Supplementary Material for: N-representability of the target density in Frozen-Density Embedding Theory based methods: numerical significance and relation to electronic polarisation

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S1. CONSTRAINED SEARCH DEFINITIONS OF DENSITY FUNCTIONALS USED IN FDET

A. Functionals in Kohn-Sham formulation of DFT

$$T_s[\rho] = \min_{\Phi \longrightarrow \rho} \left\langle \Phi | \hat{T} | \Phi \right\rangle = \left\langle \Phi^o[\rho] | \hat{T} | \Phi^o[\rho] \right\rangle = T_s[\rho] \tag{S1}$$

$$\begin{aligned} E_{xc}[\rho] &= \min_{\Psi \longrightarrow \rho} \left\langle \Psi | \hat{T} + \hat{V}^{ee} | \Psi \right\rangle - T_s[\rho] - J[\rho] \\ &= \left\langle \Psi^o[\rho] | \hat{T} + \hat{V}^{ee} | \Psi^o[\rho] \right\rangle - T_s[\rho] - J[\rho], \end{aligned} \tag{S2}$$

where $\hat{V}_{ee} = \sum_{i=1}^{N} \sum_{j>i}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$ is the electron-electron repulsion operator, $J[\rho] = \frac{1}{2} \int \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}|} \mathrm{d}\mathbf{r}' \mathrm{d}\mathbf{r}$, Φ and Ψ are N-electron wave-functions of the single-determinant or Full Configuration Interaction form, respectively.

B. Functionals used in FDET

For a) embedded wavefunctions of the Full Configuration Interaction form, b) embedded non-interacting reference (Kohn-Sham-like) system, and c) embedded one-particle spinless reduced density matrix, FDET uses the non-additive kinectic-exchange-correlation bifunctional defined as:

$$\begin{aligned} E_{xct}^{nad}[\rho_A, \rho_B] &\equiv E_{xc}[\rho_A + \rho_B] - E_{xc}[\rho_A] - E_{xc}[\rho_B] \\ &+ T_s[\rho_A + \rho_B] - T_s[\rho_A] - T_s[\rho_B]. \end{aligned} \tag{S3}$$

For embedded wavefunctions of truncated Configuration Interaction form, FDET uses another functional:

$$E_{xct}^{nad(truncCI)}[\rho_A, \rho_B] \equiv E_{xct}^{nad}[\rho_A, \rho_B] + E_c^{truncCI}[\rho] \leq E_{xct}^{nad}[\rho_A, \rho_B], \tag{S4}$$

where

$$\begin{aligned} E_c^{truncCI}[\rho] &= \min_{\Psi \longrightarrow \rho} \left\langle \Psi | \hat{T} + \hat{V}^{ee} | \Psi \right\rangle - \min_{\Psi^{truncCI} \longrightarrow \rho} \left\langle \Psi^{truncCI} | \hat{T} + \hat{V}^{ee} | \Psi^{truncCI} \right\rangle \\ &= \left\langle \Psi^o[\rho] | \hat{T} + \hat{V}^{ee} | \Psi^o[\rho] \right\rangle - \left\langle \Psi^{o(truncCI)}[\rho] | \hat{T} + \hat{V}^{ee} | \Psi^{o(truncCI)}[\rho] \right\rangle, \end{aligned} \tag{S5}$$

If the embedded wavefunction has a single-determinant form:

$$E_{xct}^{nad(SD)}[\rho_A, \rho_B] \equiv E_{xct}^{nad}[\rho_A, \rho_B] + E_c[\rho] \leq E_{xct}^{nad}[\rho_A, \rho_B], \tag{S6}$$

where

$$E_c[\rho] = \min_{\Psi \longrightarrow \rho} \left\langle \Psi | \hat{T} + \hat{V}^{ee} | \Psi \right\rangle - \min_{\Phi \longrightarrow \rho} \left\langle \Phi | \hat{T} + \hat{V}^{ee} | \Phi \right\rangle \tag{S7}$$

$$= \left\langle \Psi^o[\rho] | \hat{T} + \hat{V}^{ee} | \Psi^o[\rho] \right\rangle - \left\langle \Phi^o[\rho] | \hat{T} + \hat{V}^{ee} | \Phi^o[\rho] \right\rangle,$$

is the correlation functional defined also in the Kohn-Sham formulation of DFT.

Using variationally obtained embedded single determinant AND neglecting $E_c[\rho]$ leads to the violation of the basic FDET equality relating FDET energy functional to the Hohenberg-Kohn functional (Eq. 2) leading to the increase of the energy. The energy consistent with the Hohenberg-Kohn functional correcting this increase is given in Eq. 6.

S2.   PROOF THAT $M[\rho_B - \rho_{AB}^o] \leq P[\rho_A^o + \rho_B - \rho_{AB}^o]$

We start with the obvious equality,

$$\int \rho_A^o + \rho_B - \rho_{AB}^o = 0, \tag{S8}$$

from which it follows that:

$$\int_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o = \int_{\rho_{AB}^o > \rho_A^o + \rho_B} \rho_{AB}^o - \rho_A^o - \rho_B. \tag{S9}$$

The above relation used in the definition of P leads to:

$$P[\rho_A^o + \rho_B - \rho_{AB}^o] = \frac{1}{2} \int |\rho_A^o + \rho_B - \rho_{AB}^o| \tag{S10}$$

$$= \frac{1}{2} \int_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o +$$

$$\frac{1}{2} \int_{\rho_{AB}^o > \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o$$

$$= \int_{\rho_{AB}^o < \rho_A^o + \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o.$$

Splitting the domain of integration of the final integral above leads to:

$$P[\rho_A^o + \rho_B - \rho_{AB}^o] = \int_{\rho_{AB}^o < \rho_B} \rho_A^o + \rho_B - \rho_{AB}^o + \tag{S11}$$

$$\int_{\rho_B \leq \rho_{AB}^o < \rho_B + \rho_A^o} \rho_A^o + \rho_B - \rho_{AB}^o$$

$$= \int_{\rho_{AB}^o < \rho_B} \rho_B - \rho_{AB}^o + \tag{S12}$$

$$+ \int_{\rho_{AB}^o < \rho_B} \rho_A^o + \int_{\rho_B \leq \rho_{AB}^o < \rho_B + \rho_A^o} \rho_A^o + \rho_B - \rho_{AB}^o$$

The first integral in the right-hand-side of the equation above is equal to $M[\rho_{AB}^o - \rho_B]$ whereas the second and third are non-negative. As a result:

$$P[\rho_A^o + \rho_B - \rho_{AB}^o] \geq M[\rho_{AB}^o - \rho_B], \tag{S13}$$

which ends the proof.

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S3. DATA

A. cc-pVDZ

complex	ρ_B	$E_k[\Delta\rho^c_{v'_A},\rho'_A,\rho_B]$ [a]	$E_k[\Delta\rho^c_{v'_B},\rho'_B,\rho_A]$ [a]	$E_{int}^{FDET(\rho_B)}$ [b]	E_{int}^{ref} [c]	Δ_{CP} [d]	M [e]	P [f]	P_{cmpl} [g]
7HQ-2MeOH	ρ_B^{isol}	0.063		-11.200	-14.482	11.159	0.108	0.216	0.350
7HQ-2MeOH	ρ_B^{FAT}	0.053	0.096	-14.216	-14.482	11.159	0.007	0.066	0.350
7HQ-formate	ρ_B^{isol}	-0.009		-25.717	-38.148	11.902	0.176	0.285	0.648
7HQ-formate	ρ_B^{FAT}	-0.036	0.033	-36.933	-38.148	11.902	0.007	0.070	0.648
uracil-5H$_2$O	ρ_B^{isol}	0.166		-32.320	-34.396	23.111	0.203	0.394	0.600
uracil-5H$_2$O	ρ_B^{FAT}	0.147	0.162	-39.794	-34.396	23.111	0.014	0.126	0.600
PyrBnz-2HCOOH	ρ_B^{isol}	0.130		-26.794	-32.300	13.907	0.175	0.406	0.583
PyrBnz-2HCOOH	ρ_B^{FAT}	0.103	0.108	-33.852	-32.300	13.907	0.012	0.110	0.583

[a] defined in Eq. **??** in the manuscript

[b] defined in Eq. **??**, and Eq. **??** in the manuscript for ρ_B^{isol} and ρ_B^{FAT} respectively.

[c] Counterpoise corrected, i.e. $E_{int}^{ref} = E_{AB}^{(AB)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[d] Counterpoise correction: $\Delta_{CP} = E_A^{(A)} + E_B^{(B)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[e] $M = M[\rho^{ref} - \rho_B^{FDET(FAT)}]$ with $M[\rho]$ defined in Eq. **??** in the manuscript

[f] $P_{cmpl} = P[\rho_A^{isol} + \rho_B^{isol} - \rho^{ref}]$ (cf. Eq. **??**), with $P[\rho]$ defined in Eq. **??** in the manuscript

[g] $P = P[\rho^{ref} - \rho_{tot}^{FDET(FAT)}]$ with $P[\rho]$ defined in Eq. **??** in the manuscript

[h] $E_{int}^{FDET(FAT)}$ is given in Eq. **??** in the manuscript

TABLE S1. Supplementary data for results obtained with the *supermolecular expansion* and the cc-pVDZ basis set. Energies are given in kcal/mol and quantities related to electron densities are given in atomic units.

complex	ρ_B	$E_k[\Delta\rho^c_{v'_A},\rho'_A,\rho_B]$ [a]	$E_k[\Delta\rho^c_{v'_B},\rho'_B,\rho_A]$ [a]	$E_{int}^{FDET(\rho_B)}$ [b]	E_{int}^{ref} [c]	Δ_{CP} [d]	M [e]	P [f]	P_{cmpl} [g]
7HQ-2MeOH	ρ_B^{isol}	0.023		-10.724	-14.482	11.159	0.131	0.228	0.354
7HQ-2MeOH	$\rho_B^{pp(Mulliken)}$	0.021		-12.063	-14.482	11.159	0.091	0.171	0.354
7HQ-2MeOH	$\rho_B^{pp(ChelPG)}$	0.021		-12.343	-14.482	11.159	0.063	0.137	0.354
7HQ-2MeOH	ρ_B^{FAT}	0.020	0.036	-12.062	-14.482	11.159	0.045	0.103	0.354
7HQ-formate	ρ_B^{isol}	-0.021		-27.189	-38.148	11.902	0.226	0.306	0.645
7HQ-formate	$\rho_B^{pp(Mulliken)}$	-0.021		-29.673	-38.148	11.902	0.181	0.253	0.645
7HQ-formate	$\rho_B^{pp(ChelPG)}$	-0.021		-30.350	-38.148	11.902	0.154	0.222	0.645
7HQ-formate	ρ_B^{FAT}	-0.021	0.040	-29.917	-38.148	11.902	0.116	0.177	0.645
uracil-5H$_2$O	ρ_B^{isol}	0.068		-30.102	-34.396	23.111	0.264	0.413	0.605
uracil-5H$_2$O	$\rho_B^{pp(Mulliken)}$	0.063		-33.053	-34.396	23.111	0.183	0.303	0.605
uracil-5H$_2$O	$\rho_B^{pp(ChelPG)}$	0.061		-33.678	-34.396	23.111	0.144	0.254	0.605
uracil-5H$_2$O	ρ_B^{FAT}	0.057	0.051	-32.892	-34.396	23.111	0.120	0.206	0.605
PyrBnz-2HCOOH	ρ_B^{isol}	0.088		-24.896	-32.300	13.907	0.204	0.422	0.582
PyrBnz-2HCOOH	$\rho_B^{pp(Mulliken)}$	0.079		-28.615	-32.300	13.907	0.106	0.265	0.582
PyrBnz-2HCOOH	$\rho_B^{pp(ChelPG)}$	0.077		-29.135	-32.300	13.907	0.090	0.233	0.582
PyrBnz-2HCOOH	ρ_B^{FAT}	0.071	0.025	-28.491	-32.300	13.907	0.060	0.162	0.582

[a] defined in Eq. ?? in the manuscript

[b] defined in Eq. ??, and Eq. ?? in the manuscript for ρ_B^{isol} and ρ_B^{FAT} respectively, and in Eq. ?? for $\rho_B^{pp(Mulliken)}$ and $\rho_B^{pp(ChelPG)}$

[c] Counterpoise corrected, i.e. $E_{int}^{ref} = E_{AB}^{(AB)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[d] Counterpoise correction: $\Delta_{CP} = E_A^{(A)} + E_B^{(B)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[e] $M = M[\rho^{ref} - \rho_B^{FDET(FAT)}]$ with $M[\rho]$ defined in Eq. ?? in the manuscript

[f] $P_{cmpl} = P[\rho_A^{isol} + \rho_B^{isol} - \rho^{ref}]$ (cf. Eq. ??), with $P[\rho]$ defined in Eq. ?? in the manuscript

[g] $P = P[\rho^{ref} - \rho_{tot}^{FDET(FAT)}]$ with $P[\rho]$ defined in Eq. ?? in the manuscript

[h] $E_{int}^{FDET(FAT)}$ is given in Eq. ?? in the manuscript

TABLE S2. Supplementary data for results obtained with the *monomer expansion* and the cc-pVDZ basis set. Energies are given in kcal/mol and quantities related to electron densities are given in atomic units.

B.   aug-cc-pVDZ

complex	ρ_B	$E_k[\Delta\rho^c_{v'_A},\rho'_A,\rho_B]$ [a]	$E_k[\Delta\rho^c_{v'_B},\rho'_B,\rho_A]$ [a]	$E_{int}^{FDET(\rho_B)}$ [b]	E_{int}^{ref} [c]	Δ_{CP} [d]	M [e]	P [f]	P_{cmpl} [g]
7HQ-2MeOH	ρ_B^{isol}	0.092		-10.983	-17.473	5.632	0.121	0.228	0.362
7HQ-2MeOH	ρ_B^{FAT}	0.081	0.127	-14.269	-17.473	5.632	0.007	0.059	0.362
7HQ-formate	ρ_B^{isol}	0.020		-23.037	-36.485	3.522	0.206	0.316	0.670
7HQ-formate	ρ_B^{FAT}	-0.008	0.068	-33.325	-36.485	3.522	0.007	0.066	0.670
uracil-5H$_2$O	ρ_B^{isol}	0.224		-32.065	-38.620	7.839	0.234	0.426	0.633
uracil-5H$_2$O	ρ_B^{FAT}	0.204	0.236	-39.695	-38.620	7.839	0.014	0.114	0.633
PyrBnz-2HCOOH	ρ_B^{isol}	0.160		-26.948	-36.532	7.318	0.184	0.416	0.600
PyrBnz-2HCOOH	ρ_B^{FAT}	0.131	0.164	-34.894	-36.532	7.318	0.013	0.104	0.600

[a] defined in Eq. ?? in the manuscript

[b] defined in Eq. ??, and Eq. ?? in the manuscript for ρ_B^{isol} and ρ_B^{FAT} respectively.

[c] Counterpoise corrected, i.e. $E_{int}^{ref} = E_{AB}^{(AB)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[d] Counterpoise correction: $\Delta_{CP} = E_A^{(A)} + E_B^{(B)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[e] $M = M[\rho^{ref} - \rho_B^{FDET(FAT)}]$ with $M[\rho]$ defined in Eq. ?? in the manuscript

[f] $P_{cmpl} = P[\rho_A^{isol} + \rho_B^{isol} - \rho^{ref}]$ (cf. Eq. ??), with $P[\rho]$ defined in Eq. ?? in the manuscript

[g] $P = P[\rho^{ref} - \rho_{tot}^{FDET(FAT)}]$ with $P[\rho]$ defined in Eq. ?? in the manuscript

[h] $E_{int}^{FDET(FAT)}$ is given in Eq. ?? in the manuscript

TABLE S3. Supplementary data for results obtained with the *supermolecular expansion* and the aug-cc-pVDZ basis set. Energies are given in kcal/mol and quantities related to electron densities are given in atomic units.

complex	ρ_B	$E_k[\Delta\rho^c_{v'_A},\rho'_A,\rho_B]$ [a]	$E_k[\Delta\rho^c_{v'_B},\rho'_B,\rho_A]$ [a]	$E_{int}^{FDET(\rho_B)}$ [b]	E_{int}^{ref} [c]	Δ_{CP} [d]	M [e]	P [f]	P_{cmpl} [g]
7HQ-2MeOH	ρ_B^{isol}	0.087		-10.702	-17.473	5.632	0.123	0.231	0.368
7HQ-2MeOH	$\rho_B^{pp(Mulliken)}$	0.084		-10.688	-17.473	5.632	0.121	0.221	0.368
7HQ-2MeOH	$\rho_B^{pp(ChelPG)}$	0.084		-13.492	-17.473	5.632	0.037	0.118	0.368
7HQ-2MeOH	ρ_B^{FAT}	0.081	0.128	-13.181	-17.473	5.632	0.013	0.073	0.368
7HQ-formate	ρ_B^{isol}	0.021		-22.927	-36.485	3.522	0.205	0.316	0.673
7HQ-formate	$\rho_B^{pp(Mulliken)}$	0.016		-27.202	-36.485	3.522	0.148	0.242	0.673
7HQ-formate	$\rho_B^{pp(ChelPG)}$	0.015		-28.678	-36.485	3.522	0.096	0.186	0.673
7HQ-formate	ρ_B^{FAT}	0.011	0.117	-28.028	-36.485	3.522	0.036	0.114	0.673
uracil-5H$_2$O	ρ_B^{isol}	0.212		-31.629	-38.620	7.839	0.237	0.427	0.643
uracil-5H$_2$O	$\rho_B^{pp(Mulliken)}$	0.201		-35.221	-38.620	7.839	0.173	0.305	0.643
uracil-5H$_2$O	$\rho_B^{pp(ChelPG)}$	0.205		-38.010	-38.620	7.839	0.058	0.206	0.643
uracil-5H$_2$O	ρ_B^{FAT}	0.196	0.234	-37.182	-38.620	7.839	0.024	0.129	0.643
PyrBnz-2HCOOH	ρ_B^{isol}	0.161		-25.795	-36.532	7.318	0.185	0.419	0.606
PyrBnz-2HCOOH	$\rho_B^{pp(Mulliken)}$	0.141		-31.448	-36.532	7.318	0.152	0.281	0.606
PyrBnz-2HCOOH	$\rho_B^{pp(ChelPG)}$	0.146		-32.291	-36.532	7.318	0.057	0.215	0.606
PyrBnz-2HCOOH	ρ_B^{FAT}	0.139	0.164	-32.418	-36.532	7.318	0.016	0.127	0.606

[a] defined in Eq. ?? in the manuscript

[b] defined in Eq. ??, and Eq. ?? in the manuscript for ρ_B^{isol} and ρ_B^{FAT} respectively, and in Eq. ?? for $\rho_B^{pp(Mulliken)}$ and $\rho_B^{pp(ChelPG)}$

[c] Counterpoise corrected, i.e. $E_{int}^{ref} = E_{AB}^{(AB)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[d] Counterpoise correction: $\Delta_{CP} = E_A^{(A)} + E_B^{(B)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[e] $M = M[\rho^{ref} - \rho_B^{FDET(FAT)}]$ with $M[\rho]$ defined in Eq. ?? in the manuscript

[f] $P_{cmpl} = P[\rho_A^{isol} + \rho_B^{isol} - \rho^{ref}]$ (cf. Eq. ??), with $P[\rho]$ defined in Eq. ?? in the manuscript

[g] $P = P[\rho^{ref} - \rho_{tot}^{FDET(FAT)}]$ with $P[\rho]$ defined in Eq. ?? in the manuscript

[h] $E_{int}^{FDET(FAT)}$ is given in Eq. ?? in the manuscript

TABLE S4. Supplementary data for results obtained with the *monomer expansion* and the aug-cc-pVDZ basis set. Energies are given in kcal/mol and quantities related to electron densities are given in atomic units.

C. cc-pVTZ

complex	ρ_B	$E_k[\Delta\rho^c_{v'_A},\rho'_A,\rho_B]$ [a]	$E_k[\Delta\rho^c_{v'_B},\rho'_B,\rho_A]$ [a]	$E_{int}^{FDET(\rho_B)}$ [b]	E_{int}^{ref} [c]	Δ_{CP} [d]	M [e]	P [f]	P_{cmpl} [g]
7HQ-2MeOH	ρ_B^{isol}	0.040		-10.716	-17.858	5.681	0.125	0.226	0.358
7HQ-2MeOH	$\rho_B^{pp(Mulliken)}$	0.038		-12.684	-17.858	5.681	0.071	0.153	0.358
7HQ-2MeOH	$\rho_B^{pp(ChelPG)}$	0.037		-13.254	-17.858	5.681	0.045	0.119	0.358
7HQ-2MeOH	ρ_B^{FAT}	0.035	0.068	-13.132	-17.858	5.681	0.021	0.074	0.358
7HQ-formate	ρ_B^{isol}	0.002		-25.786	-39.521	6.011	0.214	0.310	0.661
7HQ-formate	$\rho_B^{pp(Mulliken)}$	0.003		-29.829	-39.521	6.011	0.145	0.230	0.661
7HQ-formate	$\rho_B^{pp(ChelPG)}$	0.003		-30.768	-39.521	6.011	0.116	0.196	0.661
7HQ-formate	ρ_B^{FAT}	0.003	0.064	-30.578	-39.521	6.011	0.057	0.127	0.661
uracil-5H$_2$O	ρ_B^{isol}	0.119		-32.283	-40.078	11.802	0.247	0.413	0.617
uracil-5H$_2$O	$\rho_B^{pp(Mulliken)}$	0.112		-37.341	-40.078	11.802	0.123	0.249	0.617
uracil-5H$_2$O	$\rho_B^{pp(ChelPG)}$	0.111		-37.944	-40.078	11.802	0.091	0.212	0.617
uracil-5H$_2$O	ρ_B^{FAT}	0.104	0.099	-37.489	-40.078	11.802	0.054	0.139	0.617

[a] defined in Eq. ?? in the manuscript

[b] defined in Eq. ??, and Eq. ?? in the manuscript for ρ_B^{isol} and ρ_B^{FAT} respectively, and in Eq. ?? for $\rho_B^{pp(Mulliken)}$ and $\rho_B^{pp(ChelPG)}$

[c] Counterpoise corrected, i.e. $E_{int}^{ref} = E_{AB}^{(AB)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[d] Counterpoise correction: $\Delta_{CP} = E_A^{(A)} + E_B^{(B)} - E_A^{(AB)} - E_B^{(AB)}$, where all values are obtained with MP2, the subscript denotes the subsystem, and the superscript denotes the centres involved in the basis set expansion.

[e] $M = M[\rho^{ref} - \rho_B^{FDET(FAT)}]$ with $M[\rho]$ defined in Eq. ?? in the manuscript

[f] $P_{cmpl} = P[\rho_A^{isol} + \rho_B^{isol} - \rho^{ref}]$ (cf. Eq. ??), with $P[\rho]$ defined in Eq. ?? in the manuscript

[g] $P = P[\rho^{ref} - \rho_{tot}^{FDET(FAT)}]$ with $P[\rho]$ defined in Eq. ?? in the manuscript

[h] $E_{int}^{FDET(FAT)}$ is given in Eq. ?? in the manuscript

TABLE S5. Supplementary data for results obtained with the *monomer expansion* and the cc-pVTZ basis set. Energies are given in kcal/mol and quantities related to electron densities are given in atomic units.