Geometry Optimizations in a Subsystem DFT Formalism: A Benchmark Study

Supporting Information

Kevin Klahr, Danny Schlüns, and Johannes Neugebauer[1]

Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster and Center for Multiscale Theory and Computation, Westfälische Wilhelms-Universität Münster, Corrensstraße 40, 48149 Münster, Germany.

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[1] j.neugebauer@uni-muenster.de

1 Validation

To verify the results of our implementation, analytical sDFT gradients are compared to their numerically derived counterparts. For the numerical differentiation, we used a 3-point central differences formula with a displacement of 0.003 a.u. for each atom. This value was acquired through a preliminary screening of different displacement values. Additional tests showed that the sDFT calculations are more sensitive to the choice of this step size than the corresponding Kohn–Sham DFT results. This is probably due to the additional ingredient needed in sDFT calculations: the non-additive kinetic-energy functional (and its functional derivative, during the SCF), which requires an additional numerical integration step. For every exchange–correlation functional used, the "conjoint" kinetic energy functional (see main text) is applied.

1.1 Neon Dimer

The first and simplest test system, analogously to the presentation of the sDFT gradient implementation in ADF is a neon dimer system at a distance of 1 Å. Since both atoms are displaced only along the Z-axis, gradient contributions only appear in this direction. The absolute error between the analytical and the numerical sDFT gradient in Z-direction (Tab. S1) is taken as a measure for the succesful implementation, along with a comparison of the same errors for KS-DFT calculations (Tab. S2). In addition the absolute errors between sDFT gradient calculations with and without the RI approximation are compared to assess the magnitude of the error introduced by it. It can be seen that the

Table S1: Comparison of numerical and analytical total sDFT gradient in Z direction for one neon atom of a neon dimer at 1 Å distance with and without density fitting. All results are given in atomic units.

	no-RI			RI		
XC/KEF	Analytical	Numerical	Abs. Error	Analytical	Numerical	Abs. Error
LDA/TF	2.555652	2.555662	0.000010	2.555547	2.555555	0.000008
PW91/PW91k	2.346491	2.346533	0.000038	2.346307	2.346343	0.000036

Table S2: Comparison of numerical and analytical total KS-DFT gradient in Z direction for one neon atom of a neon dimer at 1 Å distance with and without density fitting. All results are given in atomic units.

	no-RI			RI		
XC	Analytical	Numerical	Abs. Error	Analytical	Numerical	Abs. Error
LDA	3.134081	3.134090	0.000009	3.132227	3.132236	0.000009
PW91	3.169239	3.169244	0.000005	3.167367	3.167371	0.000004

deviations between numerical and analytical gradients for sDFT are around 5 orders of magnitude lower than the actual gradient, despite the fact that the absolute errors of the sDFT gradient calculations are slightly larger than the absolute errors of the KS-DFT calculations. By comparing results obtained with and without RI it can further be seen that the error introduced by this approximation is around 6 orders of magnitude lower than the actual gradient, which is negligible.

1.2 Water Dimer

The second validation test is conducted on a water dimer system. As a starting point, the water dimer geometry from the S22 test set is used. The first water molecule in the coordinate file will be treated as the active system for the purpose of this test. For clarity, only the gradient norms of each atom will be compared between analytical and numerical sDFT gradients and the resulting absolute errors will be compared to the respective absolute errors between a numerical and analytical KS-DFT gradient calculation. Moreover, the absolute errors between sDFT gradient calculations with and without the RI approximation are compared to assess the magnitude of the error introduced by it.

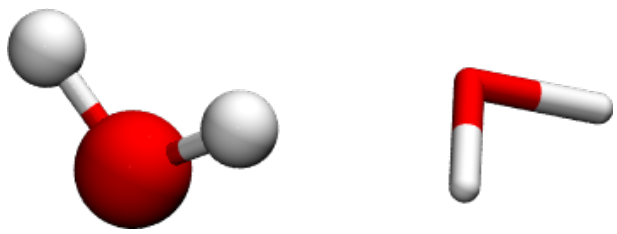

Figure S1: Structure of the water dimer from the S22 test set. The first water molecule in the coordinate file is shown in ball-and-stick representation.

Table S3: Comparison of numerical and analytical total sDFT gradient norms per atom for the first water molecule of the complex with LDA/TF. Results are given with and without the RI approximation. All results are given in atomic units.

	LDA/TF			LDA/TF - RI		
Atom	Analytical	Numerical	Abs. Error	Analytical	Numerical	Abs. Error
O	0.011977	0.011918	0.000059	0.011819	0.011758	0.000061
H	0.012105	0.012088	0.000017	0.011996	0.011977	0.000019
H	0.009935	0.009982	0.000047	0.009833	0.009890	0.000057

Table S4: Comparison of numerical and analytical total sDFT gradient norms per atom for the first water molecule of the complex with PW91/PW91k. Results are given with and without the RI approximation. All results are given in atomic units.

	PW91/PW91k			PW91/PW91k - RI		
Atom	Analytical	Numerical	Abs. Error	Analytical	Numerical	Abs. Error
O	0.010366	0.010296	0.000070	0.010198	0.010127	0.000071
H	0.009763	0.009742	0.000019	0.009639	0.009615	0.000024
H	0.008577	0.008625	0.000048	0.008459	0.008519	0.000060

The deviations between analytical and numerical sDFT gradients are around 2–3 orders of magnitude smaller than the actual gradient values, which are about two orders of magnitude smaller than in the previous example. The errors of sDFT and KS-DFT are of the same magnitude (see Tabs. S5 and S6) as was the case with the neon dimer system, the error introduced by the density fitting approximation is even lower than this (3–4 orders of magnitude lower than the actual gradient). The gradient errors also appear to be largely independent of the choice of functional.

Table S5: Comparison of numerical and analytical total KS-DFT gradient norms per atom for the first water molecule of the complex with LDA. Results are given with and without the RI approximation. All results are given in atomic units.

	LDA			LDA - RI		
Atom	Analytical	Numerical	Abs. Error	Analytical	Numerical	Abs. Error
O	0.014840	0.014789	0.000051	0.014721	0.014670	0.000049
H	0.012379	0.012359	0.000020	0.012275	0.012255	0.000020
H	0.019508	0.019540	0.000032	0.019422	0.019454	0.000032

Table S6: Comparison of numerical and analytical total KS-DFT gradient norms per atom for the first water molecule of the complex with PW91. Results are given with and without the RI approximation. All results are given in atomic units.

	PW91			PW91 - RI		
Atom	Analytical	Numerical	Abs. Error	Analytical	Numerical	Abs. Error
O	0.012847	0.012790	0.000057	0.012726	0.012670	0.000056
H	0.009920	0.009895	0.000025	0.009802	0.009776	0.000026
H	0.012833	0.012867	0.000034	0.012743	0.012777	0.000034

2 Data Tables

Table S7: Comparison of the sDFT optimized structures with reference data in the S22 test set with LDA/TF. ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	3.21	3.08	0.13	0.07
2	2.91	2.95	−0.04	0.04
3	2.99	3.13	−0.14	0.09
4	3.23	3.26	−0.03	0.04
5	6.08	6.13	−0.05	0.04
6	5.14	5.14	0.00	0.25
7	5.97	5.95	0.02	0.02
8	3.72	3.72	0.00	0.01
9	3.72	3.72	0.00	0.01
10	3.72	3.95	−0.23	0.11
11	3.76	4.05	−0.29	0.15
12	3.48	3.73	−0.25	0.14
13	3.17	5.48	−2.31	2.35
14	3.50	5.22	−1.72	1.20
15	3.17	3.54	−0.37	0.36
16	4.42	4.20	0.22	0.11
17	3.38	3.49	−0.11	0.05
18	3.56	3.70	−0.14	0.07
19	3.95	4.07	−0.12	0.05
20	4.91	5.22	−0.31	0.16
21	4.88	5.10	−0.22	0.11
22	4.92	5.72	−0.80	0.68
MAD			0.34	0.28

Table S8: Comparison of the sDFT optimized structures with reference data in the S22 test set with PW91/PW91k. ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	3.21	2.86	0.35	0.17
2	2.91	2.83	0.08	0.04
3	2.99	3.00	0.01	0.05
4	3.23	3.12	0.11	0.05
5	6.08	6.02	0.06	0.04
6	5.14	5.02	0.12	0.26
7	5.97	5.85	0.12	0.06
8	3.72	3.25	0.47	0.23
9	3.72	3.36	0.36	0.18
10	3.72	3.72	0.0	0.01
11	3.76	3.66	0.10	0.08
12	3.48	3.39	0.09	0.05
13	3.17	2.99	0.18	0.11
14	3.50	4.66	−1.16	1.23
15	3.17	3.11	0.06	0.18
16	4.42	4.01	0.41	0.20
17	3.38	3.08	0.30	0.26
18	3.56	3.11	0.45	0.41
19	3.95	3.83	0.12	0.05
20	4.91	4.91	0.0	0.01
21	4.88	4.88	0.0	0.01
22	4.92	5.34	−0.42	0.56
MAD			0.23	0.19

Table S9: Comparison of the sDFT optimized structures with reference data in the A24 test set with LDA/TF. ΔCoM is calculated as $\Delta\mathrm{CoM} = \mathrm{CoM}_{\mathrm{ref}} - \mathrm{CoM}_{\mathrm{Ser}}$. The RMSD is given by $\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\mathrm{ref}} - \vec{R}^i_{\mathrm{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\mathrm{ref}} - \vec{R}^i_{\mathrm{Ser}}|^2 = ((R^i_{\mathrm{ref}_x} - R^i_{\mathrm{Ser}_x})^2 + (R^i_{\mathrm{ref}_y} - R^i_{\mathrm{Ser}_y})^2 + (R^i_{\mathrm{ref}_z} - R^i_{\mathrm{Ser}_z})^2)$. $\vec{R}^i_{\mathrm{ref}}$ and $\vec{R}^i_{\mathrm{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	$\mathrm{CoM}_{\mathrm{ref}}$	$\mathrm{CoM}_{\mathrm{Ser}}$	ΔCoM	RMSD
1	2.98	3.01	−0.03	0.02
2	2.92	2.95	−0.03	0.02
3	4.46	4.30	0.16	0.08
4	2.72	2.82	−0.10	0.07
5	3.23	3.08	0.15	0.07
6	3.19	3.34	−0.15	0.06
7	3.95	3.61	0.34	0.17
8	3.78	3.64	0.14	0.07
9	2.91	3.15	−0.24	0.15
10	3.32	3.40	−0.08	0.04
11	3.70	3.80	−0.10	0.07
12	4.36	4.19	0.17	0.09
13	3.70	3.70	0.0	0.01
14	3.81	3.81	0.0	0.01
15	4.21	3.94	0.27	0.14
16	2.98	3.14	−0.16	0.20
17	3.71	3.71	0.0	0.01
18	4.38	4.38	0.0	0.01
19	3.64	3.64	0.0	0.01
20	3.68	3.68	0.0	0.01
21	3.90	3.71	0.19	0.07
22	3.50	3.99	−0.49	0.24
23	3.50	3.98	−0.48	0.24
24	3.50	19.65	−16.15	8.07
MAD			0.80	0.41

Table S10: Comparison of the sDFT optimized structures with reference data in the A24 test set with PW91/PW91k. ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	2.98	2.88	0.10	0.05
2	2.92	2.82	0.10	0.06
3	4.46	4.17	0.29	0.14
4	2.72	2.71	0.01	0.05
5	3.23	2.86	0.37	0.18
6	3.19	3.20	−0.01	0.01
7	3.95	3.42	0.53	0.26
8	3.78	3.46	0.32	0.15
9	2.91	2.87	0.04	0.05
10	3.32	3.22	0.10	0.05
11	3.70	3.52	0.18	0.12
12	4.36	4.00	0.36	0.18
13	3.70	3.42	0.28	0.13
14	3.81	3.61	0.20	0.10
15	4.21	3.72	0.49	0.25
16	2.98	2.77	0.21	0.22
17	3.71	3.39	0.32	0.16
18	4.38	4.03	0.35	0.17
19	3.64	3.25	0.39	0.19
20	3.68	3.35	0.33	0.12
21	3.90	3.42	0.48	0.17
22	3.50	3.50	0.0	0.00
23	3.50	3.50	0.0	0.01
24	3.50	4.02	−0.52	0.26
MAD			0.24	0.13

Table S11: Comparison of the sDFT optimized structures with reference data in the S22 test set with BP86/LLP91. ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	3.21	2.97	0.24	0.11
2	2.91	2.90	0.01	0.01
3	2.99	3.06	−0.07	0.06
4	3.23	3.17	0.06	0.03
5	6.08	6.08	0.00	0.04
6	5.14	5.09	0.05	0.23
7	5.97	5.91	0.06	0.03
8	3.72	7.17	−3.45	1.72
9	3.72	3.72	0.00	0.01
10	3.72	7.40	−3.68	1.68
11	3.76	11.39	−7.63	3.85
12	3.48	6.64	−3.16	1.72
13	3.17	5.45	−2.28	2.35
14	3.50	7.25	−3.75	1.93
15	3.17	5.56	−2.39	2.46
16	4.42	4.20	0.22	0.11
17	3.38	3.51	−0.13	0.06
18	3.56	3.77	−0.21	0.10
19	3.95	4.02	−0.07	0.03
20	4.91	8.03	−3.12	1.56
21	4.88	5.15	−0.27	0.14
22	4.92	5.89	−0.97	0.86
MAD			1.45	0.87

Table S12: Comparison of the sDFT optimized structures with reference data in the S22 test set with BP86/LLP91 + D3(BJ). ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	3.21	2.94	0.27	0.13
2	2.91	2.89	0.02	0.01
3	2.99	3.04	−0.05	0.06
4	3.23	3.15	0.08	0.04
5	6.08	6.03	0.05	0.03
6	5.14	5.03	0.11	0.23
7	5.97	5.86	0.11	0.06
8	3.72	3.38	0.34	0.17
9	3.72	3.39	0.33	0.16
10	3.72	3.48	0.24	0.11
11	3.76	3.23	0.53	0.30
12	3.48	3.07	0.41	0.39
13	3.17	2.86	0.31	0.21
14	3.50	3.19	0.31	0.26
15	3.17	2.96	0.21	0.15
16	4.42	4.04	0.38	0.19
17	3.38	3.08	0.30	0.26
18	3.56	3.07	0.49	0.42
19	3.95	3.79	0.16	0.06
20	4.91	4.69	0.22	0.11
21	4.88	4.74	0.14	0.07
22	4.92	4.57	0.35	0.34
MAD			0.24	0.17

Table S13: Comparison of the sDFT optimized structures with reference data in the A24 test set with BP86/LLP91. ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	2.98	2.95	0.03	0.03
2	2.92	2.91	0.01	0.01
3	4.46	4.25	0.21	0.10
4	2.72	2.80	−0.08	0.06
5	3.23	2.97	0.26	0.12
6	3.19	3.43	−0.24	0.10
7	3.95	3.62	0.33	0.16
8	3.78	3.78	0.00	0.01
9	2.91	3.08	−0.17	0.13
10	3.32	3.42	−0.10	0.05
11	3.70	4.29	−0.59	0.56
12	4.36	4.18	0.18	0.09
13	3.70	3.70	0.00	0.01
14	3.81	7.24	−3.43	1.72
15	4.21	4.21	0.00	0.01
16	2.98	3.20	−0.22	0.19
17	3.71	7.47	−3.76	1.84
18	4.38	-	-	-
19	3.64	7.17	−3.53	1.77
20	3.68	7.30	−3.62	1.35
21	3.90	7.42	−3.52	1.23
22	3.50	18.51	−15.01	7.35
23	3.50	15.70	−12.20	6.10
24	3.50	19.55	−16.05	8.03
MAD			2.76	1.29

Table S14: Comparison of the sDFT optimized structures with reference data in the A24 test set with BP86/LLP91 + D3(BJ). ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{Ser}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}^i_{\text{ref}} - \vec{R}^i_{\text{Ser}}|^2 = ((R^i_{\text{ref}_x} - R^i_{\text{Ser}_x})^2 + (R^i_{\text{ref}_y} - R^i_{\text{Ser}_y})^2 + (R^i_{\text{ref}_z} - R^i_{\text{Ser}_z})^2)$. $\vec{R}^i_{\text{ref}}$ and $\vec{R}^i_{\text{Ser}}$ refer to a vector of the cartesian components (x, y, z) of atom i of the reference structure and the sDFT SERENITY-optimized structure, respectively. All results are given in units of Å.

compound	CoM_{ref}	CoM_{Ser}	ΔCoM	RMSD
1	2.98	2.93	0.05	0.04
2	2.92	2.89	0.03	0.02
3	4.46	4.22	0.24	0.12
4	2.72	2.80	−0.08	0.05
5	3.23	2.94	0.29	0.14
6	3.19	3.33	−0.14	0.06
7	3.95	3.50	0.45	0.22
8	3.78	3.62	0.16	0.07
9	2.91	2.98	−0.07	0.07
10	3.32	3.30	0.02	0.03
11	3.70	3.47	0.23	0.18
12	4.36	4.04	0.32	0.16
13	3.70	3.46	0.24	0.13
14	3.81	3.57	0.24	0.12
15	4.21	3.72	0.49	0.24
16	2.98	2.90	0.08	0.19
17	3.71	3.45	0.26	0.13
18	4.38	4.14	0.24	0.12
19	3.64	3.38	0.26	0.13
20	3.68	3.67	0.01	0.01
21	3.90	3.47	0.43	0.15
22	3.50	3.36	0.14	0.07
23	3.50	3.32	0.18	0.09
24	3.50	3.50	0.00	0.00
MAD			0.19	0.11

3 Structure Overlays

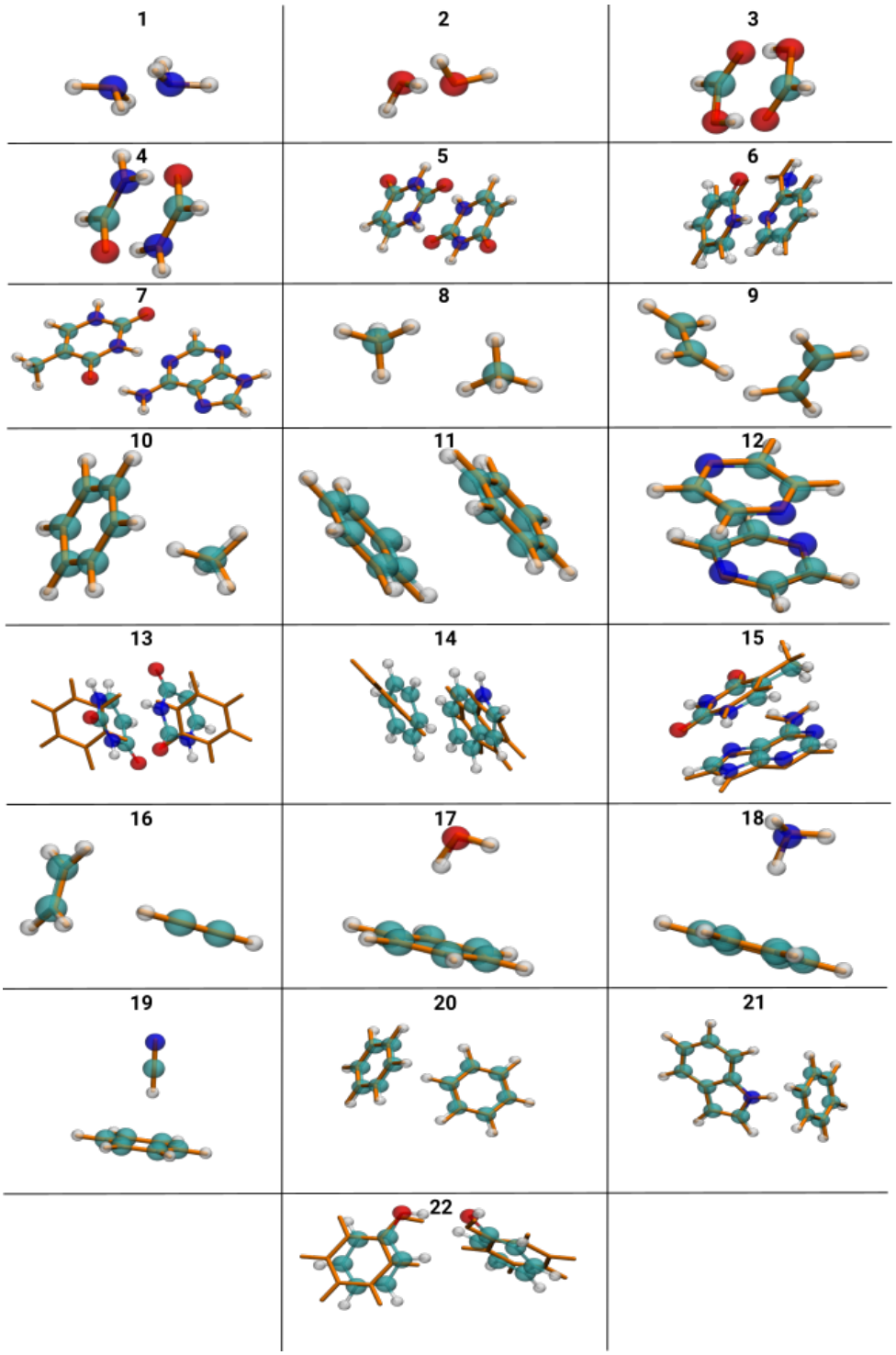

Figure S2: Structural overlays of S22 structures (ball-and-stick models) and sDFT-LDA/TF optimized structures (displayed as wireframe in orange).

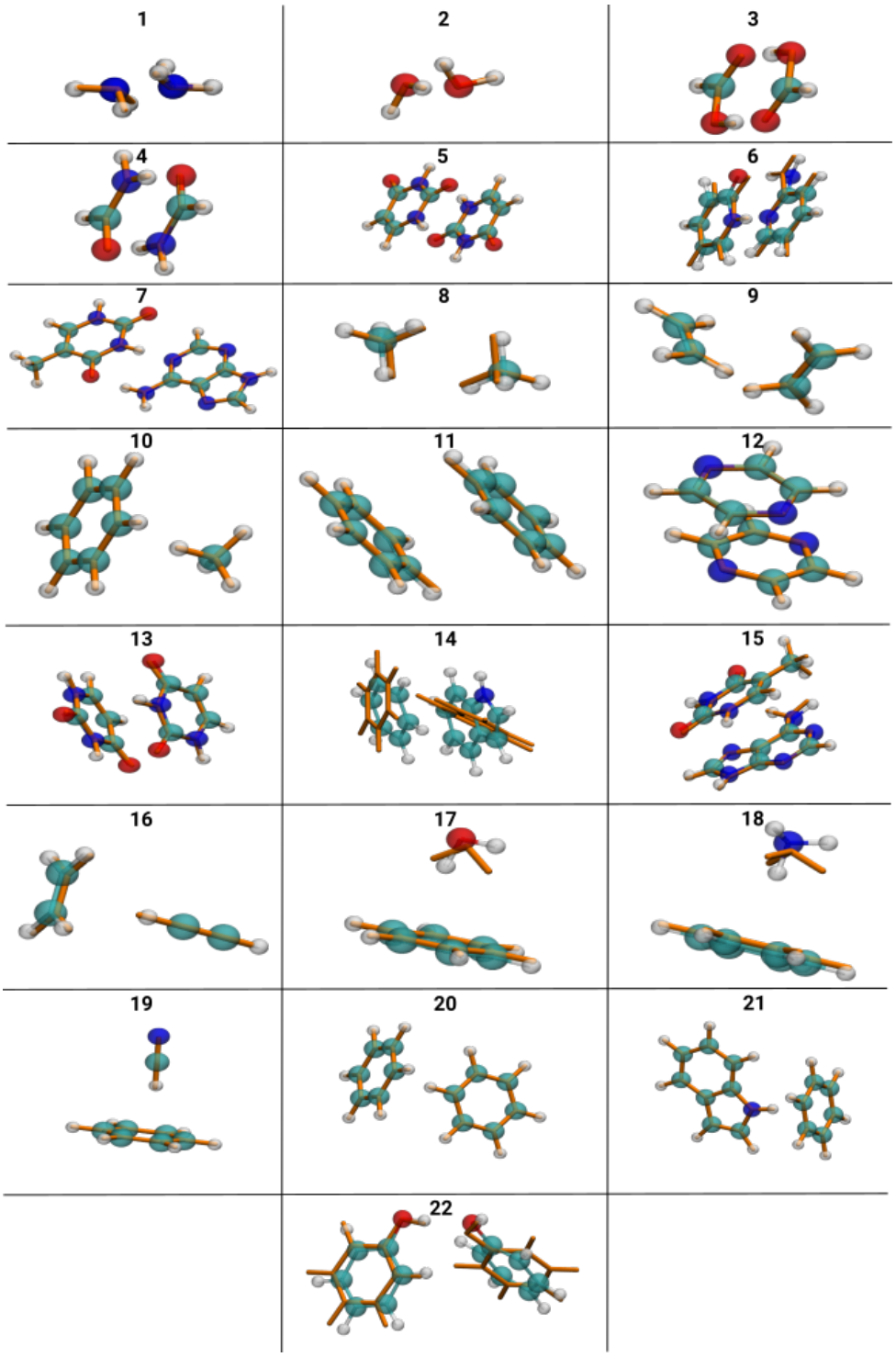

Figure S3: Structural overlays of S22 (ball-and-stick models) structures and sDFT-PW91/PW91k optimized structures (displayed as wireframe in orange).

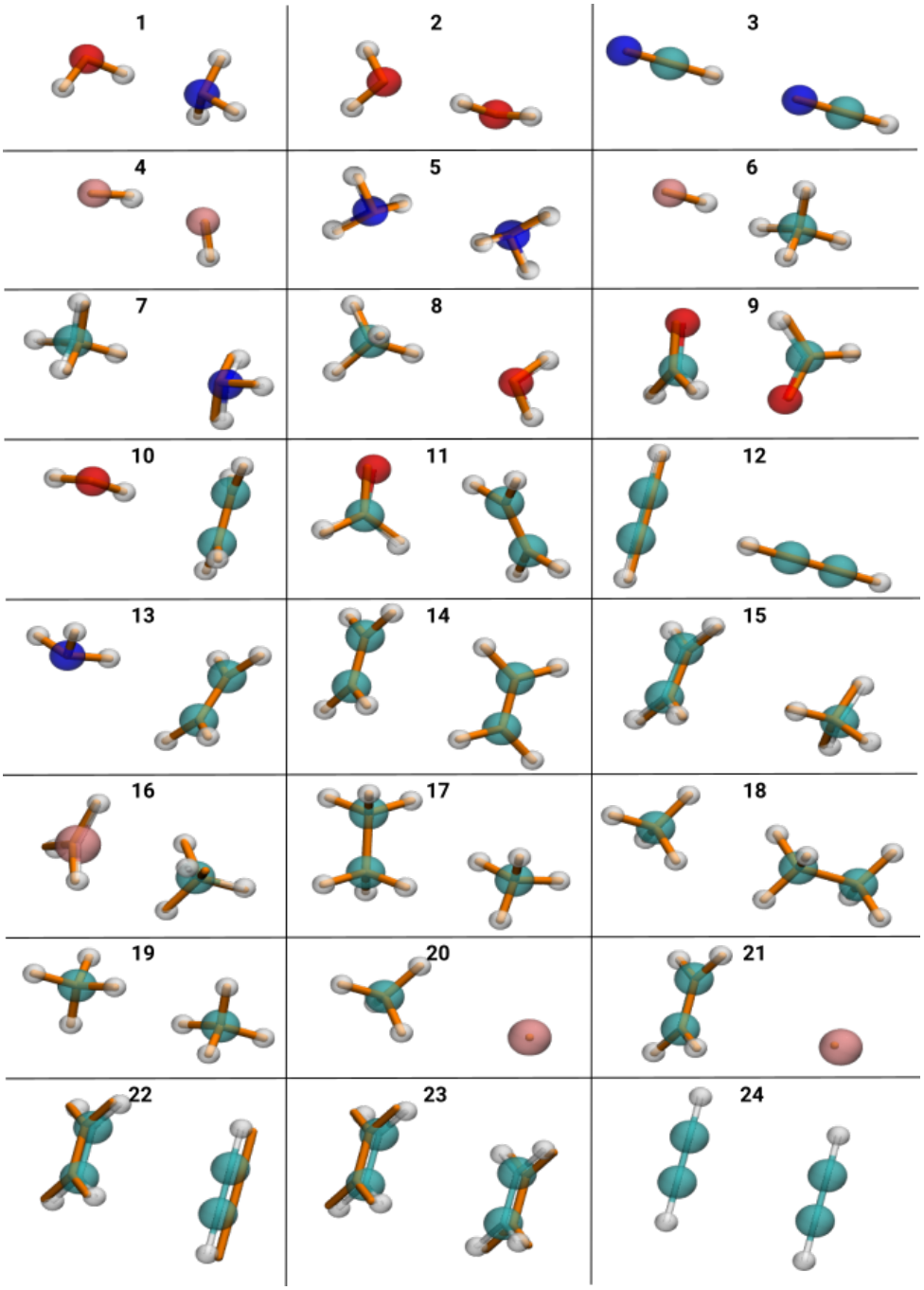

Figure S4: Structural overlays of A24 structures (ball-and-stick models) and sDFT-LDA/TF optimized structures (displayed as wireframe in orange).

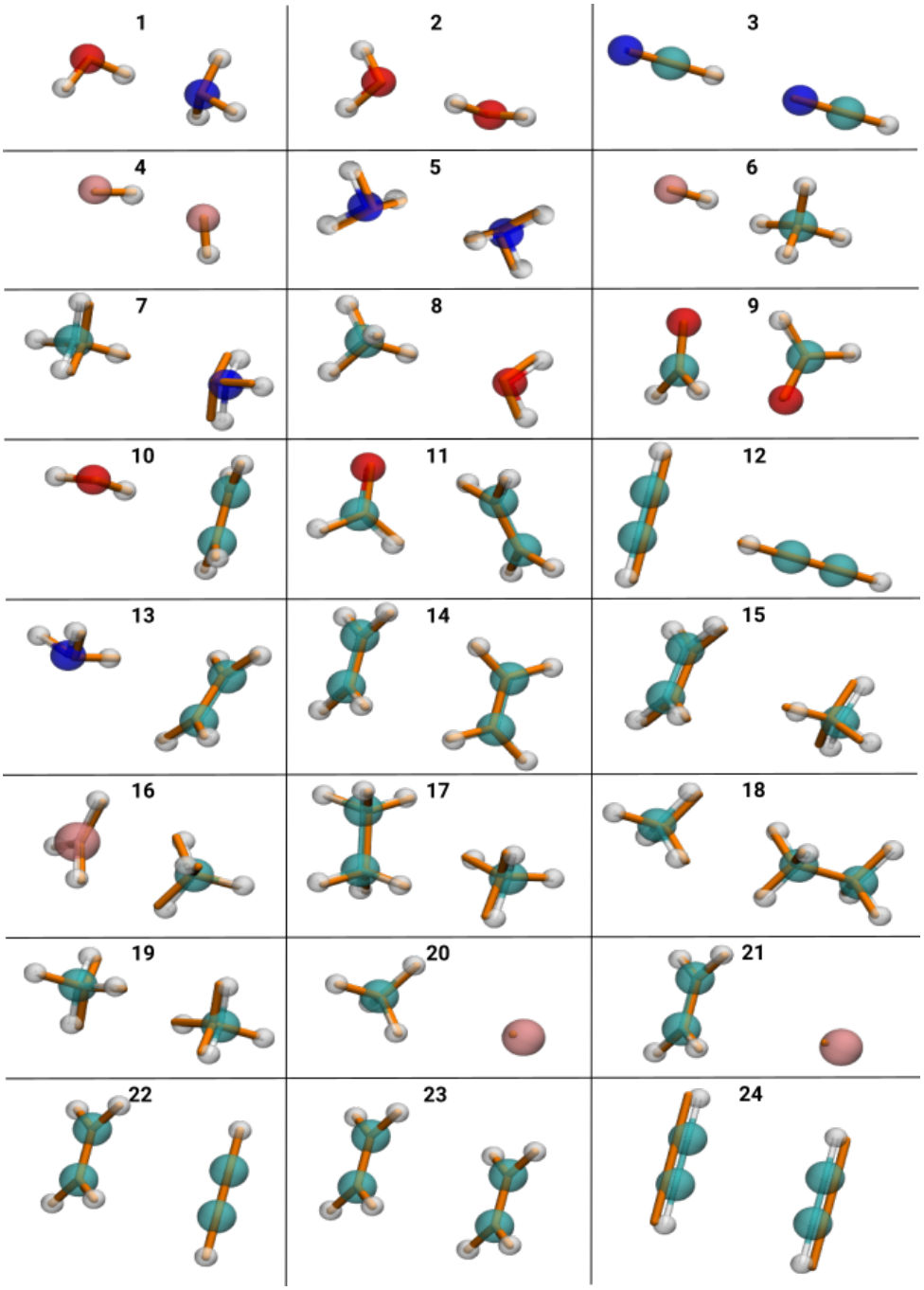

Figure S5: Structural overlays of A24 structures (ball-and-stick models) and sDFT-PW91/PW91k optimized structures (displayed as wireframe in orange).

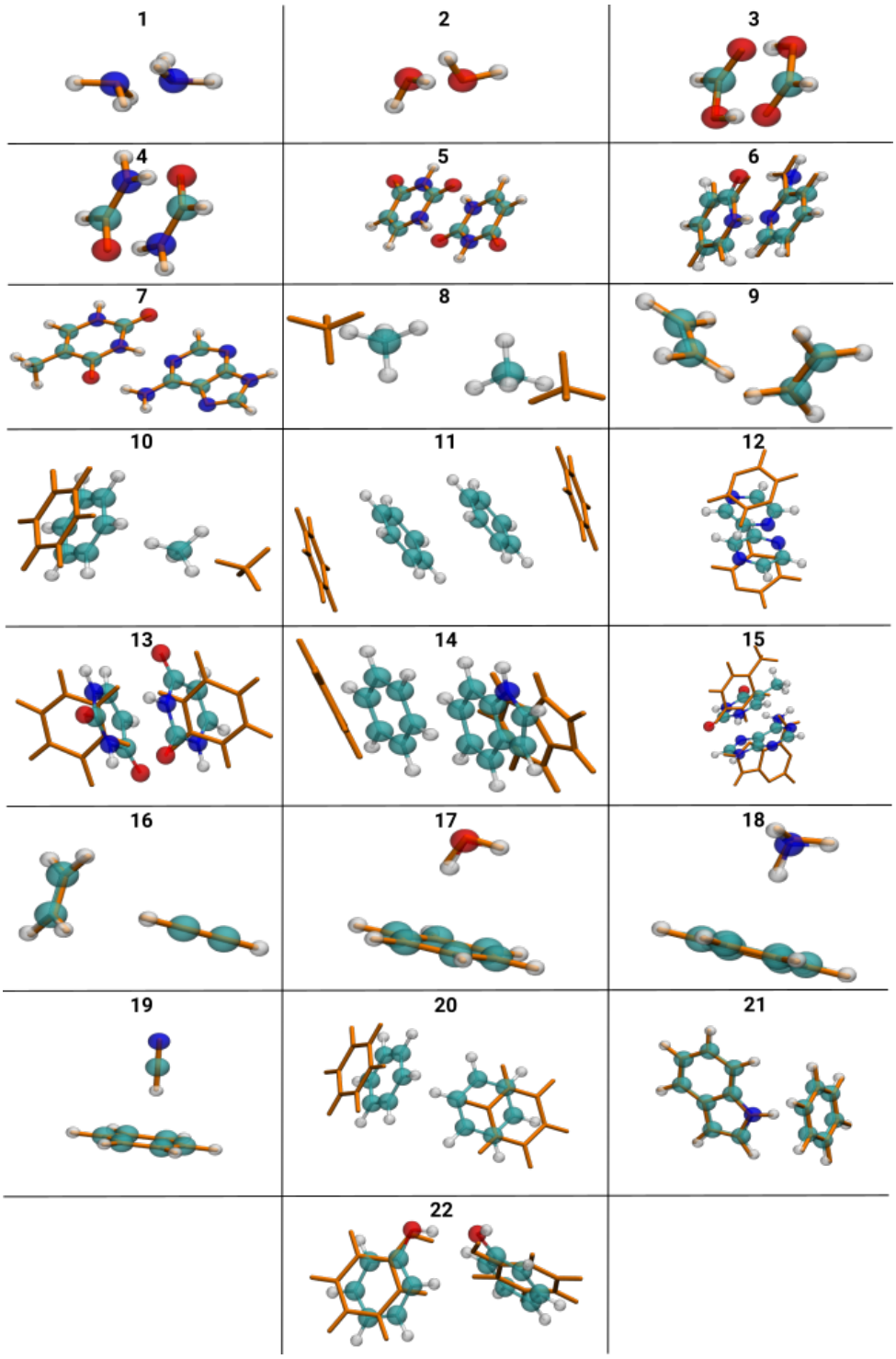

Figure S6: Structural overlays of S22 structures (ball-and-stick models) and sDFT-BP86/LLP91 optimized structures (displayed as wireframe in orange).

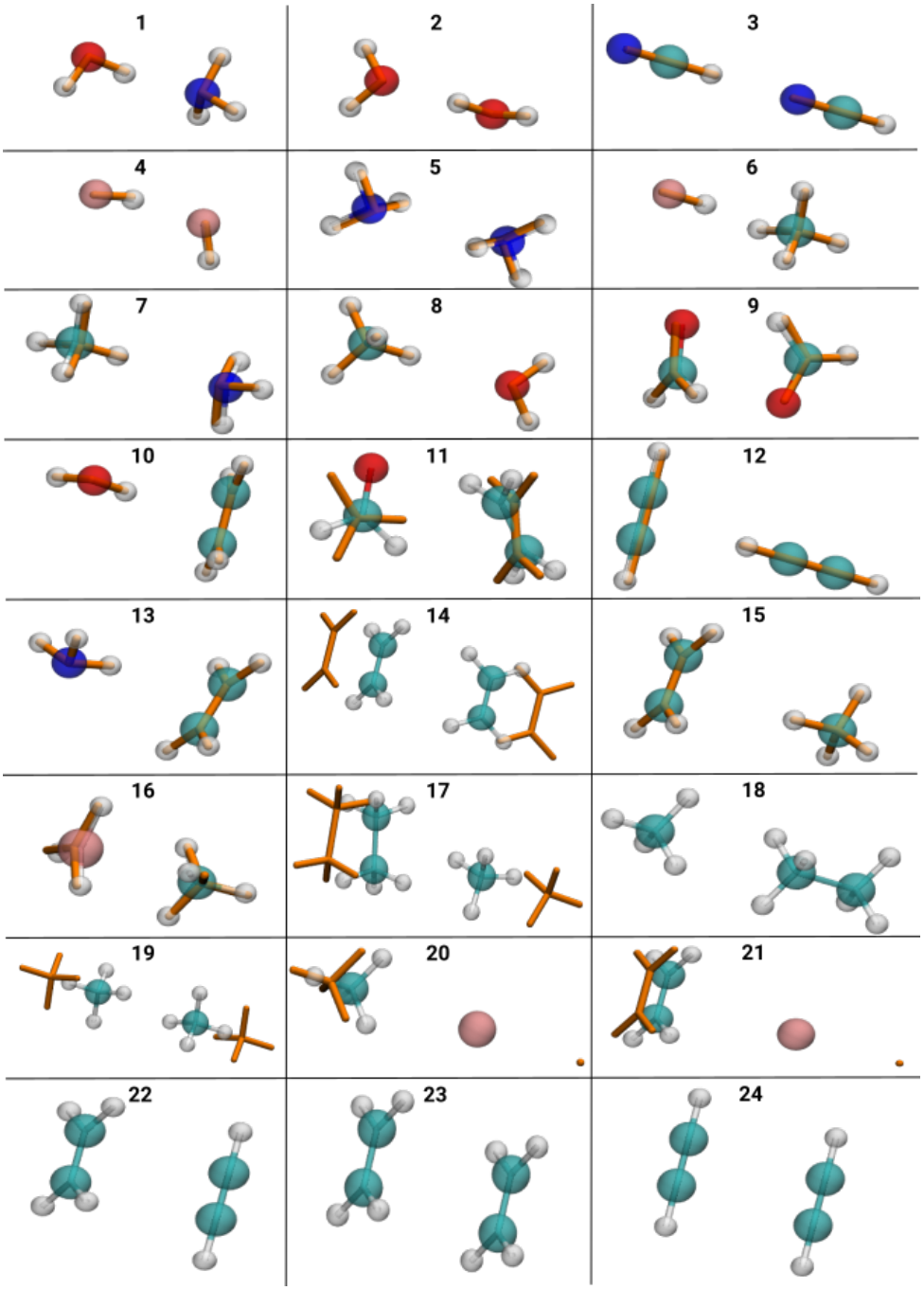

Figure S7: Structural overlays of A24 structures (ball-and-stick models) and sDFT-BP86/LLP91 optimized structures (displayed as wireframe in orange).

4 Comparison of GTOs vs. STOs

In the main manuscript, it is mentioned that in the comparison between the GTO-based implementation in Serenity and the STO-based implementation in Adf some of the Adf-optimizations were restarted from the Serenity results for a better comparability of corresponding structures. In the case of the S22 test set with the LDA/TF functional combination, only the structures 13, 14 and 22 showed significant differences when optimizing from the reference geometry, but the geometry optimizations are in good agreement after using the Serenity-optimized structure as a starting point for the Adf geometry optimization. For the S22 test set with the PW91/PW91k functional combination, significant differences between the STO and GTO optimized structures are observed for the structures 14, 18 and 22 when optimized from the reference structure, which vanished once again after using the Serenity-optimized structure as a starting point for the Adf geometry optimization. In the case of the A24 test set with LDA/TF, only one notable difference between STO and GTO optmized structures can be found. Structure 24, the ethyne dimer, is optimized to a lower-lying stationary point of the potential-energy surface. Also in this case, an additional optimization with Adf using the Serenity-optimized structure as a starting point gives a good agreement between the two implementations.

In the following section, data are provided for both sets of results, i.e., using the reference structures or the Serenity-optimized structures (in the cases mentioned above).

Table S15: Comparison of optimized sDFT structures obtained with S22 LDA/TF using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (Serenity implementation). ΔCoM is calculated as $\Delta\mathrm{CoM} = \mathrm{CoM}_{\mathrm{ref}} - \mathrm{CoM}_{\mathrm{DFT}}$. The RMSD is given by $\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R^i_{1_x} - R^i_{2_x})^2 + (R^i_{1_y} - R^i_{2_y})^2 + (R^i_{1_z} - R^i_{2_z})^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	$\mathrm{CoM}_{\mathrm{ref}}$	$\mathrm{CoM}_{\mathrm{ADF}}$	$\Delta\mathrm{CoM}_{\mathrm{ref}}^{\mathrm{ADF}}$	$\mathrm{CoM}_{\mathrm{Ser}}$	$\Delta\mathrm{CoM}_{\mathrm{Ser}}^{\mathrm{ADF}}$	$\mathrm{RMSD}_{\mathrm{ADF}}$	$\mathrm{RMSD}_{\mathrm{Ser}}$	$\Delta\mathrm{RMSD}_{\mathrm{ADF}}^{\mathrm{Ser}}$
1	3.21	3.11	0.10	3.08	0.03	0.05	0.07	0.02
2	2.91	2.99	−0.08	2.95	0.04	0.05	0.04	0.02
3	2.99	3.14	−0.15	3.13	0.01	0.09	0.09	0.01
4	3.23	3.26	−0.03	3.26	0.00	0.04	0.04	0.00
5	6.08	6.12	−0.04	6.13	−0.	0.04	0.04	0.01
6	5.14	5.14	0.00	5.14	0.00	0.12	0.25	0.14
7	5.97	5.95	0.02	5.95	0.00	0.02	0.02	0.01
8	3.72	3.69	0.03	3.72	−0.03	0.02	0.01	0.01
9	3.72	3.72	0.00	3.72	0.00	0.01	0.01	0.00
10	3.72	3.84	−0.12	3.95	−0.11	0.06	0.11	0.05
11	3.76	3.98	−0.22	4.05	−0.07	0.11	0.15	0.05
12	3.48	3.67	−0.19	3.73	−0.06	0.12	0.14	0.04
13	3.17	3.31	−0.14	5.48	−2.17	0.08	2.35	2.31
14	3.50	4.08	−0.58	5.22	−1.14	0.39	1.20	0.82
15	3.17	3.46	−0.29	3.54	−0.08	0.18	0.36	0.23
16	4.42	4.23	0.19	4.20	0.03	0.09	0.11	0.02
17	3.38	3.47	−0.09	3.49	−0.02	0.05	0.05	0.01
18	3.56	3.66	−0.10	3.70	−0.04	0.05	0.07	0.02
19	3.95	4.06	−0.11	4.07	−0.01	0.05	0.05	0.00
20	4.91	5.10	−0.19	5.22	−0.12	0.10	0.16	0.06
21	4.88	5.06	−0.18	5.10	−0.04	0.09	0.11	0.02
22	4.92	5.07	−0.15	5.72	−0.65	0.08	0.68	0.62
MAD			0.13		0.21	0.09	0.28	0.20

Table S16: Comparison of optimized sDFT structures obtained with S22 PW91/PW91k using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (SERENITY implementation). ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{DFT}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R_{1_x}^i - R_{2_x}^i)^2 + (R_{1_y}^i - R_{2_y}^i)^2 + (R_{1_z}^i - R_{2_z}^i)^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	CoM_{ref}	CoM_{ADF}	$\Delta\text{CoM}_{\text{ref}}^{\text{ADF}}$	CoM_{Ser}	$\Delta\text{CoM}_{\text{Ser}}^{\text{ADF}}$	RMSD_{ADF}	RMSD_{Ser}	$\Delta\text{RMSD}_{\text{ADF}}^{\text{Ser}}$
1	3.21	2.89	0.32	2.86	0.03	0.15	0.17	0.01
2	2.91	2.86	0.05	2.83	0.03	0.03	0.04	0.03
3	2.99	3.01	−0.02	3.00	0.01	0.05	0.05	0.01
4	3.23	3.12	0.11	3.12	0.00	0.05	0.05	0.00
5	6.08	6.02	0.06	6.02	0.00	0.04	0.04	0.00
6	5.14	5.02	0.12	5.02	0.00	0.12	0.26	0.16
7	5.97	5.85	0.12	5.85	0.00	0.06	0.06	0.01
8	3.72	3.31	0.41	3.25	0.06	0.21	0.23	0.03
9	3.72	3.42	0.30	3.36	0.06	0.15	0.18	0.03
10	3.72	3.70	0.02	3.72	−0.02	0.01	0.01	0.01
11	3.76	3.70	0.06	3.66	0.04	0.06	0.08	0.02
12	3.48	3.40	0.08	3.39	0.01	0.05	0.05	0.02
13	3.17	3.02	0.15	2.99	0.03	0.08	0.11	0.04
14	3.50	3.56	−0.06	4.66	−1.10	0.20	1.23	1.13
15	3.17	3.11	0.06	3.11	0.00	0.11	0.18	0.09
16	4.42	4.04	0.38	4.01	0.03	0.19	0.20	0.01
17	3.38	3.09	0.29	3.08	0.01	0.24	0.26	0.04
18	3.56	3.48	0.08	3.11	0.37	0.07	0.41	0.36
19	3.95	3.88	0.07	3.83	0.05	0.03	0.05	0.02
20	4.91	4.91	0.00	4.91	0.00	0.01	0.01	0.00
21	4.88	4.89	−0.01	4.88	0.01	0.01	0.01	0.01
22	4.92	4.91	0.01	5.34	−0.43	0.05	0.56	0.53
MAD			0.12		0.10	0.09	0.19	0.12

Table S17: Comparison of optimized sDFT structures obtained with A24 LDA/TF using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (SERENITY implementation). ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{DFT}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R_{1_x}^i - R_{2_x}^i)^2 + (R_{1_y}^i - R_{2_y}^i)^2 + (R_{1_z}^i - R_{2_z}^i)^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	CoM_{ref}	CoM_{ADF}	$\Delta\text{CoM}_{\text{ref}}^{\text{ADF}}$	CoM_{Ser}	$\Delta\text{CoM}_{\text{Ser}}^{\text{ADF}}$	RMSD_{ADF}	RMSD_{Ser}	$\Delta\text{RMSD}_{\text{ADF}}^{\text{Ser}}$
1	2.98	3.02	−0.04	3.01	0.01	0.02	0.02	0.01
2	2.92	2.99	−0.07	2.95	0.04	0.03	0.02	0.02
3	4.46	4.31	0.15	4.30	0.01	0.07	0.08	0.01
4	2.72	2.86	−0.14	2.82	0.04	0.08	0.07	0.02
5	3.23	3.11	0.12	3.08	0.03	0.06	0.07	0.02
6	3.19	3.29	−0.10	3.34	−0.05	0.04	0.06	0.02
7	3.95	3.68	0.27	3.61	0.07	0.14	0.17	0.03
8	3.78	3.73	0.05	3.64	0.09	0.03	0.07	0.04
9	2.91	3.13	−0.22	3.15	−0.02	0.13	0.15	0.03
10	3.32	3.37	−0.05	3.40	−0.03	0.02	0.04	0.01
11	3.70	3.77	−0.07	3.80	−0.03	0.06	0.07	0.02
12	4.36	4.21	0.15	4.19	0.02	0.08	0.09	0.01
13	3.70	3.68	0.02	3.70	−0.02	0.01	0.01	0.01
14	3.81	3.82	−0.01	3.81	0.01	0.01	0.01	0.00
15	4.21	4.05	0.16	3.94	0.11	0.08	0.14	0.06
16	2.98	3.14	−0.16	3.14	0.00	0.16	0.20	0.05
17	3.71	3.71	0.00	3.71	0.00	0.01	0.01	0.00
18	4.38	4.38	0.00	4.38	0.00	0.01	0.01	0.00
19	3.64	3.63	0.01	3.64	−0.01	0.01	0.01	0.00
20	3.68	3.65	0.03	3.68	−0.03	0.01	0.01	0.01
21	3.90	3.73	0.17	3.71	0.02	0.06	0.07	0.01
22	3.50	3.73	−0.23	3.99	−0.26	0.11	0.24	0.13
23	3.50	3.72	−0.22	3.98	−0.26	0.11	0.24	0.13
24	3.50	3.94	−0.44	19.65	−15.71	0.22	8.07	7.85
MAD			0.12		0.70	0.07	0.41	0.35

Table S18: Comparison of optimized sDFT structures obtained with A24 PW91/PW91k using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (SERENITY implementation). ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{DFT}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R_{1_x}^i - R_{2_x}^i)^2 + (R_{1_y}^i - R_{2_y}^i)^2 + (R_{1_z}^i - R_{2_z}^i)^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	CoM_{ref}	CoM_{ADF}	$\Delta\text{CoM}_{\text{ref}}^{\text{ADF}}$	CoM_{Ser}	$\Delta\text{CoM}_{\text{Ser}}^{\text{ADF}}$	RMSD_{ADF}	RMSD_{Ser}	$\Delta\text{RMSD}_{\text{ADF}}^{\text{Ser}}$
1	2.98	2.89	0.09	2.88	0.01	0.04	0.05	0.01
2	2.92	2.86	0.06	2.82	0.04	0.05	0.06	0.02
3	4.46	4.18	0.28	4.17	0.01	0.14	0.14	0.01
4	2.72	2.74	−0.02	2.71	0.03	0.05	0.05	0.01
5	3.23	2.89	0.34	2.86	0.03	0.16	0.18	0.02
6	3.19	3.15	0.04	3.20	−0.05	0.02	0.01	0.02
7	3.95	3.47	0.48	3.42	0.05	0.24	0.26	0.02
8	3.78	3.56	0.22	3.46	0.10	0.11	0.15	0.05
9	2.91	2.87	0.04	2.87	0.00	0.04	0.05	0.01
10	3.32	3.23	0.09	3.22	0.01	0.04	0.05	0.01
11	3.70	3.51	0.19	3.52	−0.01	0.12	0.12	0.03
12	4.36	4.01	0.35	4.00	0.01	0.18	0.18	0.01
13	3.70	3.47	0.23	3.42	0.05	0.11	0.13	0.02
14	3.81	3.67	0.14	3.61	0.06	0.07	0.10	0.03
15	4.21	3.76	0.45	3.72	0.04	0.22	0.25	0.04
16	2.98	2.79	0.19	2.77	0.02	0.18	0.22	0.04
17	3.71	3.47	0.24	3.39	0.08	0.12	0.16	0.04
18	4.38	4.12	0.26	4.03	0.09	0.13	0.17	0.04
19	3.64	3.30	0.34	3.25	0.05	0.17	0.19	0.03
20	3.68	3.36	0.32	3.35	0.01	0.12	0.12	0.01
21	3.90	3.41	0.49	3.42	−0.01	0.17	0.17	0.00
22	3.50	3.50	0.00	3.50	0.00	0.00	0.00	0.00
23	3.50	3.50	0.00	3.50	0.00	0.01	0.01	0.00
24	3.50	3.59	−0.09	4.02	−0.43	0.04	0.26	0.22
MAD			0.20		0.04	0.11	0.13	0.03

Table S19: Comparison of optimized sDFT structures obtained with S22 LDA/TF using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (SERENITY implementation). Starting point for the ADF structure optimization of complex 13, 14 and 22 were the SERENITY sDFT optimized structures. ΔCoM is calculated as $\Delta\text{CoM} = \text{CoM}_{\text{ref}} - \text{CoM}_{\text{DFT}}$. The RMSD is given by $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R_{1_x}^i - R_{2_x}^i)^2 + (R_{1_y}^i - R_{2_y}^i)^2 + (R_{1_z}^i - R_{2_z}^i)^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	CoM_{ref}	CoM_{ADF}	$\Delta\text{CoM}_{\text{ref}}^{\text{ADF}}$	CoM_{Ser}	$\Delta\text{CoM}_{\text{Ser}}^{\text{ADF}}$	RMSD_{ADF}	RMSD_{Ser}	$\Delta\text{RMSD}_{\text{ADF}}^{\text{Ser}}$
1	3.21	3.11	0.10	3.08	0.03	0.05	0.07	0.02
2	2.91	2.99	−0.08	2.95	0.04	0.05	0.04	0.02
3	2.99	3.14	−0.15	3.13	0.01	0.09	0.09	0.01
4	3.23	3.26	−0.03	3.26	0.00	0.04	0.04	0.00
5	6.08	6.12	−0.04	6.13	−0.01	0.04	0.04	0.01
6	5.14	5.14	0.00	5.14	0.00	0.12	0.25	0.14
7	5.97	5.95	0.02	5.95	0.00	0.02	0.02	0.01
8	3.72	3.69	0.03	3.72	−0.03	0.02	0.01	0.01
9	3.72	3.72	0.00	3.72	0.00	0.01	0.01	0.00
10	3.72	3.84	−0.12	3.95	−0.11	0.06	0.11	0.05
11	3.76	3.98	−0.22	4.05	−0.07	0.11	0.15	0.05
12	3.48	3.67	−0.19	3.73	−0.06	0.12	0.14	0.04
13	3.17	5.49	−2.32	5.48	0.01	2.35	2.35	0.00
14	3.50	5.22	−1.72	5.22	0.00	1.20	1.20	0.00
15	3.17	3.46	−0.29	3.54	−0.08	0.18	0.36	0.23
16	4.42	4.23	0.19	4.20	0.03	0.09	0.11	0.02
17	3.38	3.47	−0.09	3.49	−0.02	0.05	0.05	0.01
18	3.56	3.66	−0.10	3.70	−0.04	0.05	0.07	0.02
19	3.95	4.06	−0.11	4.07	−0.01	0.05	0.05	0.00
20	4.91	5.10	−0.19	5.22	−0.12	0.10	0.16	0.06
21	4.88	5.06	−0.18	5.10	−0.04	0.09	0.11	0.02
22	4.92	5.73	−0.81	5.72	0.01	0.68	0.68	0.01
MAD			0.31		0.03	0.25	0.28	0.03

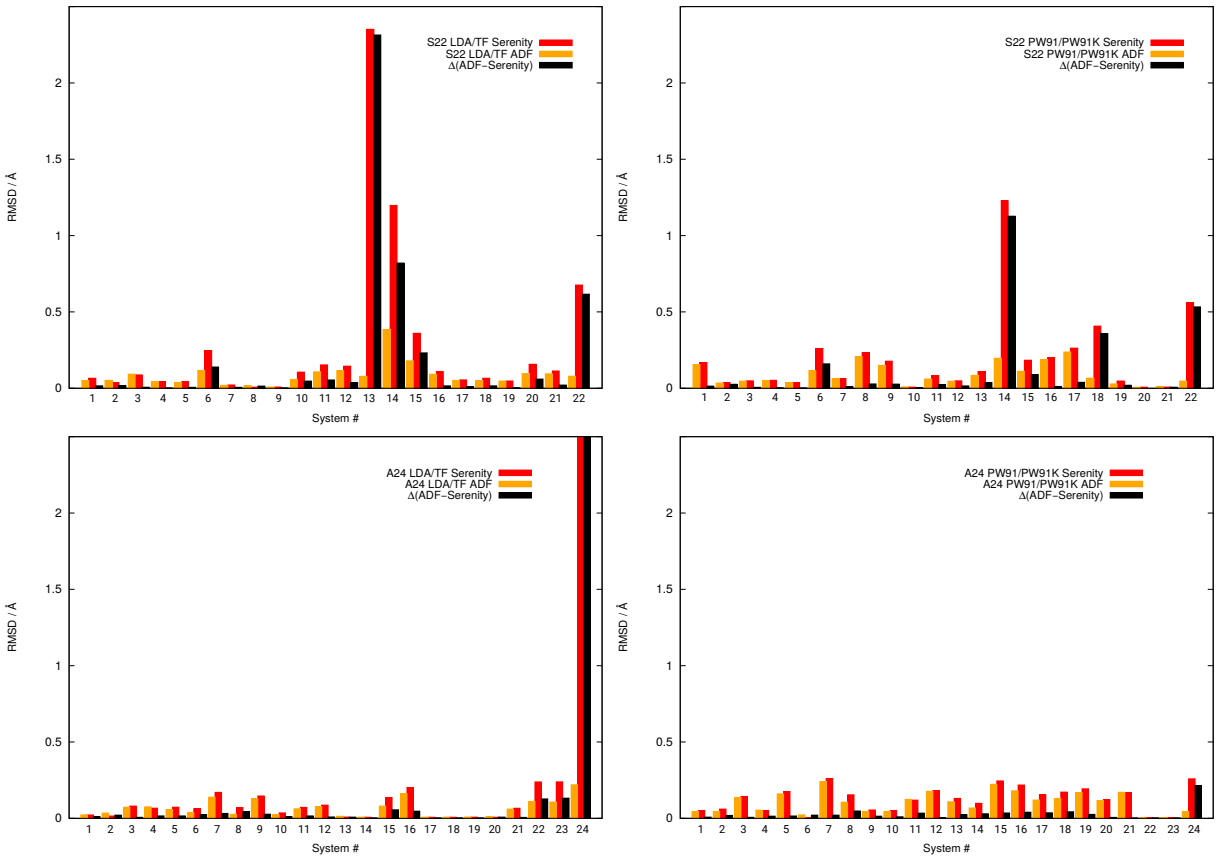

Figure S8: RMSD between the the reference structures from the S22 and A24 test sets and sDFT optimized structures by ADF and Serenity, as well as RMSD between ADF and Serenity sDFT optimized structures for the LDA/TF and PW91/PW91k functional combinations.

Table S20: Comparison of optimized sDFT structures obtained with S22 PW91/PW91k using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (SERENITY implementation). Starting point for the ADF structure optimization of complex 14, 18 and 22 were the SERENITY sDFT optimized structures. ΔCoM is calculated as $\Delta\mathrm{CoM} = \mathrm{CoM}_{\mathrm{ref}} - \mathrm{CoM}_{\mathrm{DFT}}$. The RMSD is given by $\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R_{1_x}^i - R_{2_x}^i)^2 + (R_{1_y}^i - R_{2_y}^i)^2 + (R_{1_z}^i - R_{2_z}^i)^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	$\mathrm{CoM}_{\mathrm{ref}}$	$\mathrm{CoM}_{\mathrm{ADF}}$	$\Delta\mathrm{CoM}_{\mathrm{ref}}^{\mathrm{ADF}}$	$\mathrm{CoM}_{\mathrm{Ser}}$	$\Delta\mathrm{CoM}_{\mathrm{Ser}}^{\mathrm{ADF}}$	$\mathrm{RMSD}_{\mathrm{ADF}}$	$\mathrm{RMSD}_{\mathrm{Ser}}$	$\Delta\mathrm{RMSD}_{\mathrm{ADF}}^{\mathrm{Ser}}$
1	3.21	2.89	0.32	2.86	0.03	0.15	0.17	0.01
2	2.91	2.86	0.05	2.83	0.03	0.03	0.04	0.03
3	2.99	3.01	−0.02	3.00	0.01	0.05	0.05	0.01
4	3.23	3.12	0.11	3.12	0.00	0.05	0.05	0.00
5	6.08	6.02	0.06	6.02	0.00	0.04	0.04	0.00
6	5.14	5.02	0.12	5.02	0.00	0.12	0.26	0.16
7	5.97	5.85	0.12	5.85	0.00	0.06	0.06	0.01
8	3.72	3.31	0.41	3.25	0.06	0.21	0.23	0.03
9	3.72	3.42	0.30	3.36	0.06	0.15	0.18	0.03
10	3.72	3.70	0.02	3.72	−0.02	0.01	0.01	0.01
11	3.76	3.70	0.06	3.66	0.04	0.06	0.08	0.02
12	3.48	3.40	0.08	3.39	0.01	0.05	0.05	0.02
13	3.17	3.02	0.15	2.99	0.03	0.08	0.11	0.04
14	3.50	4.67	−1.17	4.66	0.01	1.23	1.23	0.01
15	3.17	3.11	0.06	3.11	0.00	0.11	0.18	0.09
16	4.42	4.04	0.38	4.01	0.03	0.19	0.20	0.01
17	3.38	3.09	0.29	3.08	0.01	0.24	0.26	0.04
18	3.56	3.12	0.44	3.11	0.01	0.40	0.41	0.01
19	3.95	3.88	0.07	3.83	0.05	0.03	0.05	0.02
20	4.91	4.91	0.00	4.91	0.00	0.01	0.01	0.00
21	4.88	4.89	−0.01	4.88	0.01	0.01	0.01	0.01
22	4.92	5.35	−0.43	5.34	0.01	0.56	0.56	0.01
MAD			0.21		0.02	0.17	0.19	0.03

Table S21: Comparison of optimized sDFT structures obtained with A24 LDA/TF using either a TZ2P STO basis (ADF implementation) or a def2-TZVPP GTO basis (SERENITY implementation). Starting point for the ADF structure optimization of complex 24 was the SERENITY sDFT optimized structure. ΔCoM is calculated as $\Delta\mathrm{CoM} = \mathrm{CoM}_{\mathrm{ref}} - \mathrm{CoM}_{\mathrm{DFT}}$. The RMSD is given by $\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} |\vec{R}_1^i - \vec{R}_2^i|^2}{N}}$ after minimization with the Kabsch algorithm, where $|\vec{R}_1^i - \vec{R}_2^i|^2 = ((R_{1_x}^i - R_{2_x}^i)^2 + (R_{1_y}^i - R_{2_y}^i)^2 + (R_{1_z}^i - R_{2_z}^i)^2)$. $\vec{R}_1^i$ and $\vec{R}_2^i$ refer to a vector of the cartesian components (x, y, z) of atom i of the respective structures to compare. All results are given in units of Å.

compound	$\mathrm{CoM}_{\mathrm{ref}}$	$\mathrm{CoM}_{\mathrm{ADF}}$	$\Delta\mathrm{CoM}_{\mathrm{ref}}^{\mathrm{ADF}}$	$\mathrm{CoM}_{\mathrm{Ser}}$	$\Delta\mathrm{CoM}_{\mathrm{Ser}}^{\mathrm{ADF}}$	$\mathrm{RMSD}_{\mathrm{ADF}}$	$\mathrm{RMSD}_{\mathrm{Ser}}$	$\Delta\mathrm{RMSD}_{\mathrm{ADF}}^{\mathrm{Ser}}$
1	2.98	3.02	−0.04	3.01	0.01	0.02	0.02	0.01
2	2.92	2.99	−0.07	2.95	0.04	0.03	0.02	0.02
3	4.46	4.31	0.15	4.30	0.01	0.07	0.08	0.01
4	2.72	2.86	−0.14	2.82	0.04	0.08	0.07	0.02
5	3.23	3.11	0.12	3.08	0.03	0.06	0.07	0.02
6	3.19	3.29	−0.10	3.34	−0.05	0.04	0.06	0.02
7	3.95	3.68	0.27	3.61	0.07	0.14	0.17	0.03
8	3.78	3.73	0.05	3.64	0.09	0.03	0.07	0.04
9	2.91	3.13	−0.22	3.15	−0.02	0.13	0.15	0.03
10	3.32	3.37	−0.05	3.40	−0.03	0.02	0.04	0.01
11	3.70	3.77	−0.07	3.80	−0.03	0.06	0.07	0.02
12	4.36	4.21	0.15	4.19	0.02	0.08	0.09	0.01
13	3.70	3.68	0.02	3.70	−0.02	0.01	0.01	0.01
14	3.81	3.82	−0.01	3.81	0.01	0.01	0.01	0.00
15	4.21	4.05	0.16	3.94	0.11	0.08	0.14	0.06
16	2.98	3.14	−0.16	3.14	0.00	0.16	0.20	0.05
17	3.71	3.71	0.00	3.71	0.00	0.01	0.01	0.00
18	4.38	4.38	0.00	4.38	0.00	0.01	0.01	0.00
19	3.64	3.63	0.01	3.64	−0.01	0.01	0.01	0.00
20	3.68	3.65	0.03	3.68	−0.03	0.01	0.01	0.01
21	3.90	3.73	0.17	3.71	0.02	0.06	0.07	0.01
22	3.50	3.73	−0.23	3.99	−0.26	0.11	0.24	0.13
23	3.50	3.72	−0.22	3.98	−0.26	0.11	0.24	0.13
24	3.50	19.65	−16.15	19.65	0.00	8.07	8.07	0.00
MAD			0.77		0.05	0.39	0.41	0.03