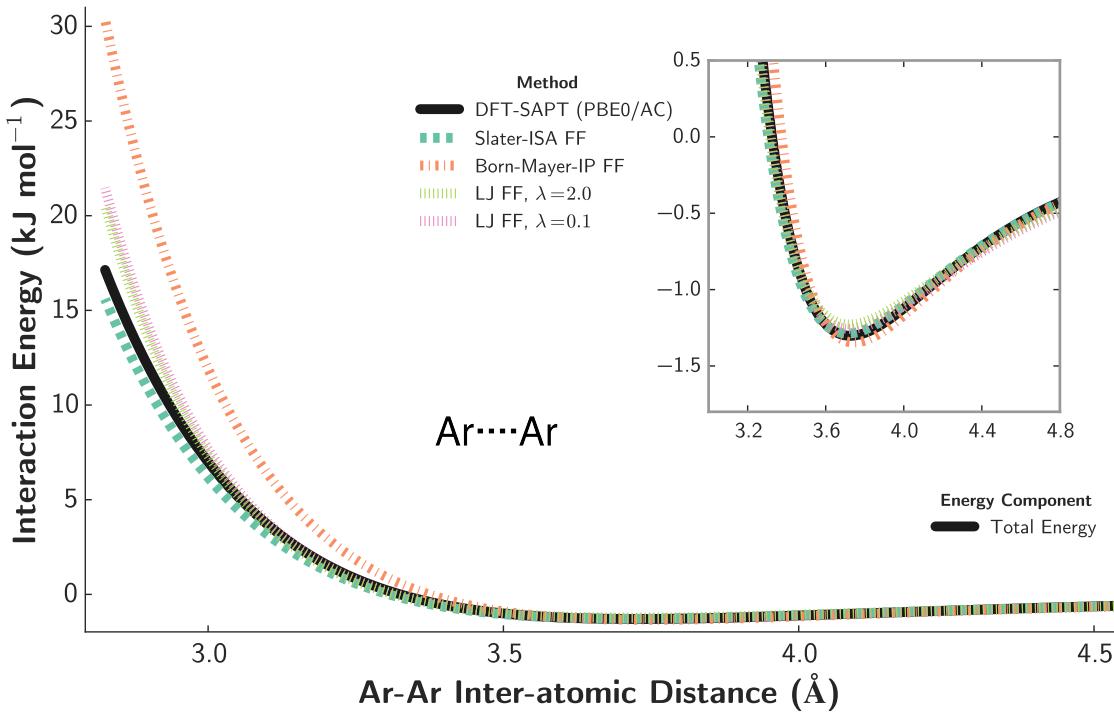


Figure S5. Potential energy surface for the argon dimer. Interaction energies for the Slater-ISA FF (dashed curves), Born-Mayer-IP FF (dash-dotted curves), and LJ FF (dotted curves) are shown alongside benchmark DFT-SAPT (PBE0/AC) energies (solid curves). Note that, for the LJ FF force fields, the magnitude of the attractive tail region is overestimated by the effective $C_{ij,6}$ dispersion parameter.

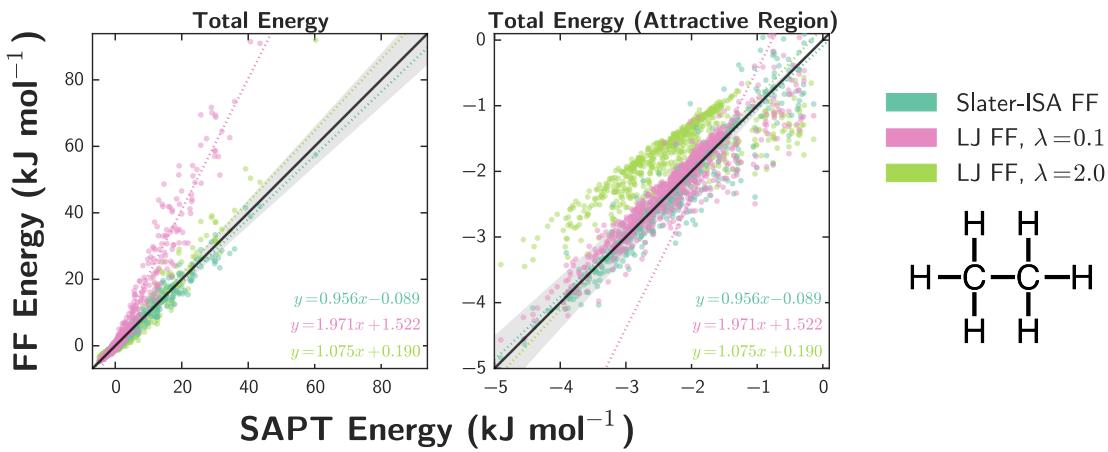


Figure S6. Fits for two views of the total interaction energy for the ethane dimer using the Slater-ISA (teal), LJ $\lambda = 0.1$ (pink) and LJ $\lambda = 2.0$ (lime green) FFs. The diagonal line (black) indicates perfect agreement between reference energies and each force field, while shaded grey areas represent points within $\pm 10\%$ agreement of the benchmark. To guide the eye, a line of best fit (dotted line) has been computed for each force field.

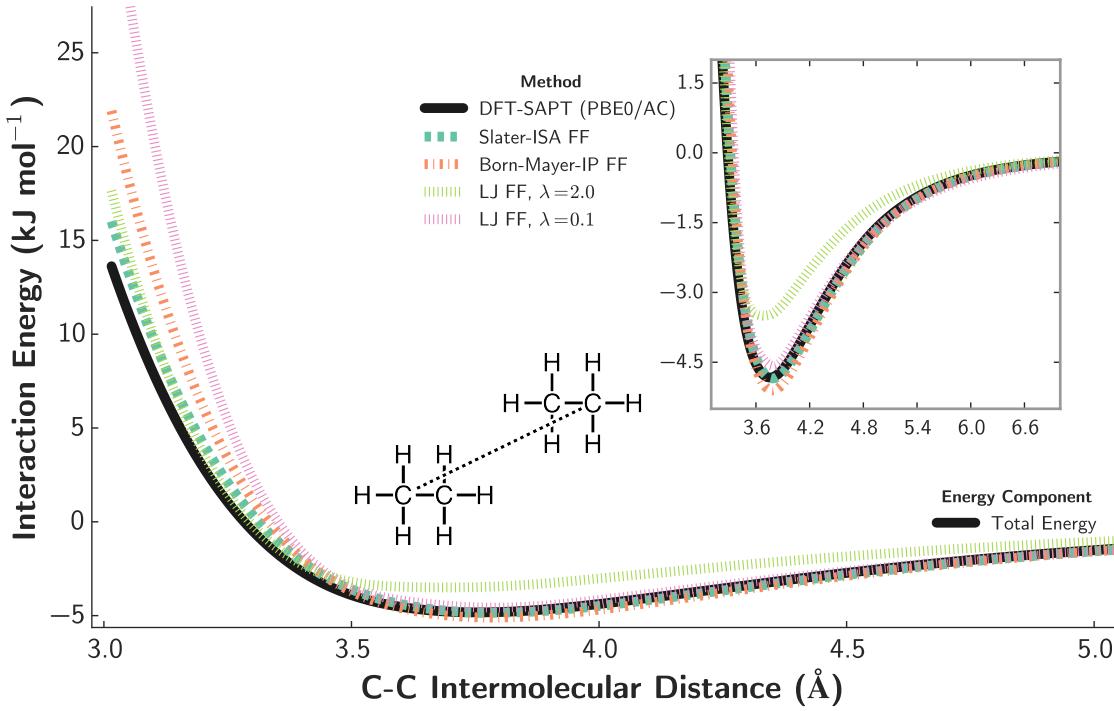


Figure S7. A representative potential energy scan near a local minimum for the ethane dimer. Interaction energies for the Slater-ISA FF (dashed curves), Born-Mayer-IP FF (dash-dotted curves), and LJ FF (dotted curves) are shown alongside benchmark DFT-SAPT (PBE0/AC) energies (solid curves). The energy decomposition for DFT-SAPT and for each force field is shown for reference. The ethane dimer configuration in this scan corresponds to the most energetically attractive dimer included in the training set; other points along this scan are not included in the training set.

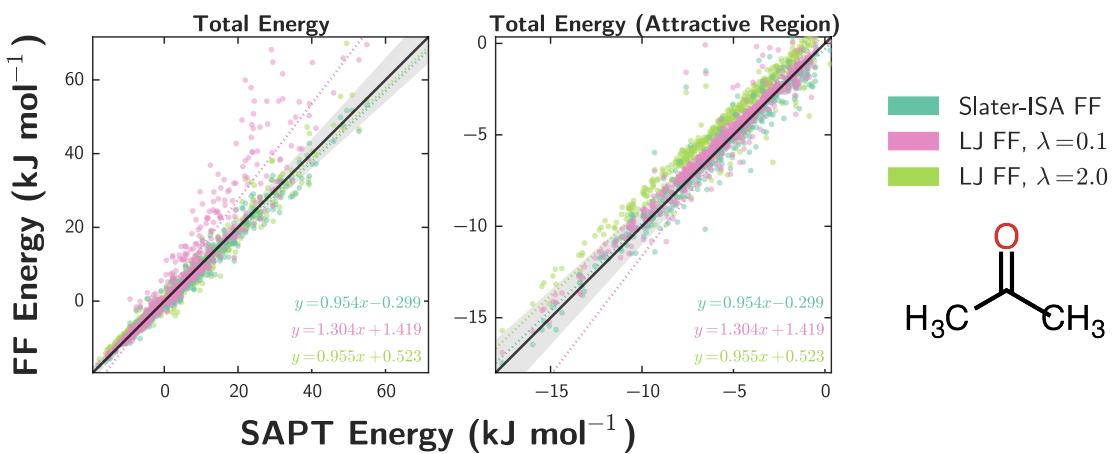


Figure S8. Force field fits for the acetone dimer using the Slater-ISA (teal), LJ $\lambda = 0.1$ (pink) and LJ $\lambda = 2.0$ (lime green) FFs. Fits for two views of the total interaction energy are displayed. The diagonal line (black) indicates perfect agreement between reference energies and each force field, while shaded grey areas represent points within $\pm 10\%$ agreement of the benchmark. To guide the eye, a line of best fit (dotted line) has been computed for each force field.

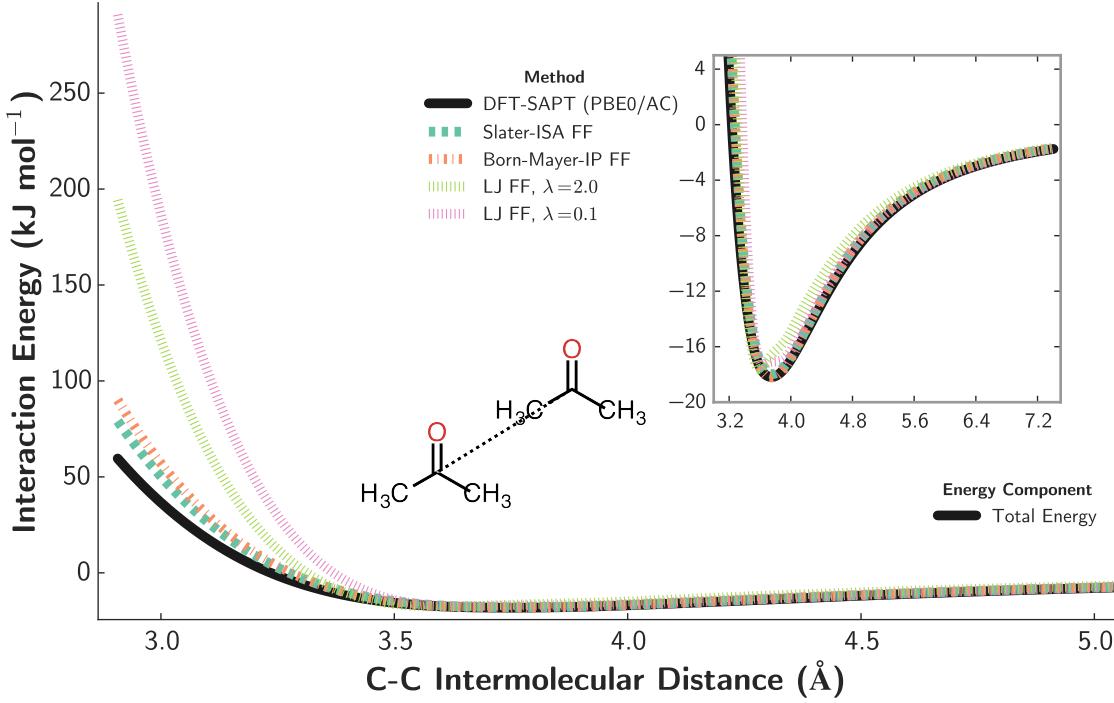


Figure S9. A representative potential energy scan near a local minimum for the acetone dimer. Interaction energies for the Slater-ISA FF (dashed curves), Born-Mayer-IP FF (dash-dotted curves), and LJ FF (dotted curves) are shown alongside benchmark DFT-SAPT (PBE0/AC) energies (solid curves). The energy decomposition for DFT-SAPT and for each force field is shown for reference. The intermolecular distance is taken to be the internuclear distance between the two carbonyl carbons on each acetone monomer. The acetone dimer configuration in this scan corresponds to the most energetically attractive dimer included in the training set; other points along this scan are not included in the training set.

S11 Parameter Robustness for Argon

Argon parameters were tested for robustness by changing the weighting function as described in the main text. As with ethane, optimized Slater-ISA FF A_{ij} parameters are much less sensitive to the choice of weighting function compared to the Born-Mayer-IP FF. As a result, the Slater-ISA FF shows decreased uncertainty when computing the 2nd virial coefficient. Virial coefficients for the Born-Mayer-IP FF, on the other hand, depend more strongly on the choice of weighting function. The fortuitous agreement with experiment for the Born-Mayer-IP FF with $\lambda = 0.5$ may point to inaccuracies in the DFT-SAPT potential itself, but is not indicative of enhanced force field fitting quality. (Indeed, Figure S11 shows that this weighting function leads to the worst agreement with DFT-SAPT compared to other λ values). Overall, the argon fits demonstrate increased parameter robustness for the Slater-ISA FF.

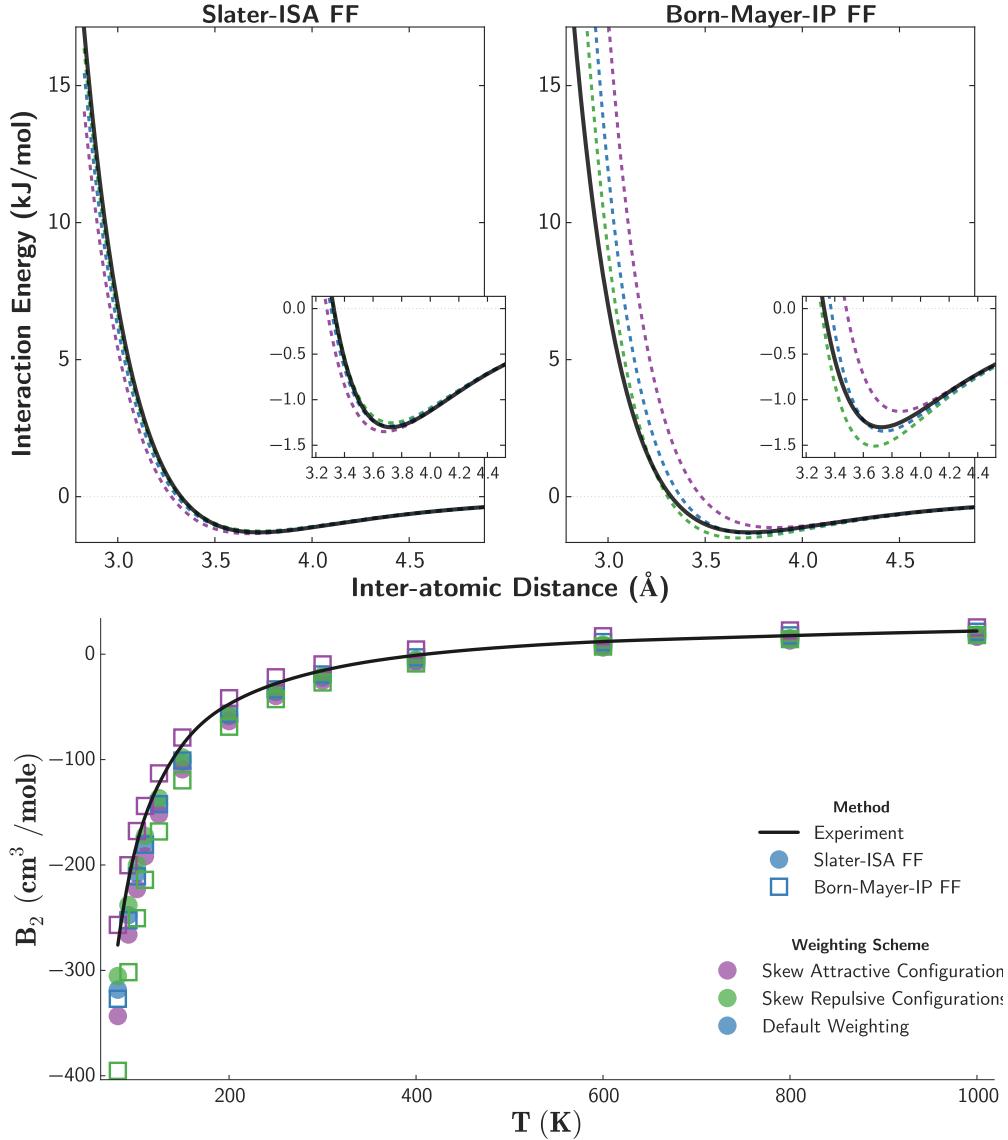


Figure S10. Comparison of the Slater-ISA FF and the Born-Mayer-IP FF in terms of sensitivity to the weighting function employed in parameter optimization for the Ar dimer. Three weighting functions, $\lambda = 0.5$ (purple), $\lambda = 2.0$ (blue), and $\lambda = 5.0$ (green) are shown, with higher λ values indicating more weighting of repulsive configurations.

(top) Total interaction energies for the Slater-ISA FF (left) and the Born-Mayer-IP FF (right) indicating the accuracy of each force field with respect to DFT-SAPT (PBE0/AC) benchmark energies. DFT-SAPT energies are shown as black solid lines, force field fits with dotted lines. Colors for the different weighting functions is as above.

(bottom) Computed 2nd virial coefficients for argon. Data for the Slater-ISA FF and Born-Mayer-IP FF are depicted using open circles and shaded squares, respectively; coloration for the different weighting functions is as above. Experimental data from Dymond and Smith (black line) is also shown.

S12 Parameter Robustness for Ethane; LJ FF results

Ethane parameters were tested for robustness by changing the weighting function as described in the main text. Optimized Slater-ISA FF A_{ij} parameters are much less sensitive to the choice of weighting function compared to the LJ FF. As a result, the Slater-ISA FF shows decreased uncertainty when computing the 2nd virial coefficient. Virial coefficients for the LJ FF, on the other hand, depend more strongly on the choice of weighting function.

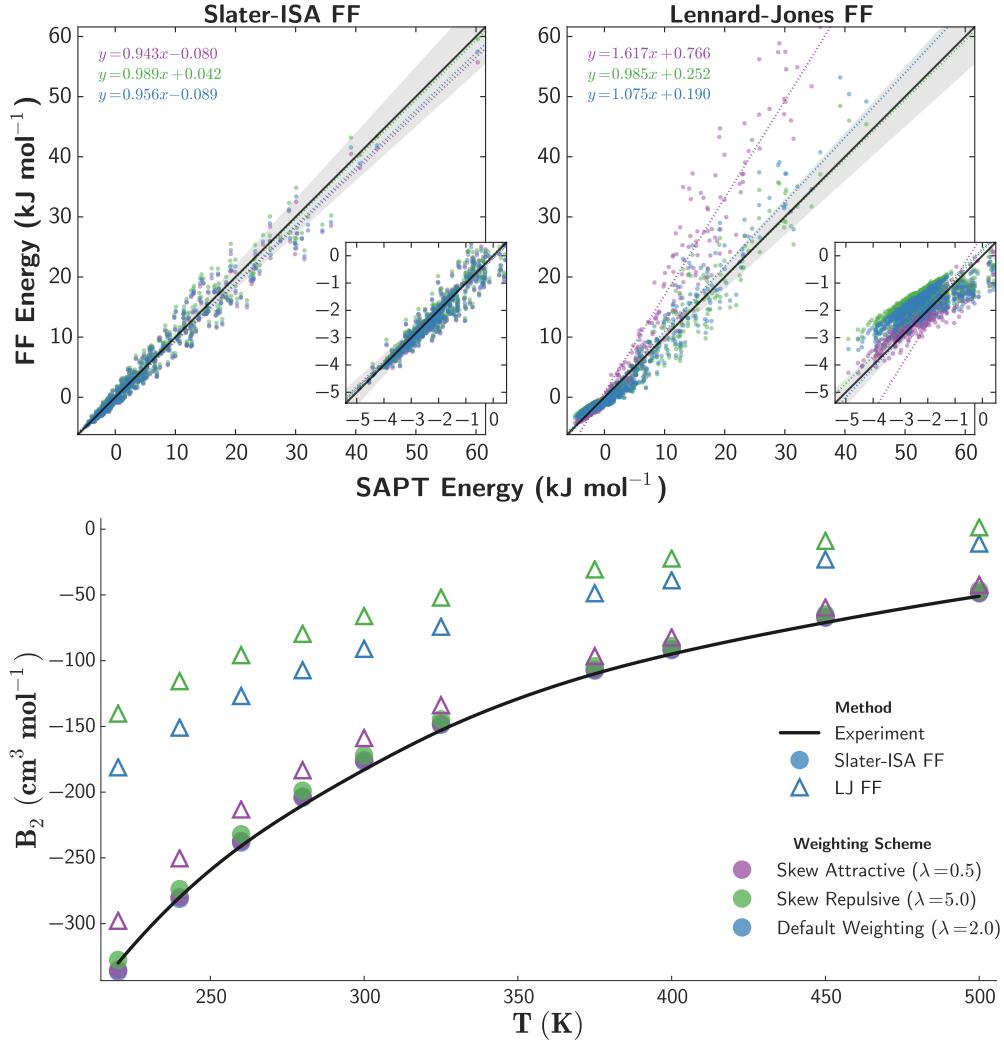


Figure S11. Comparison of the Slater-ISA FF and the LJ FF in terms of sensitivity to the weighting function employed in parameter optimization for the ethane dimer. Three weighting functions, $\lambda = 0.5$ (purple), $\lambda = 2.0$ (blue), and $\lambda = 5.0$ (green) are shown, with higher λ values indicating more weighting of repulsive configurations.

(top) Total interaction energies for the Slater-ISA FF (left) and the LJ FF (right) indicating the accuracy of each force field with respect to DFT-SAPT (PBE0/AC) benchmark energies. The diagonal line (black) indicates perfect agreement between reference energies and each force field, while shaded grey areas represent points within $\pm 10\%$ agreement of the benchmark. To guide the eye, a line of best fit (dotted line) has been computed for each force field and for each weighting function.

(bottom) Computed 2nd virial coefficients for argon. Data for the Slater-ISA FF and the Born-Mayer-IP FF are depicted using open circles and shaded squares, respectively; coloration for the different weighting functions is as above. Experimental data from Dymond and Smith (black line) is also shown.

Table S11. Fitted values for B_{ij} for a variety of element pairs. All values are given in atomic units, except for RMS errors, which are a unitless normalized overlap.

i	j	B_i	B_j	B_{ij}	RMSE	MAPE
H	He	1.99946394	2.68859863	2.31740474	0.00044277657	0.882930
H	Li	1.99946394	1.25901971	1.59404909	0.00064319203	1.106033
H	Be	1.99946394	1.65554322	1.82052039	0.00012960395	0.217206
H	B	1.99946394	1.56191136	1.76768239	0.00022762336	0.498291
H	C	1.99946394	1.81946896	1.90742066	3.6383389e-05	0.074853
H	N	1.99946394	2.06711073	2.03302187	4.9406068e-06	0.009742
H	O	1.99946394	2.00091172	2.00019722	9.9506754e-08	0.000183
H	F	1.99946394	2.26322976	2.12730789	7.0666272e-05	0.137228
H	Ne	1.99946394	2.51791099	2.24270366	0.00026455338	0.578093
H	Na	1.99946394	1.22917354	1.57023314	0.00074952732	1.738728
H	Mg	1.99946394	1.49931366	1.73354253	0.0002881065	0.529739
H	Al	1.99946394	1.32657183	1.63349076	0.00053449852	0.976877
H	Si	1.99946394	1.54808130	1.75910683	0.00024917876	0.617006
H	P	1.99946394	1.75585679	1.87377325	6.8182489e-05	0.148197
H	S	1.99946394	1.74521745	1.86810662	7.4332699e-05	0.160880
H	Cl	1.99946394	1.95253790	1.97586738	2.5436846e-06	0.005705
H	Ar	1.99946394	2.15249556	2.07440522	2.5899665e-05	0.068500
H	Br	1.99946394	1.86365053	1.93033996	2.112332e-05	0.048965
H	I	1.99946394	1.75289066	1.87194355	7.1892596e-05	0.178949
He	Li	2.68859863	1.25901971	1.83579487	0.0020586815	4.802329
He	Be	2.68859863	1.65554322	2.10352673	0.0010603604	2.573450
He	B	2.68859863	1.56191136	2.03442611	0.00129508	3.918107
He	C	2.68859863	1.81946896	2.20238570	0.00075763278	2.262394
He	N	2.68859863	2.06711073	2.35237454	0.0003780889	1.127971
He	O	2.68859863	2.00091172	2.31393264	0.00046386026	1.314845
He	F	2.68859863	2.26322976	2.46423057	0.0001731239	0.522637
He	Ne	2.68859863	2.51791099	2.60133215	2.7253815e-05	0.094670
He	Na	2.68859863	1.22917354	1.79792813	0.0021797532	6.560866
He	Mg	2.68859863	1.49931366	1.99849093	0.0014277708	3.668547
He	Al	2.68859863	1.32657183	1.88040364	0.0018777097	4.668027
He	Si	2.68859863	1.54808130	2.02089719	0.001334628	4.489483
He	P	2.68859863	1.75585679	2.16119527	0.00087958401	2.730605
He	S	2.68859863	1.74521745	2.15451616	0.00090006465	2.778815
He	Cl	2.68859863	1.95253790	2.28271739	0.00054130424	1.785225
He	Ar	2.68859863	2.15249556	2.39953728	0.00028412395	1.122892
He	Br	2.68859863	1.86365053	2.22767127	0.00068597032	2.295912
He	I	2.68859863	1.75289066	2.15618545	0.0008917	3.122234
Li	Be	1.25901971	1.65554322	1.44552618	0.00021566494	0.459735
Li	B	1.25901971	1.56191136	1.40276036	0.00013669061	0.361720
Li	C	1.25901971	1.81946896	1.51465672	0.00042489929	1.056460
Li	N	1.25901971	2.06711073	1.61476325	0.00080816618	1.922263
Li	O	1.25901971	2.00091172	1.58945583	0.00069142836	1.593136

Table S11 – continued from previous page

<i>i</i>	<i>j</i>	B_i	B_j	B_{ij}	RMSE	MAPE
Li	F	1.25901971	2.26322976	1.68919749	0.0011668895	2.718352
Li	Ne	1.25901971	2.51791099	1.77555429	0.0017026265	4.273871
Li	Na	1.25901971	1.22917354	1.24402068	1.5533688e-06	0.004373
Li	Mg	1.25901971	1.49931366	1.37457277	8.4735331e-05	0.195212
Li	Al	1.25901971	1.32657183	1.29242716	7.1019258e-06	0.016335
Li	Si	1.25901971	1.54808130	1.39618447	0.00012793291	0.374607
Li	P	1.25901971	1.75585679	1.48750641	0.00034426274	0.896554
Li	S	1.25901971	1.74521745	1.48302253	0.00033062213	0.858653
Li	Cl	1.25901971	1.95253790	1.56786800	0.00063028803	1.664314
Li	Ar	1.25901971	2.15249556	1.64158799	0.00099309611	2.932927
Li	Br	1.25901971	1.86365053	1.53172970	0.00049638053	1.350986
Li	I	1.25901971	1.75289066	1.48527643	0.00034799167	1.009017
Be	B	1.65554322	1.56191136	1.60804807	1.1972231e-05	0.031893
Be	C	1.65554322	1.81946896	1.73554580	3.3972736e-05	0.085743
Be	N	1.65554322	2.06711073	1.84956812	0.0001992019	0.484038
Be	O	1.65554322	2.00091172	1.82001716	0.00014155775	0.330806
Be	F	1.65554322	2.26322976	1.93457449	0.00041123838	0.983581
Be	Ne	1.65554322	2.51791099	2.03628351	0.00078343308	2.059895
Be	Na	1.65554322	1.22917354	1.42686604	0.00026737271	0.745777
Be	Mg	1.65554322	1.49931366	1.57563633	3.2478195e-05	0.074055
Be	Al	1.65554322	1.32657183	1.48286105	0.00014866739	0.335525
Be	Si	1.65554322	1.54808130	1.60086762	1.615263e-05	0.048036
Be	P	1.65554322	1.75585679	1.70494709	1.3101092e-05	0.034696
Be	S	1.65554322	1.74521745	1.69977980	1.0504303e-05	0.027715
Be	Cl	1.65554322	1.95253790	1.79750301	0.00010922498	0.297117
Be	Ar	1.65554322	2.15249556	1.88512628	0.00029576275	0.923403
Be	Br	1.65554322	1.86365053	1.75630627	5.5219463e-05	0.154638
Be	I	1.65554322	1.75289066	1.70346914	1.2636043e-05	0.037713
B	C	1.56191136	1.81946896	1.68526246	8.896852e-05	0.279460
B	N	1.56191136	2.06711073	1.79465183	0.00031660316	0.962841
B	O	1.56191136	2.00091172	1.76649990	0.00024246047	0.712022
B	F	1.56191136	2.26322976	1.87554766	0.00057369687	1.719903
B	Ne	1.56191136	2.51791099	1.97105959	0.00099084843	3.222525
B	Na	1.56191136	1.22917354	1.38509763	0.00017473338	0.590078
B	Mg	1.56191136	1.49931366	1.53029477	5.6807294e-06	0.016154
B	Al	1.56191136	1.32657183	1.43954012	8.2359665e-05	0.230371
B	Si	1.56191136	1.54808130	1.55498504	3.4970147e-07	0.001260
B	P	1.56191136	1.75585679	1.655571982	5.1764703e-05	0.169673
B	S	1.56191136	1.74521745	1.65073751	4.6359978e-05	0.151426
B	Cl	1.56191136	1.95253790	1.74462228	0.00019882685	0.668654
B	Ar	1.56191136	2.15249556	1.82774537	0.00043254436	1.644894
B	Br	1.56191136	1.86365053	1.70507656	0.00012232055	0.422076
B	I	1.56191136	1.75289066	1.65418604	5.1089297e-05	0.186574
C	N	1.81946896	2.06711073	1.93878424	7.2588349e-05	0.213967
C	O	1.81946896	2.00091172	1.90779431	3.9381872e-05	0.111509

Table S11 – continued from previous page

<i>i</i>	<i>j</i>	B_i	B_j	B_{ij}	RMSE	MAPE
C	F	1.81946896	2.26322976	2.02729827	0.00022128603	0.646349
C	Ne	1.81946896	2.51791099	2.13356824	0.00051712548	1.665041
C	Na	1.81946896	1.22917354	1.49359005	0.00049650546	1.590315
C	Mg	1.81946896	1.49931366	1.65145683	0.00013523926	0.364498
C	Al	1.81946896	1.32657183	1.55375705	0.00032909645	0.868090
C	Si	1.81946896	1.54808130	1.67745495	0.00010070423	0.351275
C	P	1.81946896	1.75585679	1.78734889	5.2847945e-06	0.016690
C	S	1.81946896	1.74521745	1.78191233	7.1848878e-06	0.022600
C	Cl	1.81946896	1.95253790	1.88462580	2.1955555e-05	0.071858
C	Ar	1.81946896	2.15249556	1.97704725	0.0001323859	0.499304
C	Br	1.81946896	1.86365053	1.84141110	2.5492317e-06	0.008538
C	I	1.81946896	1.75289066	1.78581710	5.8824253e-06	0.020847
N	O	2.06711073	2.00091172	2.03371451	5.041231e-06	0.013929
N	F	2.06711073	2.26322976	2.16254689	4.15042e-05	0.119485
N	Ne	2.06711073	2.51791099	2.27840189	0.00020910088	0.673215
N	Na	2.06711073	1.22917354	1.58958212	0.00090815621	2.796799
N	Mg	2.06711073	1.49931366	1.75954426	0.00039310972	1.019328
N	Al	2.06711073	1.32657183	1.65570661	0.00068105488	1.722447
N	Si	2.06711073	1.54808130	1.78559923	0.00033982883	1.150687
N	P	2.06711073	1.75585679	1.90415582	0.00011669305	0.359120
N	S	2.06711073	1.74521745	1.89832775	0.00012494822	0.382742
N	Cl	2.06711073	1.95253790	2.00885032	1.5404889e-05	0.049510
N	Ar	2.06711073	2.15249556	2.10924579	8.3837241e-06	0.031515
N	Br	2.06711073	1.86365053	1.96222048	4.938888e-05	0.162281
N	I	2.06711073	1.75289066	1.90214169	0.00012093134	0.419448
O	F	2.00091172	2.26322976	2.12742019	7.4513608e-05	0.204667
O	Ne	2.00091172	2.51791099	2.24105845	0.00027602296	0.845765
O	Na	2.00091172	1.22917354	1.56546880	0.00078625246	2.354990
O	Mg	2.00091172	1.49931366	1.73176044	0.00031061975	0.777382
O	Al	2.00091172	1.32657183	1.62980355	0.00057319586	1.403523
O	Si	2.00091172	1.54808130	1.75782981	0.00026287602	0.860753
O	P	2.00091172	1.75585679	1.87387688	7.3175089e-05	0.216650
O	S	2.00091172	1.74521745	1.86815729	7.9760452e-05	0.235090
O	Cl	2.00091172	1.95253790	1.97655937	2.8387158e-06	0.008742
O	Ar	2.00091172	2.15249556	2.07494432	2.6479263e-05	0.095246
O	Br	2.00091172	1.86365053	1.93085797	2.2760392e-05	0.071837
O	I	2.00091172	1.75289066	1.87203787	7.6356395e-05	0.255064
F	Ne	2.26322976	2.51791099	2.38617019	6.4967098e-05	0.211473
F	Na	2.26322976	1.22917354	1.66029149	0.0012830926	3.875179
F	Mg	2.26322976	1.49931366	1.83986590	0.00066962961	1.706670
F	Al	2.26322976	1.32657183	1.73140874	0.0010196712	2.528620
F	Si	2.26322976	1.54808130	1.86526151	0.00060490347	2.020578
F	P	2.26322976	1.75585679	1.99065290	0.00029360355	0.894671
F	S	2.26322976	1.74521745	1.98453998	0.00030630021	0.928727
F	Cl	2.26322976	1.95253790	2.10087150	0.00010755539	0.344316

Table S11 – continued from previous page

<i>i</i>	<i>j</i>	B_i	B_j	B_{ij}	RMSE	MAPE
F	Ar	2.26322976	2.15249556	2.20694293	1.3485721e-05	0.050987
F	Br	2.26322976	1.86365053	2.05158173	0.00018081195	0.590554
F	I	2.26322976	1.75289066	1.98794200	0.00030142935	1.036990
Ne	Na	2.51791099	1.22917354	1.74146757	0.0018171227	5.842510
Ne	Mg	2.51791099	1.49931366	1.93474540	0.0011134419	3.086201
Ne	Al	2.51791099	1.32657183	1.81962923	0.001531155	4.095464
Ne	Si	2.51791099	1.54808130	1.95888870	0.0010266525	3.702217
Ne	P	2.51791099	1.75585679	2.09400464	0.00062146304	2.076964
Ne	S	2.51791099	1.74521745	2.08750459	0.00063928574	2.124924
Ne	Cl	2.51791099	1.95253790	2.21174754	0.00033656173	1.193911
Ne	Ar	2.51791099	2.15249556	2.32497739	0.00013843693	0.584890
Ne	Br	2.51791099	1.86365053	2.15873868	0.0004557	1.639505
Ne	I	2.51791099	1.75289066	2.09004196	0.00063134274	2.372214
Na	Mg	1.22917354	1.49931366	1.35766104	0.00011473889	0.341738
Na	Al	1.22917354	1.32657183	1.27699602	1.5803838e-05	0.046721
Na	Si	1.22917354	1.54808130	1.37861851	0.00016394224	0.606312
Na	P	1.22917354	1.75585679	1.46734689	0.00040724885	1.358887
Na	S	1.22917354	1.74521745	1.46301699	0.00039233117	1.305796
Na	Cl	1.22917354	1.95253790	1.54462666	0.00071489747	2.415615
Na	Ar	1.22917354	2.15249556	1.61475657	0.0010865392	4.048855
Na	Br	1.22917354	1.86365053	1.50991318	0.00057095415	1.982122
Na	I	1.22917354	1.75289066	1.46507909	0.00040898615	1.502211
Mg	Al	1.49931366	1.32657183	1.41054381	4.3759475e-05	0.106460
Mg	Si	1.49931366	1.54808130	1.52349731	3.5595022e-06	0.011234
Mg	P	1.49931366	1.75585679	1.62233525	8.9250076e-05	0.251892
Mg	S	1.49931366	1.74521745	1.61744114	8.2197924e-05	0.231214
Mg	Cl	1.49931366	1.95253790	1.70986111	0.00026403315	0.761802
Mg	Ar	1.49931366	2.15249556	1.79169870	0.00052474149	1.715332
Mg	Br	1.49931366	1.86365053	1.67083027	0.00017608345	0.522795
Mg	I	1.49931366	1.75289066	1.62071071	8.9123446e-05	0.281480
Al	Si	1.32657183	1.54808130	1.43295795	7.4878405e-05	0.231698
Al	P	1.32657183	1.75585679	1.52615042	0.00025709446	0.709802
Al	S	1.32657183	1.74521745	1.52156219	0.00024519155	0.674974
Al	Cl	1.32657183	1.95253790	1.60826232	0.00051441718	1.443233
Al	Ar	1.32657183	2.15249556	1.68396084	0.0008502512	2.673094
Al	Br	1.32657183	1.86365053	1.57145555	0.00039199648	1.132597
Al	I	1.32657183	1.75289066	1.52414100	0.00025909364	0.796534
Si	P	1.54808130	1.75585679	1.64816385	6.0537472e-05	0.219836
Si	S	1.54808130	1.74521745	1.64322319	5.4646042e-05	0.197756
Si	Cl	1.54808130	1.95253790	1.73616531	0.00021653004	0.806893
Si	Ar	1.54808130	2.15249556	1.81809419	0.00045725342	1.916727
Si	Br	1.54808130	1.86365053	1.69704848	0.00013598439	0.519161
Si	I	1.54808130	1.75289066	1.64662155	5.971014e-05	0.240522
P	S	1.75585679	1.74521745	1.75053498	2.2383111e-07	0.000726
P	Cl	1.75585679	1.95253790	1.85109487	4.8767404e-05	0.166222

Table S11 – continued from previous page

<i>i</i>	<i>j</i>	B_i	B_j	B_{ij}	RMSE	MAPE
P	Ar	1.75585679	2.15249556	1.94118289	0.00019034099	0.743408
P	Br	1.75585679	1.86365053	1.80880477	1.5089803e-05	0.052666
P	I	1.75585679	1.75289066	1.75438024	8.3311914e-08	0.000297
S	Cl	1.74521745	1.95253790	1.84542979	5.4259063e-05	0.184109
S	Ar	1.74521745	2.15249556	1.93516069	0.00020092813	0.780785
S	Br	1.74521745	1.86365053	1.80328668	1.8231579e-05	0.063360
S	I	1.74521745	1.75289066	1.74905593	1.5042953e-07	0.000542
Cl	Ar	1.95253790	2.15249556	2.04925011	4.7026489e-05	0.193758
Cl	Br	1.95253790	1.86365053	1.90746100	9.8799774e-06	0.035850
Cl	I	1.95253790	1.75289066	1.84935929	5.0999292e-05	0.194814
Ar	Br	2.15249556	1.86365053	2.00111347	9.9755127e-05	0.417023
Ar	I	2.15249556	1.75289066	1.93889388	0.00019497498	0.849907
Br	I	1.86365053	1.75289066	1.80721936	1.6163908e-05	0.063089

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