Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

DFT and spatial confinement: A benchmark study on structure and electric properties of hydrogen bonded complexes

Justyna Kozłowska,* Paweł Lipkowski,* Agnieszka Roztoczyńska, and Wojciech Bartkowiak

Department of Physical and Quantum Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, PL–50370 Wrocław, Poland

E-mail: justyna.kozlowska@pwr.edu.pl; pawel.lipkowski@pwr.edu.pl

Electronic Supporting Information

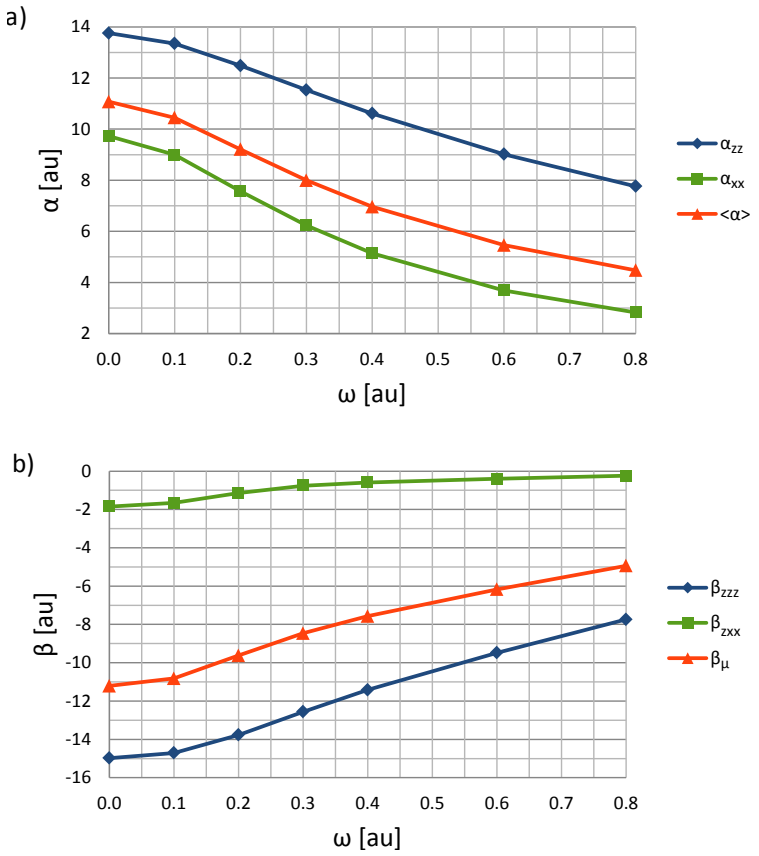

Figure S1: Electronic contribution to a) dominant tensor elements (α_{zz}, α_{xx}) and average dipole polarizability $< \alpha >$ as well as b) dominant tensor elements (β_{zzz}, β_{xx}) and vector component (β_{μ}) of first hyperpolarizability of the HF$\cdots$HF dimer in the presence of two-dimensional harmonic confining potential. Calculations were performed at the CCSD(T)/aug-cc-pVQZ level of theory.

Table S1: The Rutishauser-Romberg convergence triangles for μ_z, α_{zz} and β_{zzz} components of static electric properties of the isolated HF$\cdots$HF dimer obtained from energy differentiation. The calculations were performed at the CCSD(T)/aug-cc-pVQZ level of theory. All data are given in au.

dipole moment (μ_z): $\omega = 0.0$ au

field	0	1	2	3	4	5	6
0.0002	1.585256	1.585256	1.585256	1.585256	1.585256	1.585256	1.585256
0.0004	1.585255	1.585256	1.585256	1.585256	1.585256	1.585256	
0.0008	1.585254	1.585256	1.585256	1.585256	1.585256		
0.0016	1.585249	1.585256	1.585256	1.585256			
0.0032	1.585230	1.585256	1.585256				
0.0064	1.585153	1.585256					
0.0128	1.584845						

polarizability(α_{zz}): $\omega = 0.0$ au

field	0	1	2	3	4	5	6
0.0002	13.756845	13.756882	13.756892	13.756894	13.756895	13.756895	13.756895
0.0004	13.756735	13.756728	13.756729	13.756730	13.756730	13.756730	
0.0008	13.756756	13.756707	13.756707	13.756707	13.756707		
0.0016	13.756904	13.756704	13.756704	13.756704			
0.0032	13.757507	13.756700	13.756701				
0.0064	13.759929	13.756681					
0.0128	13.769673						

first hyperpolarizability(β_{zzz}): $\omega = 0.0$ au

field	0	1	2	3	4	5
0.0002	−15.0404	−15.0539	−15.0571	−15.0579	−15.0581	−15.0581
0.0004	−15.0000	−15.0058	−15.0075	−15.0079	−15.0081	
0.0008	−14.9826	−14.9801	−14.9798	−14.9798		
0.0016	−14.9901	−14.9844	−14.9845			
0.0032	−15.0073	−14.9828				
0.0064	−15.0808					

Table S2: The Rutishauser-Romberg convergence triangles for μ_z, α_{zz} and β_{zzz} components of static electric properties of the spatially confined HF$\cdots$HF dimer obtained from energy differentiation. The calculations were performed at the CCSD(T)/aug-cc-pVQZ level of theory. All data are given in au.

dipole moment (μ_z): $\omega = 0.8$ au

field	0	1	2	3	4	5	6
0.0002	1.445452	1.445452	1.445452	1.445452	1.445452	1.445452	1.445452
0.0004	1.445452	1.445452	1.445452	1.445452	1.445452	1.445452	
0.0008	1.445452	1.445452	1.445452	1.445452	1.445452		
0.0016	1.445449	1.445452	1.445452	1.445452			
0.0032	1.445439	1.445452	1.445452				
0.0064	1.445400	1.445453					
0.0128	1.445240						

polarizability(α_{zz}): $\omega = 0.8$ au

field	0	1	2	3	4	5	6
0.0002	7.764076	7.764093	7.764098	7.764099	7.764099	7.764099	7.764099
0.0004	7.764023	7.764022	7.764023	7.764023	7.764023	7.764023	
0.0008	7.764026	7.764016	7.764016	7.764016	7.764016		
0.0016	7.764057	7.764014	7.764014	7.764014			
0.0032	7.764184	7.764014	7.764014				
0.0064	7.764695	7.764012					
0.0128	7.766745						

first hyperpolarizability(β_{zzz}): $\omega = 0.8$ au

field	0	1	2	3	4	5
0.0002	−7.8320	−7.8631	−7.8715	−7.8737	−7.8742	−7.8744
0.0004	−7.7385	−7.7367	−7.7363	−7.7361	−7.7361	
0.0008	−7.7438	−7.7435	−7.7436	−7.7436		
0.0016	−7.7446	−7.7426	−7.7425			
0.0032	−7.7506	−7.7439				
0.0064	−7.7707					

Table S3: The values of μ_z, α_{zz} and β_{zzz} of the isolated HF$\cdots$HF dimer obtained analytically and by numerical differentiation. All results have been computed using the aug-cc-pVQZ basis set and are given in au.

analytical results	μ_z	α_{zz}	β_{zzz}
HF	1.681	12.34	-14.1
MP2	1.594	13.80	–
CCSD	1.598	–	–
B3LYP	1.598	14.42	-17.0
ωB97X-D	1.599	14.05	-12.7

numerical results	μ_z	α_{zz}	β_{zzz}
HF	1.681	12.34	-14.1
MP2	1.594	13.80	–
CCSD	1.598	–	–
B3LYP	1.598	14.43	-17.0
ωB97X-D	1.599	14.05	-12.6

Table S4: The values of electric dipole moment (μ_z) and **% error** computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**dipole moment (μ_z) [au]**							**% error**						
CCSD(T)	1.585	1.579	1.562	1.539	1.517	1.483	1.446	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	1.598	1.591	1.573	1.549	1.526	1.489	1.451	0.8	0.8	0.7	0.6	0.6	0.5	0.4
MP2	1.594	1.588	1.571	1.549	1.528	1.493	1.455	0.5	0.6	0.6	0.6	0.7	0.7	0.7
HF	1.681	1.673	1.651	1.622	1.594	1.546	1.498	6.0	6.0	5.7	5.4	5.1	4.3	3.6
B2PLYP	1.636	1.628	1.608	1.582	1.556	1.514	1.472	3.2	3.1	3.0	2.8	2.5	2.1	1.8
B3LYP	1.598	1.590	1.572	1.548	1.525	1.489	1.451	0.8	0.7	0.7	0.6	0.5	0.4	0.4
B3PW91	1.593	1.585	1.568	1.544	1.523	1.488	1.452	0.5	0.4	0.4	0.3	0.4	0.4	0.4
B97-2	1.590	1.582	1.565	1.542	1.521	1.486	1.450	0.3	0.2	0.2	0.2	0.2	0.2	0.3
B97D	1.564	1.558	1.542	1.521	1.502	1.472	1.439	-1.3	-1.3	-1.3	-1.2	-1.0	-0.7	-0.5
BLYP	1.564	1.557	1.540	1.518	1.497	1.464	1.431	-1.3	-1.4	-1.4	-1.4	-1.3	-1.2	-1.0
BMK	1.628	1.620	1.600	1.574	1.550	1.511	1.470	2.7	2.6	2.5	2.3	2.2	1.9	1.7
CAM-B3LYP	1.616	1.609	1.589	1.564	1.540	1.502	1.462	1.9	1.9	1.7	1.6	1.5	1.3	1.2
HCTH	1.564	1.558	1.542	1.521	1.501	1.471	1.438	-1.3	-1.3	-1.3	-1.2	-1.1	-0.8	-0.5
HISS	1.633	1.625	1.606	1.580	1.555	1.515	1.475	3.0	2.9	2.8	2.7	2.5	2.2	2.0
HSE06	1.597	1.590	1.572	1.549	1.526	1.490	1.453	0.7	0.7	0.7	0.6	0.6	0.5	0.5
LC-BLYP	1.653	1.644	1.624	1.597	1.570	1.528	1.486	4.3	4.1	4.0	3.8	3.5	3.0	2.8
LC-HCTH	1.653	1.645	1.624	1.597	1.569	1.526	1.485	4.3	4.2	4.0	3.8	3.4	2.9	2.7
LC-revTPSS	1.633	1.625	1.605	1.579	1.553	1.513	1.472	3.0	2.9	2.8	2.6	2.4	2.0	1.8
LC-τHCTH	1.669	1.660	1.638	1.609	1.581	1.537	1.495	5.3	5.1	4.9	4.5	4.2	3.7	3.4
LSDA	1.602	1.596	1.580	1.558	1.538	1.506	1.472	1.1	1.1	1.2	1.2	1.4	1.6	1.8
M06	1.607	1.600	1.583	1.561	1.540	1.504	1.465	1.4	1.3	1.4	1.4	1.5	1.5	1.4
M06-2X	1.622	1.614	1.594	1.568	1.542	1.501	1.459	2.3	2.2	2.1	1.9	1.6	1.2	0.9
M06-HF	1.673	1.665	1.643	1.614	1.585	1.535	1.487	5.5	5.5	5.2	4.9	4.5	3.5	2.8
M06L	1.562	1.555	1.538	1.517	1.498	1.466	1.430	-1.5	-1.5	-1.5	-1.4	-1.3	-1.1	-1.1
M11	1.640	1.632	1.611	1.584	1.559	1.517	1.474	3.5	3.4	3.2	2.9	2.7	2.3	2.0
M11-L	1.545	1.540	1.526	1.509	1.493	1.465	1.430	-2.5	-2.5	-2.3	-2.0	-1.6	-1.2	-1.1
MN12-L	1.622	1.615	1.598	1.576	1.555	1.522	1.484	2.3	2.3	2.3	2.4	2.5	2.6	2.6
MN12-SX	1.620	1.612	1.594	1.571	1.550	1.514	1.474	2.2	2.1	2.1	2.1	2.2	2.1	2.0
mPW1PW91	1.598	1.590	1.572	1.549	1.527	1.491	1.454	0.8	0.7	0.7	0.6	0.6	0.6	0.6
N12	1.617	1.609	1.592	1.569	1.548	1.514	1.479	2.0	1.9	1.9	1.9	2.0	2.1	2.3
N12-SX	1.639	1.631	1.612	1.587	1.564	1.526	1.486	3.4	3.3	3.2	3.1	3.1	2.9	2.8
PBE	1.558	1.551	1.535	1.514	1.494	1.464	1.431	-1.7	-1.8	-1.7	-1.6	-1.5	-1.3	-1.0
PBE0	1.596	1.589	1.571	1.547	1.525	1.490	1.453	0.7	0.7	0.6	0.5	0.5	0.5	0.5
revTPSS	1.553	1.546	1.528	1.506	1.484	1.452	1.417	-2.0	-2.1	-2.2	-2.2	-2.2	-2.1	-2.0
SOGGA11-X	1.601	1.594	1.575	1.550	1.527	1.487	1.447	1.0	1.0	0.9	0.7	0.6	0.3	0.1
τHCTH	1.570	1.564	1.548	1.528	1.509	1.478	1.445	-1.0	-0.9	-0.9	-0.7	-0.5	-0.3	0.0
τHCTHHYB	1.588	1.581	1.564	1.541	1.520	1.486	1.451	0.2	0.1	0.1	0.1	0.2	0.2	0.4
TPSSH	1.577	1.570	1.552	1.529	1.507	1.472	1.436	-0.5	-0.6	-0.6	-0.7	-0.7	-0.7	-0.7
ωB97	1.598	1.590	1.570	1.545	1.522	1.485	1.447	0.8	0.7	0.5	0.4	0.3	0.1	0.1
ωB97X	1.600	1.593	1.574	1.549	1.526	1.490	1.452	0.9	0.9	0.8	0.6	0.6	0.5	0.4
ωB97X-D	1.600	1.592	1.574	1.550	1.528	1.493	1.456	0.9	0.9	0.8	0.7	0.7	0.7	0.7

Table S5: The values of electric dipole moment (μ_z) and **% error** computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**dipole moment (μ_z) [au]**							**% error**						
CCSD(T)	2.693	2.677	2.638	2.587	2.535	2.454	2.390	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	2.725	2.708	2.666	2.612	2.556	2.468	2.400	1.2	1.2	1.1	0.9	0.8	0.6	0.4
MP2	2.702	2.683	2.638	2.582	2.525	2.437	2.369	0.3	0.2	0.0	-0.2	-0.4	-0.7	-0.9
HF	2.930	2.915	2.876	2.819	2.758	2.656	2.572	8.8	8.9	9.0	9.0	8.8	8.3	7.6
B2PLYP	2.815	2.799	2.760	2.704	2.646	2.550	2.473	4.5	4.6	4.6	4.5	4.4	3.9	3.5
B3LYP	2.731	2.714	2.675	2.622	2.567	2.479	2.410	1.4	1.4	1.4	1.3	1.2	1.0	0.8
B3PW91	2.720	2.705	2.668	2.617	2.566	2.483	2.416	1.0	1.0	1.1	1.2	1.2	1.2	1.1
B97-2	2.717	2.702	2.666	2.617	2.566	2.485	2.419	0.9	0.9	1.0	1.2	1.2	1.3	1.2
B97D	2.669	2.653	2.617	2.570	2.522	2.444	2.382	-0.9	-0.9	-0.8	-0.7	-0.5	-0.4	-0.3
BLYP	2.672	2.655	2.617	2.566	2.513	2.431	2.369	-0.8	-0.8	-0.8	-0.8	-0.9	-0.9	-0.9
BMK	2.782	2.765	2.724	2.670	2.613	2.517	2.434	3.3	3.3	3.3	3.2	3.1	2.6	1.8
CAM-B3LYP	2.776	2.757	2.714	2.656	2.596	2.500	2.426	3.1	3.0	2.9	2.7	2.4	1.9	1.5
HCTH	2.659	2.643	2.607	2.560	2.512	2.439	2.384	-1.3	-1.3	-1.2	-1.1	-0.9	-0.6	-0.3
HISS	2.799	2.783	2.743	2.687	2.630	2.535	2.459	3.9	4.0	4.0	3.9	3.7	3.3	2.9
HSE06	2.733	2.717	2.680	2.629	2.577	2.493	2.425	1.5	1.5	1.6	1.6	1.6	1.6	1.5
LC-BLYP	2.845	2.824	2.774	2.708	2.640	2.530	2.447	5.6	5.5	5.2	4.7	4.1	3.1	2.4
LC-HCTH	2.850	2.829	2.777	2.707	2.637	2.531	2.455	5.8	5.7	5.3	4.6	4.0	3.1	2.7
LC-REVTPSS	2.819	2.800	2.753	2.691	2.629	2.527	2.446	4.7	4.6	4.3	4.0	3.7	3.0	2.3
LC-τHCTH	2.880	2.858	2.802	2.729	2.655	2.544	2.460	6.9	6.8	6.2	5.5	4.7	3.7	2.9
LSDA	2.719	2.702	2.663	2.610	2.556	2.472	2.405	1.0	0.9	0.9	0.9	0.8	0.7	0.6
M06	2.690	2.676	2.644	2.601	2.556	2.478	2.407	-0.1	0.0	0.2	0.5	0.8	1.0	0.7
M06-2X	2.746	2.728	2.685	2.629	2.571	2.480	2.409	2.0	1.9	1.8	1.6	1.4	1.1	0.8
M06-HF	2.822	2.803	2.755	2.690	2.619	2.503	2.422	4.8	4.7	4.4	4.0	3.3	2.0	1.3
M06L	2.630	2.616	2.586	2.548	2.511	2.449	2.387	-2.3	-2.3	-2.0	-1.5	-1.0	-0.2	-0.1
M11	2.818	2.796	2.743	2.674	2.604	2.486	2.390	4.6	4.5	4.0	3.4	2.7	1.3	0.0
M11-L	2.649	2.633	2.598	2.553	2.504	2.411	2.317	-1.6	-1.6	-1.5	-1.3	-1.2	-1.7	-3.1
MN12-L	2.709	2.695	2.663	2.618	2.567	2.475	2.388	0.6	0.7	1.0	1.2	1.3	0.9	-0.1
MN12-SX	2.710	2.693	2.653	2.597	2.537	2.428	2.330	0.6	0.6	0.6	0.4	0.1	-1.1	-2.5
MPW1PW91	2.731	2.716	2.679	2.630	2.578	2.493	2.425	1.4	1.5	1.6	1.6	1.7	1.6	1.5
N12	2.696	2.680	2.642	2.592	2.539	2.452	2.384	0.1	0.1	0.2	0.2	0.2	-0.1	-0.3
N12-SX	2.765	2.748	2.707	2.653	2.597	2.504	2.428	2.7	2.6	2.6	2.6	2.4	2.0	1.6
PBE	2.661	2.645	2.609	2.561	2.513	2.437	2.378	-1.2	-1.2	-1.1	-1.0	-0.9	-0.7	-0.5
PBE0	2.731	2.715	2.679	2.629	2.577	2.494	2.427	1.4	1.4	1.5	1.6	1.6	1.6	1.5
REVTPSS	2.665	2.649	2.612	2.563	2.514	2.436	2.374	-1.0	-1.0	-1.0	-0.9	-0.8	-0.7	-0.7
SOGGA11-X	2.750	2.736	2.702	2.655	2.603	2.518	2.448	2.1	2.2	2.4	2.6	2.7	2.6	2.4
τHCTH	2.674	2.659	2.624	2.577	2.528	2.450	2.386	-0.7	-0.7	-0.5	-0.4	-0.3	-0.2	-0.2
τHCTHHYB	2.717	2.702	2.664	2.613	2.560	2.474	2.404	0.9	0.9	1.0	1.0	1.0	0.8	0.6
TPSSH	2.701	2.686	2.648	2.598	2.547	2.465	2.399	0.3	0.3	0.4	0.4	0.5	0.5	0.4
ωB97	2.772	2.752	2.706	2.646	2.587	2.494	2.420	2.9	2.8	2.6	2.3	2.0	1.6	1.3
ωB97X	2.767	2.748	2.704	2.646	2.589	2.499	2.425	2.7	2.7	2.5	2.3	2.1	1.8	1.5
ωB97X-D	2.751	2.733	2.693	2.639	2.585	2.498	2.425	2.1	2.1	2.1	2.0	2.0	1.8	1.4

Table S6: The values of interaction-induced dipole moment ($\Delta\mu_z$) and **% error** computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The values of $\Delta\mu_z$ were corrected according to the Boys and Bernardi counterpoise scheme. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**interaction-induced dipole moment ($\Delta\mu_z$) [au]**							**% error**						
CCSD(T)	0.164	0.165	0.167	0.171	0.180	0.201	0.204	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	0.163	0.164	0.166	0.171	0.179	0.200	0.203	-0.6	-0.6	-0.6	0.0	-0.6	-0.4	-0.4
MP2	0.165	0.167	0.168	0.173	0.181	0.200	0.203	0.6	1.2	0.6	1.2	0.6	-0.3	-0.4
HF	0.159	0.161	0.164	0.169	0.178	0.196	0.198	-3.0	-2.4	-1.8	-1.2	-1.1	-2.4	-2.6
B2PLYP	0.167	0.168	0.171	0.176	0.185	0.206	0.209	1.6	1.8	2.2	2.9	2.9	2.4	2.5
B3LYP	0.174	0.175	0.178	0.184	0.193	0.215	0.218	6.1	6.1	6.6	7.6	7.2	6.9	7.3
B3PW91	0.173	0.174	0.177	0.182	0.193	0.214	0.218	5.5	5.5	6.0	6.4	7.2	6.6	7.1
B97-2	0.171	0.171	0.175	0.180	0.190	0.212	0.216	4.3	3.6	4.8	5.3	5.6	5.7	6.2
B97D	0.177	0.179	0.182	0.187	0.198	0.220	0.224	7.9	8.5	9.0	9.4	10.0	9.5	10.1
BLYP	0.179	0.181	0.184	0.190	0.200	0.222	0.226	9.1	9.7	10.2	11.1	11.1	10.5	11.0
BMK	0.173	0.174	0.176	0.181	0.190	0.210	0.214	5.5	5.5	5.4	5.8	5.6	4.4	5.0
CAM-B3LYP	0.173	0.174	0.176	0.182	0.192	0.213	0.217	5.5	5.5	5.4	6.4	6.7	6.2	6.6
HCTH	0.174	0.176	0.178	0.184	0.194	0.217	0.221	6.1	6.7	6.6	7.6	7.8	8.0	8.7
HISS	0.168	0.169	0.173	0.178	0.187	0.209	0.212	2.4	2.4	3.6	4.1	3.9	3.9	4.3
HSE06	0.170	0.172	0.175	0.181	0.191	0.212	0.216	3.7	4.2	4.8	5.8	6.1	5.6	5.9
LC-BLYP	0.173	0.173	0.177	0.183	0.191	0.213	0.217	5.5	4.8	6.0	7.0	6.1	6.1	6.5
LC-HCTH	0.170	0.171	0.173	0.180	0.190	0.210	0.214	3.7	3.6	3.6	5.3	5.6	4.7	5.0
LC-revTPSS	0.170	0.171	0.174	0.180	0.189	0.211	0.215	3.7	3.6	4.2	5.3	5.0	5.0	5.6
LC-τHCTH	0.174	0.175	0.177	0.183	0.192	0.212	0.215	6.1	6.1	6.0	7.0	6.7	5.7	5.7
LSDA	0.180	0.181	0.185	0.190	0.201	0.222	0.227	9.8	9.7	10.8	11.1	11.7	10.8	11.3
M06	0.173	0.174	0.176	0.181	0.190	0.211	0.215	5.5	5.5	5.4	5.8	5.6	4.9	5.5
M06-2X	0.169	0.171	0.173	0.178	0.187	0.209	0.213	3.0	3.6	3.6	4.1	3.9	4.0	4.4
M06-HF	0.170	0.172	0.176	0.182	0.191	0.212	0.215	3.7	4.2	5.4	6.4	6.1	5.8	5.8
M06L	0.174	0.175	0.177	0.181	0.190	0.211	0.215	6.1	6.1	6.0	5.8	5.6	5.1	5.7
M11	0.171	0.172	0.175	0.181	0.192	0.213	0.217	4.3	4.2	4.8	5.8	6.7	6.2	6.4
M11-L	0.167	0.168	0.170	0.175	0.184	0.206	0.210	1.8	1.8	1.8	2.3	2.2	2.4	3.1
MN12-L	0.172	0.174	0.176	0.182	0.190	0.211	0.215	4.9	5.5	5.4	6.4	5.6	5.2	5.7
MN12-SX	0.171	0.172	0.175	0.179	0.189	0.211	0.216	4.3	4.2	4.8	4.7	5.0	5.2	5.9
mPW1PW91	0.171	0.171	0.174	0.181	0.190	0.212	0.216	4.3	3.6	4.2	5.8	5.6	5.5	6.0
N12	0.176	0.177	0.180	0.185	0.196	0.218	0.222	7.3	7.3	7.8	8.2	8.9	8.5	9.0
N12-SX	0.173	0.174	0.177	0.183	0.193	0.214	0.218	5.5	5.5	6.0	7.0	7.2	6.7	7.3
PBE	0.177	0.178	0.181	0.188	0.198	0.220	0.225	7.9	7.9	8.4	9.9	10.0	9.7	10.3
PBE0	0.171	0.172	0.175	0.179	0.190	0.212	0.216	4.3	4.2	4.8	4.7	5.6	5.4	5.9
revTPSS	0.176	0.177	0.179	0.186	0.195	0.217	0.222	7.3	7.3	7.2	8.8	8.3	8.3	8.8
SOGGA11-X	0.168	0.169	0.172	0.176	0.186	0.207	0.210	2.4	2.4	3.0	2.9	3.3	2.9	3.2
τHCTH	0.175	0.177	0.180	0.186	0.196	0.219	0.223	6.7	7.3	7.8	8.8	8.9	9.1	9.7
τHCTHHYB	0.173	0.174	0.178	0.183	0.193	0.216	0.220	5.5	5.5	6.6	7.0	7.2	7.4	7.9
TPSSH	0.174	0.175	0.178	0.183	0.194	0.215	0.220	6.1	6.1	6.6	7.0	7.8	7.2	7.8
ωB97	0.173	0.173	0.176	0.181	0.192	0.212	0.216	5.5	4.8	5.4	5.8	6.7	5.7	6.2
ωB97X	0.173	0.174	0.177	0.182	0.191	0.212	0.216	5.4	5.4	5.7	6.2	6.1	5.5	5.9
ωB97X-D	0.173	0.174	0.177	0.182	0.191	0.212	0.216	5.4	5.4	5.7	6.4	6.3	5.8	6.2

Table S7: The values of interaction-induced dipole moment ($\Delta\mu_z$) and **% error** computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The values of $\Delta\mu_z$ were corrected according to the Boys and Bernardi counterpoise scheme. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**interaction-induced dipole moment ($\Delta\mu_z$) [au]**							**% error**						
CCSD(T)	0.316	0.313	0.305	0.292	0.275	0.241	0.220	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	0.315	0.312	0.304	0.290	0.273	0.240	0.218	-0.6	-0.5	-0.6	-0.5	-0.6	-0.6	-0.7
MP2	0.309	0.306	0.298	0.285	0.268	0.235	0.214	-2.5	-2.5	-2.5	-2.5	-2.5	-2.5	-2.6
HF	0.331	0.328	0.319	0.306	0.288	0.253	0.231	4.6	4.6	4.6	4.7	4.8	5.0	5.2
B2PLYP	0.331	0.328	0.321	0.308	0.290	0.256	0.234	4.7	4.8	5.1	5.4	5.7	6.2	6.5
B3LYP	0.335	0.333	0.326	0.313	0.296	0.262	0.240	6.0	6.2	6.7	7.3	7.8	8.6	9.1
B3PW91	0.334	0.332	0.325	0.313	0.296	0.262	0.240	5.6	5.9	6.5	7.2	7.8	8.7	9.2
B97-2	0.332	0.330	0.323	0.311	0.294	0.260	0.238	5.0	5.2	5.8	6.4	7.0	7.9	8.5
B97D	0.338	0.336	0.329	0.317	0.300	0.266	0.244	7.0	7.2	7.9	8.6	9.2	10.1	11.1
BLYP	0.340	0.338	0.331	0.319	0.302	0.267	0.244	7.6	7.9	8.5	9.2	9.8	10.7	11.1
BMK	0.334	0.331	0.324	0.312	0.295	0.259	0.235	5.5	5.7	6.3	6.9	7.2	7.5	6.9
CAM-B3LYP	0.334	0.331	0.324	0.311	0.294	0.260	0.238	5.6	5.7	6.1	6.6	7.0	7.8	8.3
HCTH	0.332	0.330	0.324	0.312	0.296	0.263	0.242	4.8	5.2	6.0	6.9	7.7	9.0	10.1
HISS	0.333	0.330	0.323	0.310	0.293	0.259	0.237	5.2	5.4	5.7	6.2	6.6	7.3	7.8
HSE06	0.335	0.332	0.325	0.313	0.296	0.262	0.240	5.8	6.0	6.6	7.1	7.7	8.6	9.2
LC-BLYP	0.334	0.331	0.324	0.310	0.293	0.259	0.237	5.6	5.7	6.0	6.3	6.7	7.4	7.9
LC-HCTH	0.330	0.327	0.319	0.306	0.288	0.255	0.234	4.3	4.3	4.5	4.7	5.0	5.8	6.7
LC-REVTPSS	0.331	0.328	0.321	0.308	0.290	0.257	0.234	4.6	4.7	5.0	5.4	5.8	6.3	6.6
LC-τHCTH	0.340	0.336	0.327	0.312	0.294	0.259	0.237	7.4	7.3	7.1	7.0	7.1	7.4	7.9
LSDA	0.349	0.347	0.340	0.328	0.311	0.276	0.253	10.4	10.7	11.5	12.3	13.1	14.4	15.1
M06	0.336	0.333	0.325	0.311	0.293	0.258	0.234	6.3	6.4	6.5	6.6	6.8	6.9	6.6
M06-2X	0.331	0.328	0.320	0.306	0.289	0.255	0.232	4.5	4.6	4.8	5.0	5.2	5.6	5.7
M06-HF	0.332	0.329	0.322	0.308	0.289	0.252	0.229	4.8	5.1	5.4	5.4	5.1	4.3	4.2
M06L	0.333	0.331	0.324	0.312	0.295	0.260	0.237	5.4	5.7	6.2	6.8	7.4	7.9	8.0
M11	0.337	0.334	0.325	0.311	0.292	0.257	0.235	6.6	6.7	6.6	6.5	6.5	6.7	7.1
M11-L	0.347	0.343	0.332	0.315	0.292	0.248	0.217	9.8	9.5	8.8	7.7	6.4	2.8	-1.5
MN12-L	0.339	0.336	0.327	0.312	0.293	0.254	0.229	7.2	7.2	7.1	6.9	6.6	5.5	4.1
MN12-SX	0.336	0.332	0.323	0.307	0.288	0.249	0.222	6.2	6.1	5.8	5.3	4.7	3.0	1.2
MPW1PW91	0.333	0.331	0.324	0.312	0.295	0.261	0.239	5.3	5.6	6.2	6.8	7.4	8.3	8.9
N12	0.338	0.336	0.329	0.317	0.300	0.265	0.243	6.8	7.1	7.8	8.5	9.1	10.0	10.8
N12-SX	0.334	0.331	0.324	0.312	0.295	0.261	0.240	5.6	5.8	6.3	6.9	7.4	8.3	9.0
PBE	0.340	0.338	0.331	0.319	0.303	0.269	0.246	7.4	7.8	8.6	9.4	10.2	11.4	12.1
PBE0	0.334	0.331	0.324	0.312	0.295	0.262	0.240	5.4	5.7	6.3	6.9	7.5	8.5	9.2
REVTPSS	0.334	0.331	0.324	0.312	0.295	0.261	0.237	5.4	5.7	6.3	6.9	7.4	8.0	8.0
SOGGA11-X	0.332	0.329	0.321	0.308	0.291	0.258	0.236	4.8	4.9	5.1	5.5	5.9	6.8	7.4
τHCTH	0.339	0.337	0.330	0.318	0.301	0.266	0.243	7.2	7.6	8.3	9.0	9.7	10.4	10.8
τHCTHHYB	0.337	0.335	0.328	0.316	0.299	0.264	0.241	6.6	6.9	7.5	8.2	8.7	9.5	9.8
TPSSH	0.335	0.332	0.325	0.313	0.296	0.262	0.240	5.7	6.0	6.6	7.3	7.8	8.7	9.0
ωB97	0.332	0.329	0.320	0.307	0.289	0.255	0.233	4.8	4.9	4.9	5.1	5.3	5.9	6.2
ωB97X	0.331	0.328	0.320	0.307	0.290	0.256	0.234	4.7	4.8	5.0	5.2	5.5	6.1	6.5
ωB97X-D	0.332	0.329	0.322	0.309	0.291	0.258	0.235	5.0	5.1	5.4	5.7	6.1	6.8	7.1

Table S8: The values of uncorrected interaction-induced dipole moment and basis set superposition error (BSSE) computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**uncorrected interaction-induced dipole moment [au]**							**BSSE [au]**						
CCSD(T)	0.164	0.168	0.165	0.168	0.174	0.188	0.192	0.000	-0.003	0.002	0.003	0.006	0.013	0.012
CCSD	0.163	0.164	0.165	0.169	0.172	0.187	0.191	0.000	0.000	0.001	0.002	0.007	0.013	0.012
MP2	0.165	0.167	0.167	0.171	0.175	0.188	0.191	0.000	0.000	0.001	0.002	0.006	0.012	0.012
HF	0.159	0.161	0.164	0.168	0.174	0.186	0.189	0.000	0.000	0.000	0.001	0.004	0.010	0.009
B2PLYP	0.167	0.168	0.170	0.174	0.181	0.193	0.196	0.000	0.000	0.002	0.002	0.004	0.013	0.014
B3LYP	0.174	0.175	0.177	0.182	0.187	0.202	0.203	0.000	0.000	0.001	0.002	0.006	0.013	0.015
B3PW91	0.174	0.174	0.176	0.179	0.187	0.200	0.204	-0.001	0.000	0.001	0.003	0.006	0.014	0.015
B97-2	0.171	0.174	0.174	0.177	0.183	0.200	0.203	0.000	-0.003	0.001	0.003	0.007	0.012	0.013
B97D	0.177	0.179	0.181	0.184	0.192	0.208	0.210	0.000	0.000	0.001	0.003	0.006	0.012	0.014
BLYP	0.179	0.184	0.183	0.187	0.193	0.206	0.210	0.000	-0.003	0.001	0.003	0.007	0.016	0.016
BMK	0.173	0.177	0.174	0.177	0.183	0.196	0.201	0.000	-0.003	0.002	0.004	0.007	0.014	0.013
CAM-B3LYP	0.173	0.177	0.174	0.179	0.186	0.201	0.202	0.000	-0.003	0.002	0.003	0.006	0.012	0.015
HCTH	0.173	0.179	0.177	0.182	0.189	0.204	0.208	0.001	-0.003	0.001	0.002	0.005	0.013	0.014
HISS	0.168	0.172	0.173	0.176	0.181	0.197	0.200	0.000	-0.003	0.000	0.002	0.006	0.012	0.012
HSE06	0.170	0.175	0.174	0.178	0.186	0.198	0.201	0.000	-0.003	0.001	0.003	0.005	0.014	0.015
LC-BLYP	0.173	0.176	0.176	0.181	0.185	0.199	0.201	0.000	-0.003	0.001	0.002	0.006	0.014	0.016
LC-HCTH	0.170	0.174	0.171	0.177	0.185	0.196	0.197	0.000	-0.003	0.002	0.003	0.005	0.014	0.017
LC-revTPSS	0.170	0.174	0.173	0.177	0.183	0.198	0.201	0.000	-0.003	0.001	0.003	0.006	0.013	0.014
LC-τHCTH	0.174	0.175	0.176	0.181	0.185	0.196	0.198	0.000	0.000	0.001	0.002	0.007	0.016	0.017
LSDA	0.180	0.187	0.184	0.187	0.194	0.209	0.210	0.000	-0.006	0.001	0.003	0.007	0.013	0.017
M06	0.173	0.177	0.174	0.177	0.184	0.200	0.203	0.000	-0.003	0.002	0.004	0.006	0.011	0.012
M06-2X	0.169	0.171	0.172	0.175	0.180	0.197	0.200	0.000	0.000	0.001	0.003	0.007	0.013	0.014
M06-HF	0.170	0.172	0.176	0.181	0.187	0.201	0.203	0.000	0.000	0.000	0.001	0.004	0.011	0.012
M06L	0.174	0.178	0.175	0.176	0.182	0.201	0.206	0.000	-0.003	0.002	0.005	0.008	0.010	0.009
M11	0.171	0.175	0.173	0.177	0.185	0.199	0.202	0.000	-0.003	0.002	0.004	0.007	0.014	0.015
M11-L	0.166	0.171	0.169	0.172	0.179	0.198	0.205	0.001	-0.003	0.001	0.003	0.005	0.008	0.006
MN12-L	0.173	0.174	0.175	0.180	0.185	0.201	0.205	-0.001	0.000	0.001	0.002	0.005	0.010	0.010
MN12-SX	0.171	0.175	0.173	0.175	0.182	0.202	0.205	0.000	-0.003	0.002	0.004	0.007	0.009	0.011
mPW1PW91	0.171	0.174	0.173	0.179	0.185	0.200	0.203	0.000	-0.003	0.001	0.002	0.005	0.012	0.013
N12	0.176	0.180	0.179	0.182	0.190	0.206	0.208	0.000	-0.003	0.001	0.003	0.006	0.012	0.014
N12-SX	0.173	0.174	0.175	0.181	0.188	0.202	0.206	0.000	0.000	0.002	0.002	0.005	0.012	0.013
PBE	0.177	0.184	0.179	0.185	0.192	0.206	0.210	0.000	-0.006	0.002	0.003	0.006	0.014	0.015
PBE0	0.171	0.172	0.174	0.176	0.185	0.200	0.203	0.000	0.000	0.001	0.003	0.005	0.012	0.013
revTPSS	0.176	0.177	0.177	0.184	0.189	0.204	0.208	0.000	0.000	0.002	0.002	0.006	0.013	0.014
SOGGA11-X	0.168	0.169	0.171	0.173	0.179	0.194	0.197	0.000	0.000	0.001	0.003	0.007	0.013	0.013
τHCTH	0.175	0.177	0.179	0.184	0.191	0.208	0.210	0.000	0.000	0.001	0.002	0.005	0.011	0.013
τHCTHHYB	0.173	0.180	0.177	0.180	0.186	0.204	0.207	0.000	-0.006	0.001	0.003	0.007	0.012	0.013
TPSSH	0.174	0.175	0.177	0.180	0.189	0.204	0.207	0.000	0.000	0.001	0.003	0.005	0.011	0.013
ωB97	0.173	0.179	0.175	0.177	0.186	0.199	0.202	0.000	-0.006	0.001	0.004	0.006	0.013	0.014
ωB97X	0.173	0.174	0.176	0.179	0.186	0.199	0.203	0.000	0.000	0.001	0.003	0.006	0.013	0.013
ωB97X-D	0.173	0.174	0.176	0.179	0.186	0.200	0.205	0.000	0.000	0.001	0.003	0.005	0.012	0.011

Table S9: The values of uncorrected interaction-induced dipole moment and basis set superposition error (BSSE) computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**uncorrected interaction-induced dipole moment [au]**							**BSSE [au]**						
CCSD(T)	0.317	0.314	0.306	0.295	0.280	0.250	0.238	-0.001	-0.001	-0.001	-0.003	-0.005	-0.009	-0.018
CCSD	0.315	0.312	0.304	0.293	0.279	0.248	0.236	0.000	0.000	0.000	-0.003	-0.006	-0.008	-0.018
MP2	0.309	0.306	0.298	0.288	0.274	0.245	0.233	0.000	0.000	0.000	-0.003	-0.006	-0.010	-0.019
HF	0.331	0.328	0.320	0.308	0.293	0.260	0.245	0.000	0.000	-0.001	-0.002	-0.005	-0.007	-0.014
B2PLYP	0.334	0.329	0.321	0.310	0.296	0.265	0.253	-0.003	0.000	0.000	-0.003	-0.005	-0.009	-0.019
B3LYP	0.336	0.333	0.326	0.316	0.303	0.273	0.263	-0.001	0.000	0.000	-0.003	-0.007	-0.011	-0.023
B3PW91	0.334	0.332	0.326	0.316	0.302	0.272	0.263	0.000	0.000	-0.001	-0.003	-0.006	-0.010	-0.023
B97-2	0.332	0.330	0.324	0.313	0.299	0.270	0.260	0.000	-0.001	-0.001	-0.002	-0.005	-0.010	-0.022
B97D	0.339	0.336	0.330	0.320	0.306	0.278	0.269	-0.001	0.000	-0.001	-0.003	-0.006	-0.012	-0.025
BLYP	0.341	0.338	0.332	0.322	0.309	0.281	0.272	-0.001	0.000	-0.001	-0.003	-0.007	-0.014	-0.028
BMK	0.335	0.332	0.326	0.315	0.300	0.267	0.253	-0.001	-0.001	-0.002	-0.003	-0.006	-0.008	-0.018
CAM-B3LYP	0.334	0.332	0.324	0.314	0.300	0.271	0.261	0.000	-0.001	0.000	-0.003	-0.006	-0.011	-0.023
HCTH	0.331	0.329	0.323	0.315	0.302	0.276	0.268	0.001	0.001	0.001	-0.003	-0.006	-0.013	-0.026
HISS	0.333	0.330	0.323	0.313	0.298	0.267	0.256	0.000	0.000	0.000	-0.003	-0.005	-0.008	-0.019
HSE06	0.335	0.332	0.326	0.316	0.302	0.272	0.262	0.000	0.000	-0.001	-0.003	-0.006	-0.010	-0.022
LC-BLYP	0.334	0.331	0.324	0.313	0.300	0.271	0.260	0.000	0.000	0.000	-0.003	-0.007	-0.012	-0.023
LC-HCTH	0.329	0.326	0.318	0.308	0.296	0.268	0.257	0.001	0.001	0.001	-0.002	-0.008	-0.013	-0.023
LC-REVTPSS	0.331	0.328	0.321	0.311	0.296	0.266	0.255	0.000	0.000	-0.001	-0.003	-0.006	-0.010	-0.021
LC-τHCTH	0.339	0.335	0.327	0.316	0.302	0.271	0.259	0.001	0.001	0.000	-0.004	-0.008	-0.012	-0.022
LSDA	0.349	0.347	0.341	0.331	0.317	0.288	0.278	0.000	0.000	-0.001	-0.003	-0.006	-0.012	-0.025
M06	0.336	0.333	0.326	0.314	0.297	0.266	0.257	0.000	0.000	-0.001	-0.003	-0.004	-0.008	-0.023
M06-2X	0.331	0.328	0.321	0.310	0.295	0.264	0.252	0.000	0.000	-0.001	-0.004	-0.006	-0.009	-0.020
M06-HF	0.335	0.332	0.323	0.310	0.294	0.261	0.248	-0.003	-0.003	-0.001	-0.002	-0.005	-0.009	-0.019
M06L	0.333	0.331	0.325	0.314	0.297	0.265	0.257	0.000	0.000	-0.001	-0.002	-0.002	-0.005	-0.020
M11	0.338	0.336	0.329	0.316	0.299	0.265	0.255	-0.001	-0.002	-0.004	-0.005	-0.007	-0.008	-0.020
M11-L	0.345	0.342	0.332	0.315	0.292	0.250	0.234	0.002	0.001	0.000	-0.001	0.000	-0.002	-0.017
MN12-L	0.338	0.335	0.327	0.313	0.294	0.258	0.245	0.001	0.001	0.000	-0.001	-0.001	-0.004	-0.016
MN12-SX	0.334	0.331	0.323	0.309	0.290	0.253	0.240	0.002	0.001	0.000	-0.002	-0.002	-0.005	-0.018
MPW1PW91	0.334	0.331	0.325	0.315	0.300	0.271	0.261	-0.001	0.000	-0.001	-0.003	-0.005	-0.010	-0.022
N12	0.338	0.336	0.330	0.320	0.306	0.277	0.268	0.000	0.000	-0.001	-0.003	-0.006	-0.012	-0.025
N12-SX	0.334	0.332	0.325	0.315	0.300	0.271	0.261	0.000	-0.001	-0.001	-0.003	-0.005	-0.010	-0.021
PBE	0.340	0.338	0.332	0.323	0.309	0.282	0.273	0.000	0.000	-0.001	-0.004	-0.006	-0.013	-0.027
PBE0	0.334	0.331	0.325	0.315	0.301	0.272	0.262	0.000	0.000	-0.001	-0.003	-0.006	-0.010	-0.022
REVTPSS	0.334	0.332	0.325	0.315	0.301	0.272	0.262	-0.001	-0.001	-0.001	-0.003	-0.006	-0.011	-0.025
SOGGA11-X	0.332	0.329	0.322	0.311	0.296	0.266	0.255	0.000	0.000	-0.001	-0.003	-0.005	-0.009	-0.019
τHCTH	0.340	0.338	0.331	0.321	0.306	0.277	0.269	-0.001	-0.001	-0.001	-0.003	-0.005	-0.011	-0.026
τHCTHHYB	0.337	0.335	0.329	0.319	0.304	0.274	0.264	0.000	0.000	-0.001	-0.003	-0.005	-0.010	-0.023
TPSSH	0.335	0.333	0.326	0.316	0.302	0.272	0.262	0.000	-0.001	-0.001	-0.003	-0.006	-0.010	-0.023
ωB97	0.332	0.329	0.321	0.310	0.296	0.266	0.256	0.000	0.000	-0.001	-0.003	-0.007	-0.011	-0.023
ωB97X	0.331	0.329	0.321	0.310	0.296	0.265	0.255	0.000	-0.001	-0.001	-0.003	-0.006	-0.009	-0.021
ωB97X-D	0.332	0.330	0.323	0.312	0.297	0.266	0.256	0.000	-0.001	-0.001	-0.003	-0.006	-0.009	-0.021

Table S10: The values of electric dipole polarizability (α_{zz}) and **% error** computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**polarizability (α_{zz}) [au]**							**% error**						
CCSD(T)	13.76	13.35	12.48	11.53	10.61	9.02	7.76	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	13.49	13.11	12.29	11.38	10.49	8.93	7.70	-2.0	-1.8	-1.5	-1.3	-1.1	-0.9	-0.8
MP2	13.80	13.38	12.49	11.51	10.58	8.98	7.72	0.3	0.2	0.0	-0.1	-0.3	-0.4	-0.5
HF	12.34	12.04	11.38	10.60	9.83	8.43	7.30	-10.3	-9.8	-8.9	-8.1	-7.4	-6.5	-5.9
B2PLYP	13.40	13.03	12.22	11.33	10.47	8.95	7.74	-2.6	-2.4	-2.1	-1.7	-1.3	-0.7	-0.3
B3LYP	14.43	13.96	13.01	12.01	11.07	9.44	8.15	4.9	4.6	4.2	4.2	4.3	4.7	5.0
B3PW91	14.19	13.75	12.85	11.88	10.97	9.37	8.11	3.2	3.0	2.9	3.1	3.3	3.9	4.4
B97-2	14.06	13.62	12.72	11.76	10.86	9.29	8.04	2.2	2.0	1.9	2.0	2.3	3.0	3.5
B97D	14.86	14.34	13.31	12.27	11.30	9.65	8.34	8.0	7.4	6.6	6.4	6.5	7.0	7.4
BLYP	15.38	14.81	13.72	12.61	11.59	9.86	8.51	11.8	11.0	9.9	9.4	9.2	9.4	9.6
BMK	13.80	13.43	12.57	11.56	10.66	9.07	7.87	0.3	0.6	0.7	0.3	0.5	0.6	1.4
CAM-B3LYP	14.24	13.78	12.86	11.87	10.94	9.33	8.06	3.5	3.3	3.0	3.0	3.1	3.4	3.7
HCTH	14.82	14.27	13.21	12.17	11.20	9.56	8.26	7.7	6.9	5.8	5.5	5.5	6.0	6.3
HISS	13.54	13.15	12.34	11.45	10.58	9.06	7.85	-1.6	-1.5	-1.1	-0.7	-0.3	0.5	1.1
HSE06	14.13	13.70	12.79	11.83	10.91	9.32	8.05	2.7	2.6	2.5	2.6	2.8	3.3	3.7
LC-BLYP	14.00	13.57	12.68	11.72	10.81	9.23	7.98	1.7	1.6	1.6	1.7	1.9	2.3	2.7
LC-HCTH	13.98	13.54	12.64	11.67	10.74	9.13	7.87	1.6	1.4	1.2	1.2	1.2	1.3	1.4
LC-revTPSS	13.80	13.41	12.56	11.64	10.75	9.19	7.96	0.3	0.4	0.6	0.9	1.3	2.0	2.5
LC-τHCTH	14.18	13.75	12.84	11.85	10.88	9.20	7.91	3.1	3.0	2.9	2.7	2.5	2.1	1.9
LSDA	15.14	14.60	13.55	12.47	11.46	9.74	8.40	10.0	9.4	8.6	8.1	8.0	8.1	8.1
M06	13.97	13.51	12.57	11.58	10.65	9.09	7.88	1.5	1.2	0.7	0.5	0.4	0.8	1.5
M06-2X	13.76	13.37	12.54	11.63	10.74	9.20	7.97	0.0	0.1	0.5	0.8	1.2	2.0	2.7
M06-HF	13.35	13.01	12.29	11.48	10.68	9.22	8.00	-3.0	-2.6	-1.5	-0.4	0.6	2.2	3.0
M06L	14.43	13.96	12.98	11.90	10.94	9.31	8.07	4.9	4.6	4.0	3.2	3.1	3.2	4.0
M11	13.76	13.36	12.53	11.62	10.74	9.19	7.96	0.0	0.1	0.4	0.8	1.2	1.9	2.6
M11-L	14.16	13.68	12.70	11.69	10.75	9.20	8.00	3.0	2.5	1.7	1.4	1.3	2.0	3.1
MN12-L	13.98	13.50	12.55	11.56	10.64	9.09	7.89	1.6	1.1	0.5	0.3	0.2	0.8	1.6
MN12-SX	13.96	13.50	12.58	11.61	10.70	9.16	7.96	1.5	1.1	0.7	0.7	0.8	1.6	2.6
mPW1PW91	14.04	13.61	12.71	11.76	10.86	9.28	8.03	2.1	1.9	1.8	2.0	2.3	3.0	3.5
N12	14.50	13.99	12.99	11.94	11.01	9.38	8.09	5.4	4.8	4.0	3.6	3.8	4.0	4.2
N12-SX	13.90	13.46	12.57	11.62	10.72	9.17	7.94	1.0	0.8	0.7	0.8	1.0	1.7	2.3
PBE	15.22	14.66	13.59	12.50	11.50	9.80	8.46	10.6	9.8	8.8	8.4	8.4	8.7	8.9
PBE0	14.11	13.67	12.77	11.80	10.89	9.30	8.04	2.5	2.4	2.3	2.4	2.6	3.2	3.6
revTPSS	15.01	14.49	13.48	12.44	11.46	9.78	8.45	9.1	8.5	8.0	7.8	8.0	8.5	8.8
SOGGA11-X	13.76	13.35	12.50	11.58	10.69	9.14	7.91	0.0	0.0	0.2	0.4	0.7	1.4	1.9
τHCTH	14.65	14.15	13.16	12.16	11.22	9.60	8.30	6.5	6.0	5.4	5.5	5.7	6.4	6.9
τHCTHHYB	14.34	13.89	12.97	11.98	11.06	9.44	8.17	4.2	4.0	3.9	3.9	4.2	4.7	5.2
TPSSH	14.53	14.06	13.12	12.12	11.19	9.57	8.27	5.6	5.3	5.1	5.2	5.5	6.1	6.6
ωB97	14.31	13.87	12.93	11.91	10.97	9.32	8.05	4.0	3.9	3.6	3.3	3.3	3.4	3.7
ωB97X	14.19	13.75	12.82	11.81	10.88	9.25	8.00	3.1	3.0	2.7	2.5	2.5	2.6	3.0
ωB97X-D	14.05	13.62	12.71	11.72	10.81	9.22	7.98	2.1	2.0	1.8	1.6	1.9	2.3	2.8

Table S11: The values of electric dipole polarizability (α_{zz}) and **% error** computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**polarizability (α_{zz}) [au]**							**% error**						
CCSD(T)	49.76	47.57	43.27	38.92	35.04	28.93	24.57	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	49.15	47.04	42.86	38.59	34.78	28.74	24.43	-1.2	-1.1	-1.0	-0.8	-0.8	-0.6	-0.6
MP2	48.71	46.54	42.32	38.06	34.29	28.31	24.05	-2.1	-2.2	-2.2	-2.2	-2.2	-2.1	-2.1
HF	49.98	47.88	43.72	39.48	35.68	29.65	25.32	0.5	0.7	1.0	1.4	1.8	2.5	3.1
B2PLYP	50.71	48.48	44.17	39.83	35.97	29.85	25.49	1.9	1.9	2.1	2.3	2.6	3.2	3.7
B3LYP	51.77	49.39	44.89	40.42	36.47	30.22	25.78	4.0	3.8	3.8	3.9	4.1	4.5	4.9
B3PW91	51.20	48.95	44.60	40.23	36.33	30.15	25.72	2.9	2.9	3.1	3.4	3.7	4.2	4.7
B97-2	51.17	48.90	44.53	40.16	36.26	30.07	25.66	2.8	2.8	2.9	3.2	3.5	4.0	4.4
B97D	52.64	50.15	45.52	40.95	36.91	30.54	26.01	5.8	5.4	5.2	5.2	5.3	5.6	5.8
BLYP	53.19	50.61	45.85	41.19	37.10	30.68	26.12	6.9	6.4	6.0	5.8	5.9	6.1	6.3
BMK	50.43	48.35	44.22	39.92	36.10	30.01	25.57	1.3	1.6	2.2	2.6	3.0	3.7	4.1
CAM-B3LYP	51.26	48.97	44.57	40.16	36.26	30.08	25.68	3.0	2.9	3.0	3.2	3.5	4.0	4.5
HCTH	52.34	49.80	45.14	40.58	36.57	30.27	25.80	5.2	4.7	4.3	4.3	4.4	4.6	5.0
HISS	50.15	48.05	43.88	39.63	35.82	29.77	25.43	0.8	1.0	1.4	1.8	2.2	2.9	3.5
HSE06	51.26	48.98	44.60	40.20	36.28	30.08	25.66	3.0	3.0	3.1	3.3	3.5	4.0	4.4
LC-BLYP	50.41	48.27	44.05	39.77	35.95	29.89	25.55	1.3	1.5	1.8	2.2	2.6	3.3	4.0
LC-HCTH	50.76	48.49	44.08	39.69	35.82	29.74	25.41	2.0	1.9	1.9	2.0	2.2	2.8	3.4
LC-REVTPSS	49.89	47.85	43.77	39.57	35.80	29.77	25.43	0.3	0.6	1.2	1.7	2.1	2.9	3.5
LC-τHCTH	51.41	49.11	44.62	40.14	36.19	29.99	25.58	3.3	3.2	3.1	3.1	3.3	3.7	4.1
LSDA	52.57	50.14	45.55	40.98	36.94	30.56	26.03	5.6	5.4	5.3	5.3	5.4	5.7	5.9
M06	51.21	48.95	44.58	40.16	36.22	29.99	25.53	2.9	2.9	3.0	3.2	3.4	3.7	3.9
M06-2X	51.08	48.87	44.57	40.20	36.29	30.11	25.72	2.6	2.7	3.0	3.3	3.6	4.1	4.7
M06-HF	50.90	48.78	44.56	40.17	36.17	29.86	25.50	2.3	2.6	3.0	3.2	3.2	3.2	3.7
M06L	50.98	48.86	44.67	40.30	36.34	30.05	25.55	2.4	2.7	3.2	3.5	3.7	3.9	4.0
M11	50.98	48.85	44.62	40.28	36.40	30.30	26.01	2.4	2.7	3.1	3.5	3.9	4.7	5.8
M11-L	53.93	51.47	46.70	41.81	37.43	30.43	25.39	8.4	8.2	7.9	7.4	6.8	5.2	3.3
MN12-L	51.70	49.36	44.88	40.35	36.31	29.88	25.25	3.9	3.8	3.7	3.7	3.6	3.3	2.7
MN12-SX	52.10	49.73	45.21	40.65	36.59	30.13	25.49	4.7	4.5	4.5	4.4	4.4	4.1	3.7
MPW1PW91	51.04	48.79	44.46	40.10	36.22	30.06	25.65	2.6	2.6	2.8	3.0	3.4	3.9	4.4
N12	52.18	49.68	45.07	40.55	36.54	30.24	25.78	4.9	4.4	4.2	4.2	4.3	4.5	4.9
N12-SX	50.80	48.55	44.24	39.91	36.06	29.96	25.60	2.1	2.1	2.2	2.6	2.9	3.6	4.2
PBE	52.78	50.27	45.62	41.03	36.99	30.61	26.07	6.1	5.7	5.4	5.4	5.5	5.8	6.1
PBE0	51.17	48.90	44.54	40.16	36.26	30.08	25.67	2.8	2.8	2.9	3.2	3.5	4.0	4.4
REVTPSS	52.22	49.82	45.28	40.76	36.74	30.38	25.83	4.9	4.7	4.6	4.7	4.8	5.0	5.1
SOGGA11-X	50.80	48.61	44.33	40.00	36.13	30.00	25.63	2.1	2.2	2.5	2.8	3.1	3.7	4.3
τHCTH	52.40	49.99	45.44	40.91	36.88	30.50	25.95	5.3	5.1	5.0	5.1	5.2	5.4	5.6
τHCTHHYB	51.74	49.43	45.01	40.56	36.59	30.32	25.84	4.0	3.9	4.0	4.2	4.4	4.8	5.1
TPSSH	51.73	49.41	44.97	40.52	36.56	30.28	25.78	4.0	3.9	3.9	4.1	4.3	4.7	4.9
ωB97	51.01	48.81	44.48	40.10	36.19	30.01	25.61	2.5	2.6	2.8	3.0	3.3	3.8	4.2
ωB97X	51.07	48.81	44.43	40.03	36.12	29.96	25.56	2.6	2.6	2.7	2.9	3.1	3.6	4.0
ωB97X-D	51.04	48.77	44.40	40.02	36.13	29.97	25.58	2.6	2.5	2.6	2.8	3.1	3.6	4.1

Table S12: The values of interaction-induced polarizability ($\Delta\alpha_{zz}$) and **% error** computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The values of $\Delta\alpha_{zz}$ were corrected according to the Boys and Bernardi counterpoise scheme. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**interaction-induced polarizability ($\Delta\alpha_{zz}$) [au]**							**% error**						
CCSD(T)	0.98	0.97	0.93	0.88	0.82	0.71	0.58	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	0.93	0.92	0.89	0.84	0.80	0.69	0.57	-5.0	-4.7	-4.3	-3.9	-3.4	-2.8	-2.4
MP2	0.97	0.95	0.92	0.87	0.82	0.70	0.58	-1.8	-1.2	-1.0	-0.9	-0.7	-0.6	-0.3
HF	0.71	0.71	0.69	0.67	0.64	0.56	0.48	-27.4	-26.6	-25.3	-23.9	-22.5	-20.5	-18.5
B2PLYP	0.94	0.93	0.90	0.86	0.82	0.72	0.60	-4.8	-4.0	-3.2	-1.9	-0.7	1.1	2.6
B3LYP	1.16	1.14	1.10	1.05	0.99	0.87	0.72	17.9	18.2	18.8	19.5	20.5	22.3	23.1
B3PW91	1.12	1.11	1.07	1.03	0.98	0.86	0.72	13.7	14.5	15.6	17.2	18.9	21.7	22.9
B97-2	1.09	1.07	1.04	1.00	0.95	0.84	0.70	10.5	11.1	11.9	13.7	15.4	18.9	20.4
B97D	1.23	1.22	1.17	1.12	1.07	0.95	0.79	25.3	25.8	25.9	28.1	29.6	33.4	34.6
BLYP	1.34	1.32	1.27	1.21	1.14	0.99	0.82	36.7	36.9	36.7	37.4	38.2	39.9	40.1
BMK	1.00	1.02	0.99	0.89	0.85	0.72	0.62	2.0	5.3	6.8	1.3	3.6	2.0	6.3
CAM-B3LYP	1.10	1.09	1.05	1.00	0.95	0.82	0.68	11.7	12.3	12.8	13.8	14.7	15.9	17.0
HCTH	1.19	1.17	1.12	1.08	1.03	0.93	0.77	21.3	21.1	20.7	22.8	25.4	30.5	32.4
HISS	1.02	1.01	0.98	0.93	0.89	0.78	0.65	3.8	4.3	5.3	6.6	8.3	10.6	12.2
HSE06	1.13	1.12	1.08	1.03	0.98	0.85	0.71	15.0	15.4	15.9	17.2	18.6	20.5	21.6
LC-BLYP	1.05	1.04	1.01	0.96	0.91	0.79	0.66	7.0	7.8	8.5	9.6	10.6	11.7	12.8
LC-HCTH	1.05	1.02	0.97	0.92	0.87	0.74	0.62	6.5	5.9	5.1	5.4	5.2	5.1	6.0
LC-revTPSS	1.02	1.01	0.98	0.94	0.90	0.79	0.66	3.7	4.5	5.8	7.4	9.0	11.1	12.8
LC-τHCTH	1.19	1.16	1.09	1.01	0.93	0.78	0.64	21.4	20.0	17.1	15.3	12.5	9.3	8.9
LSDA	1.44	1.41	1.35	1.27	1.20	1.03	0.85	46.4	46.0	44.9	44.8	45.0	45.3	45.4
M06	1.09	1.07	1.03	0.98	0.92	0.79	0.65	10.9	10.9	10.9	11.4	11.0	11.0	10.8
M06-2X	1.04	1.02	0.99	0.94	0.89	0.78	0.66	5.6	6.0	6.4	7.1	7.8	10.2	12.3
M06-HF	0.95	0.94	0.93	0.91	0.88	0.78	0.65	-3.4	-2.8	-0.2	3.4	6.3	10.3	11.1
M06L	1.14	1.12	1.08	1.01	0.97	0.84	0.71	15.5	16.0	16.6	14.8	17.5	19.2	22.1
M11	1.00	0.99	0.97	0.93	0.88	0.75	0.62	1.4	2.5	4.1	5.5	6.3	6.2	6.7
M11-L	1.02	1.01	0.97	0.92	0.88	0.77	0.64	3.6	4.1	4.5	5.5	6.9	8.9	9.8
MN12-L	0.94	0.93	0.89	0.85	0.80	0.69	0.58	-4.3	-3.8	-3.7	-3.5	-3.4	-2.5	-0.9
MN12-SX	0.97	0.96	0.92	0.87	0.82	0.72	0.60	-1.1	-1.0	-0.8	-0.6	-0.1	1.0	2.2
mPW1PW91	1.09	1.08	1.05	1.01	0.96	0.85	0.71	11.0	11.8	12.9	14.6	16.3	19.3	20.7
N12	1.17	1.17	1.14	1.07	1.04	0.91	0.75	18.8	20.9	22.7	22.3	26.2	27.8	28.1
N12-SX	1.05	1.03	1.00	0.95	0.90	0.80	0.67	6.4	7.0	7.8	8.6	9.8	12.4	14.0
PBE	1.34	1.32	1.27	1.21	1.14	1.00	0.83	36.6	36.6	36.6	37.4	38.8	41.3	42.3
PBE0	1.11	1.10	1.06	1.02	0.97	0.85	0.71	13.1	13.8	14.4	15.7	17.2	20.0	21.4
revTPSS	1.28	1.26	1.22	1.17	1.11	0.98	0.81	30.1	30.7	31.5	33.2	34.8	37.7	38.4
SOGGA11-X	1.09	1.08	1.04	0.98	0.92	0.79	0.66	11.1	11.6	11.7	11.6	11.5	12.0	12.7
τHCTH	1.24	1.22	1.17	1.13	1.08	0.96	0.79	25.7	26.0	26.4	29.2	31.1	35.0	36.0
τHCTHHYB	1.17	1.15	1.12	1.06	1.02	0.89	0.74	18.6	19.3	21.1	21.2	23.7	25.2	26.4
TPSSH	1.18	1.17	1.13	1.09	1.04	0.92	0.77	20.2	21.0	22.1	24.2	26.5	29.8	31.0
ωB97	1.12	1.11	1.07	0.99	0.94	0.80	0.66	14.2	14.9	14.8	13.2	13.8	12.7	13.0
ωB97X	1.08	1.07	1.03	0.96	0.91	0.79	0.65	9.9	10.8	10.8	9.7	10.8	10.7	11.6
ωB97X-D	1.04	1.04	1.01	0.95	0.91	0.79	0.66	6.0	7.9	8.9	8.2	10.6	11.8	12.7

Table S13: The values of interaction-induced polarizability ($\Delta\alpha_{zz}$) and **% error** computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The values of $\Delta\alpha_{zz}$ were corrected according to the Boys and Bernardi counterpoise scheme. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**interaction-induced polarizability ($\Delta\alpha_{zz}$) [au]**							**% error**						
CCSD(T)	4.74	4.55	4.12	3.63	3.15	2.36	1.82	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	4.60	4.42	4.02	3.55	3.09	2.32	1.79	-2.8	-2.7	-2.4	-2.2	-2.0	-1.8	-1.7
MP2	4.55	4.37	3.97	3.50	3.04	2.28	1.75	-3.9	-3.9	-3.8	-3.7	-3.6	-3.6	-3.8
HF	4.51	4.33	3.94	3.49	3.05	2.31	1.81	-4.9	-4.7	-4.3	-3.8	-3.3	-2.2	-0.9
B2PLYP	4.88	4.70	4.28	3.80	3.32	2.53	1.97	3.1	3.3	3.9	4.6	5.4	6.9	8.2
B3LYP	5.29	5.09	4.64	4.12	3.61	2.75	2.14	11.7	11.9	12.6	13.5	14.5	16.3	17.2
B3PW91	5.24	5.06	4.63	4.12	3.61	2.75	2.14	10.6	11.2	12.3	13.4	14.5	16.3	17.3
B97-2	5.19	5.00	4.57	4.07	3.56	2.72	2.12	9.6	10.0	10.9	12.0	13.0	14.9	16.3
B97D	5.55	5.33	4.86	4.31	3.77	2.86	2.22	17.2	17.3	17.8	18.7	19.6	21.2	21.7
BLYP	5.63	5.42	4.94	4.38	3.83	2.91	2.24	18.9	19.1	19.7	20.5	21.4	23.0	23.0
BMK	4.99	4.86	4.49	3.93	3.43	2.60	1.99	5.3	6.9	8.9	8.3	8.9	10.1	8.9
CAM-B3LYP	5.10	4.91	4.49	4.00	3.51	2.68	2.09	7.6	8.1	9.0	10.2	11.3	13.4	14.8
HCTH	5.36	5.14	4.69	4.17	3.67	2.82	2.21	13.2	13.1	13.7	15.0	16.3	19.1	21.1
HISS	5.02	4.83	4.42	3.93	3.44	2.62	2.05	6.0	6.3	7.1	8.1	9.1	10.9	12.5
HSE06	5.27	5.07	4.63	4.11	3.60	2.74	2.14	11.2	11.5	12.3	13.2	14.2	16.0	17.2
LC-BLYP	4.90	4.73	4.34	3.87	3.40	2.61	2.05	3.5	4.0	5.2	6.6	7.9	10.4	12.3
LC-HCTH	4.88	4.67	4.24	3.76	3.30	2.54	2.00	3.0	2.7	2.9	3.7	4.8	7.2	9.4
LC-REVTPSS	4.84	4.68	4.30	3.83	3.36	2.57	2.00	2.3	2.9	4.2	5.5	6.7	8.7	9.9
LC-τHCTH	5.21	4.97	4.48	3.94	3.44	2.61	2.04	10.0	9.4	8.7	8.6	9.0	10.5	12.1
LSDA	5.90	5.67	5.17	4.59	4.02	3.07	2.39	24.5	24.7	25.4	26.3	27.5	29.9	31.2
M06	5.47	5.25	4.77	4.22	3.69	2.82	2.18	15.6	15.6	15.7	16.3	17.2	19.2	19.8
M06-2X	5.09	4.90	4.46	3.96	3.45	2.61	2.03	7.5	7.7	8.3	9.0	9.4	10.2	11.4
M06-HF	5.28	5.10	4.65	4.07	3.48	2.52	1.90	11.5	12.1	12.8	12.2	10.4	6.6	4.4
M06L	5.60	5.39	4.92	4.35	3.78	2.88	2.23	18.2	18.5	19.4	19.8	20.1	21.6	22.2
M11	5.01	4.82	4.36	3.84	3.33	2.50	1.96	5.7	5.9	5.9	5.7	5.6	5.9	7.5
M11-L	5.99	5.71	5.10	4.41	3.75	2.68	1.94	26.3	25.5	23.7	21.5	19.0	13.5	6.5
MN12-L	5.13	4.90	4.41	3.87	3.36	2.54	1.97	8.2	7.7	6.9	6.6	6.6	7.4	8.3
MN12-SX	5.22	4.99	4.50	3.96	3.43	2.57	1.98	10.3	9.8	9.3	8.9	8.8	8.5	8.6
MPW1PW91	5.19	5.01	4.58	4.08	3.58	2.73	2.13	9.6	10.1	11.2	12.4	13.5	15.5	16.9
N12	5.47	5.30	4.87	4.35	3.82	2.93	2.29	15.6	16.6	18.1	19.7	21.2	23.9	25.3
N12-SX	5.14	4.96	4.54	4.05	3.56	2.73	2.15	8.5	9.0	10.1	11.5	12.9	15.5	17.7
PBE	5.67	5.45	4.98	4.42	3.87	2.95	2.29	19.6	19.9	20.7	21.8	22.8	24.9	25.6
PBE0	5.22	5.03	4.60	4.09	3.59	2.74	2.14	10.3	10.7	11.6	12.7	13.8	15.7	17.2
REVTPSS	5.44	5.23	4.77	4.22	3.68	2.77	2.12	14.7	15.0	15.6	16.2	16.7	17.3	16.5
SOGGA11-X	5.08	4.88	4.44	3.94	3.44	2.62	2.05	7.2	7.4	7.8	8.4	9.2	10.9	12.6
τHCTH	5.64	5.42	4.94	4.38	3.83	2.90	2.24	19.0	19.2	19.7	20.6	21.4	22.7	23.0
τHCTHHYB	5.43	5.24	4.79	4.25	3.72	2.82	2.18	14.6	15.2	16.3	17.0	17.9	19.5	19.7
TPSSH	5.35	5.15	4.71	4.19	3.66	2.78		12.9	13.3	14.3	15.3	16.2	17.7	
ωB97	5.06	4.87	4.43	3.93	3.43	2.60	2.02	6.9	7.1	7.5	8.1	8.7	9.9	10.5
ωB97X	5.05	4.85	4.42	3.92	3.43	2.61	2.03	6.6	6.8	7.2	8.1	8.8	10.3	11.1
ωB97X-D	5.07	4.88	4.46	3.97	3.47	2.64	2.05	7.0	7.3	8.2	9.4	10.2	11.7	12.2

Table S14: The values of uncorrected interaction-induced polarizability and basis set superposition error (BSSE) computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**uncorrected interaction-induced polarizability [au]**							**BSSE [au]**						
CCSD(T)	0.99	0.99	0.95	0.90	0.86	0.79	0.70	-0.01	-0.02	-0.02	-0.02	-0.04	-0.08	-0.12
CCSD	0.94	0.94	0.91	0.87	0.83	0.77	0.68	-0.01	-0.02	-0.02	-0.03	-0.03	-0.08	-0.11
MP2	0.98	0.98	0.95	0.90	0.86	0.79	0.70	-0.01	-0.03	-0.03	-0.03	-0.04	-0.09	-0.12
HF	0.72	0.72	0.71	0.69	0.67	0.63	0.57	-0.01	-0.01	-0.02	-0.02	-0.03	-0.07	-0.09
B2PLYP	0.95	0.95	0.93	0.89	0.86	0.80	0.72	-0.01	-0.02	-0.03	-0.03	-0.04	-0.08	-0.12
B3LYP	1.17	1.17	1.15	1.33	1.05	0.97	0.87	-0.01	-0.03	-0.05	-0.28	-0.06	-0.10	-0.15
B3PW91	1.13	1.13	1.11	1.07	1.03	0.96	0.86	-0.01	-0.02	-0.04	-0.04	-0.05	-0.10	-0.14
B97-2	1.10	1.10	1.08	1.04	1.01	0.94	0.84	-0.01	-0.03	-0.04	-0.04	-0.06	-0.10	-0.14
B97D	1.24	1.24	1.22	1.18	1.14	1.06	0.94	-0.01	-0.02	-0.05	-0.06	-0.07	-0.11	-0.15
BLYP	1.35	1.36	1.33	1.27	1.22	1.12	0.99	-0.01	-0.04	-0.06	-0.06	-0.08	-0.13	-0.17
BMK	1.01	1.03	1.01	0.92	0.92	0.84	0.77	-0.01	-0.01	-0.02	-0.03	-0.07	-0.12	-0.15
CAM-B3LYP	1.11	1.11	1.09	1.05	1.00	0.93	0.83	-0.01	-0.02	-0.04	-0.05	-0.05	-0.11	-0.15
HCTH	1.19	1.21	1.18	1.14	1.10	1.03	0.92	0.00	-0.04	-0.06	-0.06	-0.07	-0.10	-0.15
HISS	1.03	1.03	1.01	0.97	0.93	0.87	0.79	-0.01	-0.02	-0.03	-0.04	-0.04	-0.09	-0.14
HSE06	1.14	1.14	1.11	1.07	1.03	0.95	0.85	-0.01	-0.02	-0.03	-0.04	-0.05	-0.10	-0.14
LC-BLYP	1.06	1.07	1.05	1.01	0.97	0.90	0.81	-0.01	-0.03	-0.04	-0.05	-0.06	-0.11	-0.15
LC-HCTH	1.08	1.07	1.03	0.96	0.90	0.83	0.75	-0.03	-0.05	-0.06	-0.04	-0.03	-0.09	-0.13
LC-revTPSS	1.03	1.03	1.02	0.98	0.95	0.89	0.80	-0.01	-0.02	-0.04	-0.04	-0.05	-0.10	-0.14
LC-τHCTH	1.20	1.18	1.11	1.03	0.96	0.87	0.78	-0.01	-0.02	-0.02	-0.02	-0.03	-0.09	-0.14
LSDA	1.45	1.44	1.39	1.32	1.26	1.15	1.01	-0.01	-0.03	-0.04	-0.05	-0.06	-0.12	-0.16
M06	1.15	1.13	1.09	1.05	1.01	0.92	0.81	-0.06	-0.06	-0.06	-0.07	-0.09	-0.13	-0.16
M06-2X	1.05	1.04	1.02	0.97	0.93	0.87	0.78	-0.01	-0.02	-0.03	-0.03	-0.04	-0.09	-0.12
M06-HF	0.97	0.97	0.98	0.96	0.93	0.85	0.76	-0.02	-0.03	-0.05	-0.05	-0.05	-0.07	-0.11
M06L	1.21	1.19	1.15	1.10	1.09	1.01	0.90	-0.07	-0.07	-0.07	-0.09	-0.12	-0.17	-0.19
M11	1.03	1.02	1.00	0.97	0.95	0.87	0.78	-0.03	-0.03	-0.03	-0.04	-0.07	-0.12	-0.16
M11-L	1.10	1.08	1.05	1.01	0.98	0.90	0.78	-0.08	-0.07	-0.08	-0.09	-0.10	-0.13	-0.14
MN12-L	1.02	1.00	0.97	0.93	0.90	0.83	0.74	-0.08	-0.07	-0.08	-0.08	-0.10	-0.14	-0.16
MN12-SX	1.05	1.03	0.99	0.96	0.93	0.86	0.76	-0.08	-0.07	-0.07	-0.09	-0.11	-0.14	-0.16
mPW1PW91	1.10	1.10	1.09	1.05	1.01	0.94	0.84	-0.01	-0.02	-0.04	-0.04	-0.05	-0.09	-0.13
N12	1.18	1.20	1.20	1.14	1.11	1.02	0.90	-0.01	-0.03	-0.06	-0.07	-0.07	-0.11	-0.15
N12-SX	1.05	1.06	1.04	1.00	0.96	0.90	0.81	0.00	-0.03	-0.04	-0.05	-0.06	-0.10	-0.14
PBE	1.35	1.35	1.32	1.26	1.21	1.12	0.99	-0.01	-0.03	-0.05	-0.05	-0.07	-0.12	-0.16
PBE0	1.12	1.12	1.10	1.06	1.02	0.95	0.84	-0.01	-0.02	-0.04	-0.04	-0.05	-0.10	-0.13
revTPSS	1.29	1.29	1.27	1.22	1.18	1.09	0.96	-0.01	-0.03	-0.05	-0.05	-0.07	-0.11	-0.15
SOGGA11-X	1.12	1.11	1.08	1.03	0.98	0.90	0.79	-0.03	-0.03	-0.04	-0.05	-0.06	-0.11	-0.13
τHCTH	1.24	1.25	1.22	1.19	1.15	1.07	0.94	0.00	-0.03	-0.05	-0.06	-0.07	-0.11	-0.15
τHCTHHYB	1.18	1.18	1.16	1.11	1.08	0.99	0.88	-0.01	-0.03	-0.04	-0.05	-0.06	-0.10	-0.14
TPSSH	1.19	1.20	1.18	1.14	1.10	1.02	0.91	-0.01	-0.03	-0.05	-0.05	-0.06	-0.10	-0.14
ωB97	1.13	1.13	1.10	1.04	1.00	0.91	0.81	-0.01	-0.02	-0.03	-0.05	-0.06	-0.11	-0.15
ωB97X	1.09	1.09	1.06	1.01	0.97	0.90	0.80	-0.01	-0.02	-0.03	-0.05	-0.06	-0.11	-0.15
ωB97X-D	1.06	1.07	1.05	0.99	0.98	0.90	0.80	-0.02	-0.03	-0.04	-0.04	-0.07	-0.11	-0.14

Table S15: The values of uncorrected interaction-induced polarizability and basis set superposition error (BSSE) computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**uncorrected interaction-induced polarizability [au]**							**BSSE [au]**						
CCSD(T)	4.75	4.57	4.17	3.72	3.29	2.66	2.28	-0.01	-0.02	-0.05	-0.09	-0.14	-0.30	-0.46
CCSD	4.61	4.45	4.07	3.63	3.22	2.60	2.24	-0.01	-0.03	-0.05	-0.08	-0.13	-0.28	-0.45
MP2	4.57	4.40	4.02	3.59	3.19	2.58	2.22	-0.02	-0.03	-0.05	-0.09	-0.15	-0.30	-0.47
HF	4.52	4.35	3.98	3.56	3.16	2.54	2.19	-0.01	-0.02	-0.04	-0.07	-0.11	-0.23	-0.38
B2PLYP	5.02	4.72	4.33	3.89	3.47	2.83	2.46	-0.14	-0.02	-0.05	-0.09	-0.15	-0.30	-0.49
B3LYP	5.30	5.12	4.71	4.24	3.80	3.13	2.74	-0.01	-0.03	-0.07	-0.12	-0.19	-0.38	-0.60
B3PW91	5.25	5.08	4.68	4.22	3.78	3.11	2.73	-0.01	-0.02	-0.05	-0.10	-0.17	-0.36	-0.59
B97-2	5.21	5.03	4.63	4.17	3.73	3.07	2.69	-0.02	-0.03	-0.06	-0.10	-0.17	-0.35	-0.57
B97D	5.56	5.37	4.93	4.44	3.98	3.30	2.91	-0.01	-0.04	-0.07	-0.13	-0.21	-0.44	-0.69
BLYP	5.64	5.46	5.02	4.52	4.06	3.37	2.96	-0.01	-0.04	-0.08	-0.14	-0.23	-0.46	-0.72
BMK	5.00	4.89	4.54	4.02	3.58	2.93	2.51	-0.01	-0.03	-0.05	-0.09	-0.15	-0.33	-0.52
CAM-B3LYP	5.11	4.94	4.56	4.11	3.69	3.04	2.66	-0.01	-0.03	-0.07	-0.11	-0.18	-0.36	-0.57
HCTH	5.39	5.19	4.77	4.31	3.87	3.22	2.84	-0.03	-0.05	-0.08	-0.14	-0.20	-0.40	-0.63
HISS	5.03	4.86	4.46	4.01	3.58	2.93	2.55	-0.01	-0.03	-0.04	-0.08	-0.14	-0.31	-0.50
HSE06	5.28	5.10	4.68	4.21	3.76	3.09	2.70	-0.01	-0.03	-0.05	-0.10	-0.16	-0.35	-0.56
LC-BLYP	4.92	4.76	4.40	3.98	3.58	2.96	2.60	-0.02	-0.03	-0.06	-0.11	-0.18	-0.35	-0.55
LC-HCTH	4.91	4.71	4.32	3.89	3.48	2.86	2.50	-0.03	-0.04	-0.08	-0.13	-0.18	-0.32	-0.50
LC-REVTPSS	4.86	4.70	4.34	3.92	3.52	2.89	2.53	-0.02	-0.02	-0.04	-0.09	-0.16	-0.32	-0.53
LC-τHCTH	5.24	5.02	4.55	4.06	3.61	2.94	2.56	-0.03	-0.05	-0.07	-0.12	-0.17	-0.33	-0.52
LSDA	5.91	5.70	5.24	4.71	4.22	3.49	3.05	-0.01	-0.03	-0.07	-0.12	-0.20	-0.42	-0.66
M06	5.45	5.28	4.84	4.33	3.88	3.21	2.81	0.02	-0.03	-0.07	-0.11	-0.19	-0.39	-0.63
M06-2X	5.11	4.93	4.52	4.05	3.61	2.93	2.55	-0.02	-0.03	-0.06	-0.09	-0.16	-0.32	-0.52
M06-HF	5.34	5.14	4.69	4.15	3.61	2.82	2.38	-0.06	-0.04	-0.04	-0.08	-0.13	-0.30	-0.48
M06L	5.51	5.33	4.90	4.38	3.92	3.26	2.89	0.09	0.06	0.02	-0.03	-0.14	-0.38	-0.66
M11	5.02	4.85	4.44	3.96	3.52	2.90	2.58	-0.01	-0.03	-0.08	-0.12	-0.19	-0.40	-0.62
M11-L	5.92	5.71	5.19	4.57	4.01	3.15	2.63	0.07	0.00	-0.09	-0.16	-0.26	-0.47	-0.69
MN12-L	5.06	4.90	4.47	3.98	3.54	2.89	2.52	0.07	0.00	-0.06	-0.11	-0.18	-0.35	-0.55
MN12-SX	5.16	5.00	4.58	4.08	3.63	2.95	2.55	0.06	-0.01	-0.08	-0.12	-0.20	-0.38	-0.57
MPW1PW91	5.21	5.04	4.64	4.18	3.74	3.08	2.69	-0.02	-0.03	-0.06	-0.10	-0.16	-0.35	-0.56
N12	5.48	5.34	4.95	4.48	4.02	3.33	2.92	-0.01	-0.04	-0.08	-0.13	-0.20	-0.40	-0.63
N12-SX	5.15	4.99	4.60	4.15	3.72	3.07	2.70	-0.01	-0.03	-0.06	-0.10	-0.16	-0.34	-0.55
PBE	5.68	5.49	5.05	4.55	4.08	3.38	2.97	-0.01	-0.04	-0.07	-0.13	-0.21	-0.43	-0.68
PBE0	5.24	5.06	4.66	4.19	3.75	3.08	2.69	-0.02	-0.03	-0.06	-0.10	-0.16	-0.34	-0.55
REVTPSS	5.45	5.26	4.83	4.33	3.87	3.18	2.77	-0.01	-0.03	-0.06	-0.11	-0.19	-0.41	-0.65
SOGGA11-X	5.11	4.93	4.51	4.04	3.60	2.96	2.58	-0.03	-0.05	-0.07	-0.10	-0.16	-0.34	-0.53
τHCTH	5.66	5.46	5.00	4.49	4.02	3.32	2.92	-0.02	-0.04	-0.06	-0.11	-0.19	-0.42	-0.68
τHCTHHYB	5.44	5.26	4.85	4.35	3.89	3.20	2.78	-0.01	-0.02	-0.06	-0.10	-0.17	-0.38	-0.60
TPSSH	5.36	5.18	4.77	4.29	3.84	3.15	2.75	-0.01	-0.03	-0.06	-0.10	-0.18	-0.37	
ωB97	5.07	4.89	4.49	4.03	3.60	2.96	2.59	-0.01	-0.02	-0.06	-0.10	-0.17	-0.36	-0.57
ωB97X	5.06	4.88	4.47	4.02	3.60	2.96	2.59	-0.01	-0.03	-0.05	-0.10	-0.17	-0.35	-0.56
ωB97X-D	5.08	4.90	4.51	4.07	3.65	3.00	2.62	-0.01	-0.02	-0.05	-0.10	-0.18	-0.36	-0.57

Table S16: The values of first hyperpolarizability (β_{zzz}) and **% error** computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**first hyperpolarizability (β_{zzz}) [au]**							**% error**						
CCSD(T)	-15.0	-14.7	-13.8	-12.6	-11.4	-9.5	-7.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	-14.5	-14.3	-13.4	-12.3	-11.1	-9.2	-7.5	-3.0	-2.9	-2.5	-2.4	-2.5	-2.7	-2.7
MP2	-14.0	-13.8	-13.0	-11.9	-10.9	-9.1	-7.5	-6.7	-6.4	-5.9	-5.4	-5.0	-4.1	-3.6
HF	-14.1	-13.9	-13.0	-11.8	-10.6	-8.5	-6.8	-5.6	-5.6	-5.4	-5.9	-7.2	-10.2	-12.0
B2PLYP	-14.8	-14.7	-13.9	-12.7	-11.7	-10.0	-8.3	-0.9	-0.3	0.7	1.4	2.5	5.3	6.7
B3LYP	-17.0	-16.8	-15.9	-14.8	-13.9	-12.5	-10.6	13.4	14.1	15.4	17.4	21.5	31.8	37.1
B3PW91	-16.1	-15.9	-15.1	-14.1	-13.3	-12.0	-10.2	7.5	8.1	9.6	11.9	16.0	26.4	31.9
B97-2	-16.0	-15.9	-14.9	-13.8	-12.9	-11.6	-9.9	6.5	7.8	8.0	9.8	12.7	22.4	27.3
B97D	-19.0	-18.9	-17.8	-16.4	-15.5	-14.5	-12.5	27.0	28.3	28.9	30.6	35.7	52.9	61.6
BLYP	-20.7	-20.4	-19.2	-17.9	-17.0	-15.9	-13.7	38.3	38.4	39.3	42.2	49.0	67.3	76.4
BMK	-13.0	-10.0	-17.8	-12.8	-14.8	-9.9	-9.7	-13.1	-31.7	29.2	1.7	29.9	4.8	25.2
CAM-B3LYP	-14.4	-14.4	-13.8	-12.8	-12.0	-10.7	-9.1	-3.6	-2.2	-0.1	1.9	4.9	12.9	17.6
HCTH	-19.3	-19.1	-17.6	-16.0	-15.0	-14.0	-12.0	28.6	29.7	28.0	27.2	31.5	47.8	55.3
HISS	-13.8	-13.6	-12.8	-11.9	-11.1	-9.7	-8.2	-8.2	-7.7	-6.8	-5.4	-3.2	2.2	5.4
HSE06	-16.0	-15.8	-14.9	-13.8	-12.9	-11.6	-9.8	6.7	7.3	8.1	9.7	13.2	22.1	26.7
LC-BLYP	-11.7	-11.7	-11.4	-10.6	-9.9	-8.8	-7.5	-22.1	-20.2	-17.6	-15.5	-13.1	-7.1	-2.8
LC-HCTH	-12.6	-12.8	-11.4	-10.5	-9.8	-8.8	-7.4	-16.2	-13.2	-17.3	-16.3	-14.6	-7.4	-4.3
LC-revTPSS	-11.5	-11.5	-11.1	-10.4	-9.7	-8.6	-7.4	-23.5	-21.9	-19.3	-17.2	-14.8	-9.2	-4.9
LC-τHCTH	-12.2	-12.1	-11.2	-10.9	-10.1	-9.2	-7.7	-18.8	-17.7	-18.7	-13.5	-11.4	-2.6	-0.4
LSDA	-19.2	-18.8	-17.6	-16.5	-15.8	-14.7	-12.7	28.1	27.6	28.0	31.1	38.1	55.5	63.8
M06	-14.4	-14.1	-13.4	-13.0	-11.9	-10.8	-9.1	-4.2	-4.1	-2.8	3.3	3.8	13.8	17.6
M06-2X	-14.6	-14.5	-13.5	-12.7	-11.5	-9.9	-8.1	-2.3	-1.3	-2.0	1.3	1.0	4.3	4.9
M06-HF	-15.6	-15.1	-12.8	-12.5	-10.2	-8.4	-7.0	3.9	2.4	-7.1	-0.6	-11.0	-11.3	-9.9
M06L	-16.3	-16.2	-16.4	-15.8	-15.1	-13.0	-11.1	8.8	9.9	19.2	25.9	32.4	37.3	43.7
M11	-13.1	-12.7	-12.0	-11.0	-10.2	-8.9	-7.6	-12.9	-13.6	-13.1	-12.3	-10.9	-6.5	-1.7
M11-L	-18.8	-18.5	-17.8	-16.6	-15.3	-13.2	-11.2	25.3	25.5	29.0	32.1	33.9	38.8	44.3
MN12-L	-20.6	-20.0	-18.8	-17.3	-16.1	-13.9	-11.6	37.6	35.6	36.4	38.1	40.6	46.1	49.6
MN12-SX	-18.6	-18.0	-17.0	-15.7	-14.5	-12.5	-10.5	24.0	22.0	23.2	25.1	27.1	31.8	36.0
mPW1PW91	-15.6	-15.5	-14.7	-13.6	-12.7	-11.4	-9.7	4.4	5.1	6.5	8.4	11.6	19.8	24.7
N12	-19.2	-18.3	-17.4	-16.5	-15.8	-14.3	-12.0	27.8	24.5	26.1	31.5	37.9	50.9	54.4
N12-SX	-15.9	-15.8	-14.9	-14.0	-12.9	-11.6	-9.6	6.3	7.5	8.0	11.1	12.8	22.0	24.4
PBE	-19.6	-19.2	-18.1	-16.8	-16.0	-15.0	-12.9	30.6	30.7	31.2	33.8	40.3	57.9	67.2
PBE0	-15.7	-15.6	-14.7	-13.6	-12.7	-11.4	-9.7	5.1	5.7	6.8	8.4	11.6	20.2	25.1
revTPSS	-19.6	-19.3	-18.2	-17.0	-16.1	-14.8	-12.7	31.0	31.2	32.3	35.2	41.1	56.3	64.6
SOGGA11-X	-15.0	-14.8	-14.0	-12.9	-11.9	-10.3	-8.7	-0.1	0.3	1.3	2.5	4.2	9.1	12.8
τHCTH	-18.9	-18.7	-17.4	-15.9	-15.1	-14.1	-12.2	26.0	27.3	26.5	26.6	32.0	48.8	58.1
τHCTHHYB	-17.0	-16.3	-16.0	-14.6	-14.2	-12.5	-10.9	13.2	11.1	16.5	16.3	24.6	31.6	40.6
TPSSH	-18.1	-17.8	-16.8	-15.6	-14.7	-13.4	-11.4	20.8	21.1	22.1	24.1	28.5	40.8	47.5
ωB97	-10.9	-11.2	-11.0	-10.4	-10.5	-9.2	-7.9	-27.2	-23.8	-19.9	-17.0	-8.5	-3.4	1.4
ωB97X	-12.8	-12.2	-11.5	-11.2	-10.9	-9.7	-8.1	-21.3	-17.0	-16.3	-10.9	-4.6	2.3	5.0
ωB97X-D	-13.6	-13.0	-12.0	-12.0	-11.6	-10.4	-8.6	-14.9	-11.7	-12.6	-4.5	1.8	10.1	11.5

Table S17: The values of first hyperpolarizability (β_{zzz}) and **% error** computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**first hyperpolarizability (β_{zzz}) [au]**							**% error**						
CCSD(T)	27.9	25.9	23.5	21.6	20.1	18.4	17.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	30.5	28.5	25.8	23.5	21.7	19.5	17.8	9.4	9.9	9.9	9.2	8.2	5.9	4.2
MP2	39.6	36.6	32.3	28.6	25.8	22.1	19.6	41.7	41.1	37.5	32.8	28.3	20.4	14.9
HF	11.3	11.8	12.4	12.3	11.9	11.3	10.7	-59.4	-54.5	-47.2	-43.0	-40.7	-38.6	-37.3
B2PLYP	24.6	24.2	23.6	22.5	21.3	19.3	17.5	-11.8	-6.6	0.4	4.4	6.1	5.0	2.7
B3LYP	34.2	33.2	31.9	30.6	29.3	26.8	24.2	22.4	27.8	35.7	41.9	45.6	45.6	41.6
B3PW91	34.9	33.6	32.0	30.6	29.2	26.7	24.1	25.1	29.5	36.2	41.9	45.4	45.4	41.4
B97-2	31.8	30.7	30.0	29.1	28.0	25.8	23.3	13.9	18.4	27.4	34.8	39.2	40.2	36.7
B97D	35.4	33.9	33.7	33.9	33.3	31.4	28.4	26.8	30.7	43.4	57.2	65.9	70.8	66.7
BLYP	37.4	36.1	35.2	34.8	34.1	32.1	29.3	33.8	39.3	49.8	61.2	69.5	74.6	71.7
BMK	49.5	46.6	21.5	16.8	17.5	18.9	21.6	77.5	79.8	-8.7	-22.0	-12.8	2.6	26.8
CAM-B3LYP	36.8	35.0	32.6	30.3	28.3	25.1	22.4	31.8	35.0	38.8	40.7	40.8	36.6	31.4
HCTH	26.2	26.4	28.4	30.0	30.2	29.4	27.3	-6.2	1.7	20.8	39.2	50.1	60.1	59.7
HISS	27.8	27.3	26.6	25.5	24.3	22.1	20.0	-0.4	5.2	13.0	18.2	21.0	20.4	17.3
HSE06	31.7	30.9	29.9	28.8	27.6	25.3	22.9	13.5	19.2	27.2	33.5	37.4	37.9	34.5
LC-BLYP	36.4	34.5	31.7	29.1	26.8	23.3	20.7	30.4	32.8	35.0	35.0	33.3	27.0	21.3
LC-HCTH	28.3	28.6	29.4	27.3	24.9	21.7	19.4	1.3	10.1	24.9	26.6	23.7	18.0	13.8
LC-REVTPSS	34.8	32.9	30.1	27.6	25.4	22.2	19.8	24.8	26.7	28.0	27.8	26.5	20.9	15.8
LC-τHCTH	36.0	35.2	32.8	29.1	25.8	22.1	19.6	29.0	35.7	39.4	34.8	28.6	20.3	14.6
LSDA	38.5	37.3	36.4	35.6	34.7	32.4	29.3	37.8	43.9	54.8	65.2	72.7	76.4	71.5
M06	53.8	48.7	43.6	40.3	37.9	34.6	29.9	92.9	87.8	85.5	87.0	88.8	88.3	75.0
M06-2X	33.1	32.2	30.9	28.8	26.5	23.1	20.7	18.6	24.2	31.4	33.3	32.0	25.4	21.6
M06-HF	51.9	52.8	49.3	40.4	31.1	18.4	12.5	85.9	103.5	109.9	87.2	54.9	0.3	-26.7
M06L	61.4	54.1	43.8	36.7	33.8	33.0	32.0	120.0	108.6	86.3	70.3	68.0	79.3	87.7
M11	26.1	24.8	23.1	21.2	19.2	16.7	16.9	-6.5	-4.5	-1.9	-1.6	-4.2	-9.3	-0.8
M11-L	36.6	34.1	34.5	35.7	35.3	31.4	26.7	31.2	31.6	46.7	65.4	75.9	70.7	56.3
MN12-L	23.6	19.8	18.8	19.8	21.2	23.0	22.8	-15.5	-23.5	-20.2	-8.0	5.5	25.2	33.9
MN12-SX	24.0	22.5	23.4	25.0	25.8	25.5	24.0	-13.9	-13.4	-0.5	15.8	28.2	38.8	40.7
MPW1PW91	33.0	31.5	30.2	29.0	27.8	25.4	22.9	18.2	21.6	28.6	34.6	38.4	38.2	34.5
N12	40.0	36.2	34.8	36.0	35.0	32.2	29.0	43.2	39.7	48.0	67.1	74.4	75.4	69.8
N12-SX	35.6	33.7	32.1	30.8	29.5	27.0	24.3	27.4	29.9	36.3	42.9	47.0	47.1	42.3
PBE	36.0	34.8	34.2	33.9	33.4	31.6	29.0	29.0	34.3	45.3	57.1	66.1	72.1	69.9
PBE0	32.0	31.1	30.0	28.8	27.6	25.3	22.9	14.8	19.8	27.5	33.6	37.3	37.4	33.9
REVTPSS	31.5	30.2	29.3	28.8	28.4	27.0	24.8	12.8	16.5	24.4	33.6	41.2	46.8	45.5
SOGGA11-X	25.1	23.4	23.2	23.1	22.6	21.4	19.7	-10.2	-9.7	-1.4	7.0	12.5	16.2	15.6
τHCTH	30.4	30.8	32.1	32.9	32.6	30.8	28.0	9.0	18.8	36.6	52.6	62.5	67.8	64.1
τHCTHHYB	37.0	36.2	32.7	30.6	29.5	27.4	25.3	32.4	39.5	39.2	41.7	46.9	48.9	48.2
TPSSH	31.7	30.8	29.9	29.2	28.4	26.5	24.1	13.5	18.6	27.1	35.3	41.3	44.3	41.4
ωB97	42.0	38.1	34.1	29.5	26.5	23.4	21.8	50.6	47.0	44.9	36.6	32.1	27.2	27.9
ωB97X	40.7	37.1	34.5	30.1	27.0	23.7	21.8	45.6	42.8	46.7	39.4	34.1	28.8	28.0
ωB97X-D	39.6	35.4	34.7	30.6	27.5	24.3	22.6	41.8	36.5	47.6	41.9	36.8	31.9	32.3

Table S18: The values of interaction-induced first hyperpolarizability ($\Delta\beta_{zzz}$) and **% error** computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The values of $\Delta\beta_{zzz}$ were corrected according to the Boys and Bernardi counterpoise scheme. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**interaction-induced first hyperpolarizability ($\Delta\beta_{zzz}$) [au]**							**% error**						
CCSD(T)	4.7	4.4	3.8	3.2	2.6	1.7	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	4.4	4.2	3.6	3.1	2.6	1.7	1.3	-6.4	-5.3	-4.2	-2.5	-1.5	1.2	1.5
MP2	4.8	4.4	3.8	3.2	2.6	1.6	1.3	1.7	0.9	-0.3	0.0	-1.5	-1.2	-3.1
HF	3.7	3.5	3.1	2.7	2.3	1.6	1.2	-20.9	-19.4	-17.4	-14.5	-12.2	-4.2	-4.6
B2PLYP	4.2	4.0	3.4	2.8	2.2	1.1	0.7	-10.0	-9.8	-10.3	-11.3	-17.9	-36.7	-48.5
B3LYP	3.9	3.6	2.9	2.2	1.2	-0.4	-0.6	-16.2	-17.8	-22.6	-32.1	-53.6	-121.1	-146.9
B3PW91	4.3	4.0	3.3	2.5	1.6	0.0	-0.4	-7.7	-8.9	-13.2	-20.8	-39.5	-102.4	-127.7
B97-2	4.3	3.9	3.4	2.6	1.7	0.1	-0.2	-8.3	-12.1	-11.8	-18.6	-33.8	-92.8	-114.6
B97D	3.6	3.0	2.3	1.6	0.5	-1.6	-1.8	-24.0	-31.3	-38.7	-50.6	-80.6	-197.6	-238.5
BLYP	2.4	2.1	1.5	0.6	-0.6	-2.6	-2.6	-48.1	-51.8	-61.1	-81.4	-121.7	-254.8	-298.5
BMK	5.7	8.3	-0.3	3.5	-0.1	1.6	-0.3	20.2	89.7	-108.9	9.1	-104.6	-1.8	-125.4
CAM-B3LYP	5.1	4.7	4.0	3.2	2.3	0.8	0.4	8.3	7.3	4.7	0.9	-11.0	-50.6	-70.8
HCTH	3.4	2.9	2.3	1.6	0.5	-1.5	-1.6	-27.2	-34.7	-40.8	-50.9	-80.6	-192.8	-222.3
HISS	4.5	4.2	3.7	3.0	2.3	1.0	0.6	-4.0	-3.7	-3.7	-5.0	-12.9	-39.2	-53.1
HSE06	4.2	3.8	3.2	2.5	1.6	0.1	-0.2	-11.5	-12.8	-15.5	-22.0	-39.5	-95.2	-116.2
LC-BLYP	5.7	5.3	4.6	3.9	3.1	1.7	1.2	21.3	21.2	21.6	22.3	18.6	4.2	-10.0
LC-HCTH	5.6	4.9	4.7	3.8	3.1	1.7	1.3	18.9	10.7	24.5	20.4	16.0	2.4	-3.8
LC-revTPSS	5.6	5.2	4.6	3.9	3.1	1.8	1.2	18.3	19.2	20.3	21.7	18.6	7.8	-9.2
LC-τHCTH	5.4	5.0	4.7	3.7	3.1	1.7	1.2	14.7	13.9	22.9	14.8	17.9	-0.6	-10.0
LSDA	3.3	2.9	2.1	1.2	0.0	-2.0	-2.1	-30.2	-33.8	-43.7	-61.9	-99.6	-219.3	-261.5
M06	5.8	5.3	4.3	3.0	2.5	0.5	0.1	23.0	20.5	12.1	-5.0	-5.3	-70.5	-93.1
M06-2X	4.4	4.1	3.8	2.9	2.5	1.2	1.0	-5.5	-7.1	-0.5	-8.8	-4.9	-25.9	-20.8
M06-HF	3.2	3.2	4.1	2.7	3.3	2.1	1.6	-32.6	-27.4	8.7	-16.4	25.5	25.3	22.3
M06L	5.2	5.0	4.0	3.4	2.0	-0.4	-1.0	10.9	14.8	5.3	6.9	-25.9	-124.7	-175.4
M11	5.8	5.5	4.9	4.2	3.4	1.8	1.0	22.3	25.3	29.5	32.1	27.8	7.2	-20.8
M11-L	3.9	3.8	3.5	2.7	1.6	-0.5	-1.0	-17.2	-13.5	-8.7	-15.7	-41.1	-131.9	-180.0
MN12-L	4.4	4.2	3.3	2.4	1.4	-0.4	-0.8	-6.8	-4.6	-12.6	-23.9	-47.9	-122.3	-163.1
MN12-SX	4.1	4.0	3.3	2.5	1.6	0.1	-0.4	-13.2	-9.1	-13.4	-21.7	-38.0	-94.6	-128.5
mPW1PW91	4.3	4.0	3.4	2.6	1.8	0.3	-0.1	-8.1	-8.2	-11.1	-17.6	-32.7	-84.3	-106.9
N12	3.6	3.7	2.9	1.5	0.2	-1.5	-1.4	-22.8	-14.6	-24.5	-52.8	-91.6	-192.2	-210.8
N12-SX	4.5	4.1	3.6	2.7	2.0	0.3	0.1	-3.8	-5.5	-5.5	-14.8	-24.0	-80.1	-88.5
PBE	3.0	2.6	1.9	1.1	-0.1	-2.1	-2.2	-36.8	-40.2	-49.2	-66.7	-103.8	-225.9	-269.2
PBE0	4.3	4.0	3.3	2.6	1.7	0.2	-0.1	-8.7	-9.8	-12.9	-18.9	-35.0	-87.3	-109.2
revTPSS	2.8	2.5	1.8	1.0	-0.1	-1.9	-2.1	-39.8	-43.2	-51.8	-68.6	-102.7	-215.7	-258.5
SOGGA11-X	4.6	4.1	3.4	2.7	1.9	0.6	0.3	-3.2	-5.5		-15.1	-29.3	-61.4	-78.5
τHCTH	3.4	2.8	2.3	1.7	0.6	-1.5	-1.8	-27.4	-35.6	-39.7	-46.2	-78.3	-192.8	-240.8
τHCTHHYB	4.1	4.1	2.8	2.3	0.9	-0.3	-0.8	-12.3	-5.7	-25.5	-27.0	-66.5	-119.9	-163.1
TPSSH	3.5	3.2	2.5	1.8	0.8	-0.9	-1.2	-25.5	-27.6	-33.2	-44.7	-70.3	-156.0	-189.2
ωB97	6.7	6.1	5.3	4.5	3.0	1.7	1.1	43.2	39.5	38.7	40.6	14.4	3.6	-13.1
ωB97X	6.8	5.9	5.5	4.3	3.0	1.5	1.1	43.6	35.6	43.4	34.6	15.6	-10.2	-18.5
ωB97X-D	7.0	6.1	5.7	4.1	2.7	1.0	0.8	47.9	38.4	49.5	27.4	4.2	-37.3	-40.0

Table S19: The values of interaction-induced first hyperpolarizability ($\Delta\beta_{zzz}$) and **% error** computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. The values of $\Delta\beta_{zzz}$ were corrected according to the Boys and Bernardi counterpoise scheme. The **% error** was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**interaction-induced first hyperpolarizability ($\Delta\beta_{zzz}$) [au]**							**% error**						
CCSD(T)	38.3	36.1	32.3	27.8	23.6	16.7	11.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CCSD	36.3	34.4	30.9	26.7	22.8	16.2	11.4	-5.2	-4.7	-4.2	-3.7	-3.3	-2.8	-2.5
MP2	38.1	36.0	32.1	27.7	23.5	16.6	11.6	-0.5	-0.1	-0.5	0.0	-0.3	-0.3	-0.9
HF	24.2	23.0	21.1	18.7	16.2	11.9	8.6	-36.9	-36.1	-34.7	-32.6	-31.3	-28.9	-26.6
B2PLYP	34.9	33.5	30.8	27.5	23.9	17.5	12.4	-8.9	-7.1	-4.5	-0.9	1.5	5.0	5.9
B3LYP	45.7	44.1	40.9	36.8	34.6	23.7	16.2	19.2	22.3	26.9	32.7	46.8	42.0	38.8
B3PW91	46.8	45.1	41.7	37.4	34.2	24.0	16.5	22.2	25.1	29.2	34.7	45.0	44.1	41.4
B97-2	45.0	43.4	40.5	36.6	32.7	23.7	16.4	17.5	20.4	25.6	32.0	38.8	42.1	40.1
B97D	52.5	50.7	48.0	44.3	39.7	28.9	19.2	37.1	40.5	48.9	59.5	68.3	73.5	63.8
BLYP	53.0	51.4	48.3	44.1	41.4	28.6	18.8	38.2	42.6	49.8	58.8	75.3	71.4	60.6
BMK	49.2	48.6	25.3	20.5	22.0	15.4	14.2	28.4	34.7	-21.5	-26.2	-6.8	-7.7	21.1
CAM-B3LYP	41.6	40.1	37.0	33.1	33.2	21.3	14.9	8.6	11.1	14.7	19.3	40.5	27.7	27.6
HCTH	48.7	47.7	46.2	43.3	36.4	28.7	19.3	27.1	32.2	43.1	56.0	54.1	72.1	65.3
HISS	38.6	37.3	34.4	30.7	28.1	19.8	14.1	0.8	3.4	6.5	10.8	19.1	19.0	20.6
HSE06	44.7	43.2	39.9	35.8	32.3	23.1	16.1	16.6	19.7	23.7	29.1	36.9	38.6	37.5
LC-BLYP	36.3	35.0	32.4	29.0	31.1	18.9	13.6	-5.3	-2.9	0.3	4.5	31.8	13.3	16.2
LC-HCTH	31.5	31.3	31.0	28.2	29.3	18.3	13.2	-17.7	-13.3	-3.8	1.6	24.1	9.5	13.0
LC-REVTPSS	36.2	34.8	32.0	28.5	29.3	18.3	13.0	-5.6	-3.5	-0.9	2.6	24.1	9.7	11.5
LC-τHCTH	33.9	33.1	31.3	28.2	30.5	18.5	13.4	-11.6	-8.2	-3.1	1.6	29.1	10.8	14.3
LSDA	53.4	52.1	49.0	44.7	40.9	29.7	20.3	39.4	44.5	51.9	61.2	73.3	77.9	73.8
M06	56.2	52.7	48.1	43.6	42.4	29.3	19.0	46.7	46.2	49.0	57.2	79.9	75.5	62.0
M06-2X	38.3	37.0	34.3	30.3	30.7	18.9	13.2	-0.1	2.6	6.3	9.2	30.0	13.6	12.6
M06-HF	43.0	42.4	38.4	30.8	34.0	15.0	8.8	12.1	17.5	19.1	11.1	44.3	-10.3	-24.7
M06L	58.3	55.8	50.0	44.4	38.2	30.5	21.5	52.2	54.6	54.9	60.0	61.8	82.9	83.5
M11	37.8	36.4	32.9	29.0	22.9	18.2	13.8	-1.4	0.9	2.0	4.6	-3.1	9.3	18.2
M11-L	54.4	53.1	50.4	46.3	40.5	28.5	17.1	41.8	47.3	56.1	66.8	71.6	71.0	46.0
MN12-L	40.7	37.4	34.3	31.9	24.6	22.7	15.6	6.2	3.8	6.2	14.9	4.1	36.1	32.9
MN12-SX	39.4	37.1	34.6	32.0	29.3	22.1	15.3	2.8	2.8	7.3	15.5	24.4	32.8	30.6
MPW1PW91	45.0	43.2	40.0	35.8	32.4	23.1	16.1	17.5	19.9	23.8	29.0	37.3	38.5	37.9
N12	56.6	52.3	47.8	44.6	41.3	28.3	19.3	47.7	45.0	48.3	60.8	75.0	69.9	64.5
N12-SX	44.3	42.5	39.5	35.7	34.3	23.5	16.6	15.7	17.9	22.3	28.6	45.2	40.8	41.5
PBE	53.9	52.3	49.1	44.8	39.9	29.4	19.8	40.6	45.0	52.1	61.3	69.3	76.2	69.2
PBE0	44.7	43.1	39.9	35.8	32.3	23.1	16.1	16.6	19.5	23.5	29.0	36.8	38.5	37.7
REVTPSS	47.6	45.9	42.5	38.3	34.1	24.5	16.1	24.3	27.2	31.7	38.2	44.6	47.0	37.6
SOGGA11-X	40.1	37.8	34.5	30.9	26.6	20.3	14.3	4.6	4.7	6.8	11.5	12.9	21.5	22.5
τHCTH	52.3	50.9	48.1	44.1	38.5	28.6	19.2	36.6	41.1	49.1	58.8	63.3	71.6	63.7
τHCTHHYB	50.1	48.6	42.8	37.4	34.5	24.2	17.1	30.7	34.8	32.6	34.8	46.3	45.1	46.2
TPSSH	46.9	45.3	41.9	37.7	33.5	24.2	16.4	22.5	25.5	29.9	35.9	41.9	45.4	40.2
ωB97	39.1	36.9	34.3	29.6	31.1	19.0	14.2	2.0	2.2	6.2	6.7	31.8	13.7	21.4
ωB97X	39.6	37.3	35.9	31.3	31.5	19.9	14.6	3.2	3.5	11.3	12.9	33.7	19.1	24.8
ωB97X-D	44.5	39.5	39.0	33.7	32.1	20.8	15.3	16.0	9.4	20.8	21.6	36.2	24.9	30.4

Table S20: The values of uncorrected interaction-induced first hyperpolarizability and basis set superposition error (BSSE) computed for the HF$\cdots$HF complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**uncorrected interaction-induced first hyperpolarizability [au]**							**BSSE [au]**						
CCSD(T)	5.7	5.2	4.4	3.8	3.4	2.6	2.2	-1.0	-0.8	-0.6	-0.6	-0.8	-0.9	-0.9
CCSD	5.3	4.9	4.3	3.7	3.3	2.6	2.2	-0.9	-0.7	-0.7	-0.6	-0.7	-0.9	-0.9
MP2	5.6	5.3	4.5	3.9	3.4	2.6	2.2	-0.8	-0.9	-0.7	-0.7	-0.8	-1.0	-0.9
HF	4.2	4.0	3.6	3.2	2.9	2.4	2.0	-0.5	-0.5	-0.5	-0.5	-0.6	-0.8	-0.8
B2PLYP	5.1	4.8	4.2	3.7	2.9	2.0	1.6	-0.9	-0.8	-0.8	-0.9	-0.7	-0.9	-0.9
B3LYP	5.1	4.8	3.9	2.3	2.2	0.7	0.4	-1.2	-1.2	-1.0	-0.1	-1.0	-1.1	-1.0
B3PW91	5.2	4.9	4.1	3.3	2.5	1.0	0.7	-0.9	-0.9	-0.8	-0.8	-0.9	-1.0	-1.1
B97-2	5.3	4.9	4.2	3.4	2.6	1.1	0.8	-1.0	-1.0	-0.8	-0.8	-0.9	-1.0	-1.0
B97D	4.8	4.3	3.4	2.5	1.8	-0.6	-0.8	-1.2	-1.3	-1.1	-0.9	-1.3	-1.0	-1.0
BLYP	3.9	3.6	2.7	1.6	0.4	-1.4	-1.5	-1.5	-1.5	-1.2	-1.0	-1.0	-1.2	-1.1
BMK	6.2	8.9	0.3	4.2	1.0	3.1	0.8	-0.5	-0.6	-0.6	-0.7	-1.1	-1.5	-1.1
CAM-B3LYP	6.3	5.9	5.0	4.1	3.2	1.9	1.4	-1.2	-1.2	-1.0	-0.9	-0.9	-1.1	-1.0
HCTH	5.4	4.7	3.6	2.5	1.2	-0.5	-0.6	-2.0	-1.8	-1.3	-0.9	-0.7	-1.0	-1.0
HISS	5.3	5.0	4.4	3.8	3.1	2.0	1.6	-0.8	-0.8	-0.7	-0.8	-0.8	-1.0	-1.0
HSE06	5.2	4.9	4.1	3.3	2.4	1.1	0.8	-1.0	-1.1	-0.9	-0.8	-0.8	-1.0	-1.0
LC-BLYP	6.9	6.5	5.7	4.9	4.1	2.9	2.3	-1.2	-1.2	-1.1	-1.0	-1.0	-1.2	-1.1
LC-HCTH	7.2	6.3	5.8	4.8	4.0	2.8	2.5	-1.6	-1.4	-1.1	-1.0	-0.9	-1.1	-1.2
LC-revTPSS	6.5	6.2	5.4	4.7	4.1	2.9	2.3	-0.9	-1.0	-0.8	-0.8	-1.0	-1.1	-1.1
LC-τHCTH	6.3	5.9	5.6	4.7	4.2	3.1	2.6	-0.9	-0.9	-0.9	-1.0	-1.1	-1.4	-1.4
LSDA	4.5	4.2	3.2	2.2	1.0	-0.7	-0.9	-1.2	-1.3	-1.1	-1.0	-1.0	-1.3	-1.2
M06	5.9	5.7	5.0	3.7	3.2	1.4	0.9	-0.1	-0.4	-0.7	-0.7	-0.7	-0.9	-0.8
M06-2X	5.1	4.7	4.4	3.6	3.4	2.5	2.1	-0.7	-0.6	-0.6	-0.7	-0.9	-1.3	-1.1
M06-HF	4.6	4.5	5.0	3.6	6.0	2.8	2.5	-1.4	-1.3	-0.9	-0.9	-2.7	-0.7	-0.9
M06L	5.8	5.7	4.6	3.8	2.7	1.0	-0.1	-0.6	-0.7	-0.6	-0.4	-0.7	-1.4	-0.9
M11	6.3	6.2	5.7	5.0	4.3	3.0	2.2	-0.5	-0.7	-0.8	-0.8	-0.9	-1.2	-1.2
M11-L	4.5	4.4	3.7	2.9	1.0	-0.1	-0.8	-0.6	-0.6	-0.2	-0.2	0.6	-0.4	-0.2
MN12-L	4.5	4.4	3.5	2.6	1.7	0.1	-0.4	-0.1	-0.2	-0.2	-0.2	-0.3	-0.5	-0.4
MN12-SX	4.3	4.3	3.6	2.8	2.1	1.5	0.1	-0.2	-0.3	-0.3	-0.3	-0.5	-1.4	-0.5
mPW1PW91	5.3	5.0	4.2	3.4	2.6	1.3	0.9	-1.0	-1.0	-0.8	-0.8	-0.8	-1.0	-1.0
N12	4.8	5.0	3.9	2.3	1.0	-0.6	-0.5	-1.2	-1.3	-1.0	-0.8	-0.8	-0.9	-0.9
N12-SX	5.4	5.1	4.4	3.5	2.6	1.4	1.1	-0.9	-1.0	-0.8	-0.8	-0.6	-1.1	-1.0
PBE	4.4	4.1	3.1	2.0	0.9	-1.0	-1.1	-1.4	-1.5	-1.2	-0.9	-1.0	-1.1	-1.1
PBE0	5.3	5.0	4.2	3.4	2.6	1.2	0.9	-1.0	-1.0	-0.9	-0.8	-0.9	-1.0	-1.0
revTPSS	4.0	3.7	2.8	1.9	0.8	-0.9	-1.1	-1.2	-1.2	-1.0	-0.9	-0.9	-1.0	-1.0
SOGGA11-X	5.2	4.9	4.2	3.4	2.7	1.5	1.1	-0.6	-0.8	-0.8	-0.7	-0.8	-0.9	-0.8
τHCTH	4.9	4.3	3.4	2.6	1.4	-0.6	-0.9	-1.5	-1.5	-1.1	-0.9	-0.8	-0.9	-0.9
τHCTHHYB	5.2	5.2	3.7	3.1	1.7	0.7	0.2	-1.1	-1.1	-0.9	-0.8	-0.8	-1.0	-1.0
TPSSH	4.6	4.3	3.5	2.6	1.6	0.1	-0.2	-1.1	-1.1	-1.0	-0.8	-0.8	-1.0	-1.0
ωB97	7.6	7.0	6.1	5.4	4.1	2.9	2.3	-0.9	-0.9	-0.8	-0.9	-1.1	-1.2	-1.2
ωB97X	7.6	6.8	6.3	5.2	4.0	2.6	2.1	-0.8	-0.9	-0.8	-0.9	-1.0	-1.1	-1.0
ωB97X-D	7.7	6.9	6.5	4.9	3.7	2.2	1.7	-0.7	-0.8	-0.8	-0.8	-1.0	-1.2	-0.9

Table S21: The values of uncorrected interaction-induced first hyperpolarizability and basis set superposition error (BSSE) computed for the HCN$\cdots$HCN complex at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVQZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**uncorrected interaction-induced first hyperpolarizability [au]**							**BSSE [au]**						
CCSD(T)	39.1	37.3	34.0	30.9	28.2	23.2	19.6	-0.8	-1.2	-1.7	-3.1	-4.6	-6.5	-7.9
CCSD	37.0	35.5	32.6	29.7	27.2	22.5	18.7	-0.7	-1.1	-1.7	-3.0	-4.4	-6.3	-7.3
MP2	38.8	37.3	34.2	31.1	28.3	23.3	19.6	-0.7	-1.3	-2.1	-3.4	-4.8	-6.7	-8.0
HF	24.8	23.8	22.3	20.9	19.6	16.9	14.8	-0.6	-0.8	-1.2	-2.2	-3.4	-5.0	-6.2
B2PLYP	35.4	34.7	32.8	30.7	28.7	24.4	20.9	-0.5	-1.2	-2.0	-3.2	-4.7	-6.9	-8.5
B3LYP	46.7	45.8	43.8	41.3	38.6	32.6	24.1	-1.0	-1.7	-2.9	-4.5	-3.9	-8.9	-7.9
B3PW91	47.6	46.5	44.2	41.5	38.6	32.6	27.5	-0.8	-1.4	-2.5	-4.1	-4.4	-8.6	-11.0
B97-2	46.0	44.9	43.1	40.5	37.7	31.8	26.8	-1.0	-1.5	-2.6	-3.9	-4.9	-8.1	-10.4
B97D	53.8	52.8	51.4	49.3	46.2	39.1	32.5	-1.3	-2.1	-3.4	-5.0	-6.5	-10.2	-13.3
BLYP	54.3	53.9	52.3	49.9	47.0	39.7	33.1	-1.3	-2.5	-4.0	-5.8	-5.6	-11.1	-14.3
BMK	49.7	50.0	28.3	25.5	26.2	24.3	24.4	-0.5	-1.4	-3.0	-5.0	-4.2	-8.9	-10.2
CAM-B3LYP	42.6	41.7	39.7	37.3	34.8	29.7	25.4	-1.0	-1.6	-2.7	-4.2	-1.7	-8.4	-10.5
HCTH	51.4	50.9	49.9	48.1	45.2	38.2	31.7	-2.7	-3.2	-3.7	-4.8	-8.8	-9.5	-12.4
HISS	39.3	38.3	36.2	33.9	31.5	26.8	22.9	-0.7	-1.0	-1.8	-3.2	-3.4	-7.0	-8.8
HSE06	45.6	44.6	42.4	39.7	36.9	31.1	26.3	-0.9	-1.4	-2.5	-3.9	-4.6	-8.0	-10.2
LC-BLYP	37.1	36.4	34.7	32.8	30.8	26.7	23.2	-0.8	-1.4	-2.3	-3.8	0.3	-7.8	-9.6
LC-HCTH	33.9	33.5	33.1	31.4	29.7	25.8	22.2	-2.4	-2.2	-2.1	-3.2	-0.4	-7.5	-9.0
LC-REVTPSS	36.7	35.8	33.9	31.8	29.7	25.6	22.1	-0.5	-1.0	-1.9	-3.3	-0.5	-7.3	-9.1
LC-τHCTH	33.9	33.4	32.5	31.7	30.4	26.5	22.6	0.0	-0.3	-1.2	-3.5	0.1	-8.0	-9.2
LSDA	54.3	53.9	52.2	49.8	46.9	39.7	33.0	-0.9	-1.8	-3.2	-5.1	-6.0	-10.0	-12.7
M06	60.9	57.1	52.7	49.4	45.1	38.0	31.2	-4.7	-4.4	-4.6	-5.8	-2.6	-8.7	-12.2
M06-2X	38.4	37.6	36.0	33.7	31.2	26.4	22.7	-0.1	-0.6	-1.7	-3.4	-0.6	-7.5	-9.5
M06-HF	44.9	44.7	41.9	40.3	28.5	21.3	17.4	-1.9	-2.3	-3.5	-9.5	5.6	-6.3	-8.6
M06L	62.2	60.2	56.0	52.1	49.1	42.0	35.6	-3.9	-4.4	-6.0	-7.7	-11.0	-11.5	-14.1
M11	39.4	37.6	34.8	32.1	29.6	25.7	23.5	-1.6	-1.2	-1.9	-3.1	-6.8	-7.5	-9.7
M11-L	63.1	60.1	55.4	51.4	46.7	36.6	28.8	-8.7	-7.0	-5.0	-5.1	-6.3	-8.1	-11.7
MN12-L	47.2	43.8	39.6	36.9	34.4	29.4	25.2	-6.5	-6.4	-5.3	-5.0	-9.8	-6.7	-9.6
MN12-SX	45.7	42.7	39.2	36.6	34.2	29.2	25.1	-6.3	-5.6	-4.6	-4.6	-4.8	-7.1	-9.8
MPW1PW91	46.1	44.8	42.4	39.6	36.8	31.0	26.3	-1.1	-1.6	-2.4	-3.8	-4.4	-7.9	-10.2
N12	58.1	55.0	51.8	49.7	45.7	37.8	31.5	-1.5	-2.7	-4.0	-5.1	-4.4	-9.5	-12.2
N12-SX	44.7	43.8	41.9	39.6	37.1	31.6	26.7	-0.4	-1.3	-2.4	-3.9	-2.8	-8.1	-10.1
PBE	55.2	54.6	52.7	49.9	46.8	39.6	33.1	-1.3	-2.3	-3.6	-5.1	-6.9	-10.2	-13.3
PBE0	45.6	44.6	42.3	39.6	36.8	31.1	26.3	-0.9	-1.5	-2.4	-3.8	-4.6	-8.0	-10.2
REVTPSS	48.8	47.8	45.6	42.9	40.0	33.8	28.3	-1.2	-1.9	-3.1	-4.6	-5.9	-9.3	-12.2
SOGGA11-X	42.3	39.7	36.8	34.2	31.8	27.1	23.2	-2.2	-1.9	-2.3	-3.3	-5.1	-6.8	-8.9
τHCTH	53.8	53.0	51.4	48.6	45.2	38.0	31.7	-1.5	-2.1	-3.2	-4.5	-6.7	-9.4	-12.5
τHCTHHYB	51.2	50.3	45.5	41.5	38.6	32.8	28.3	-1.1	-1.7	-2.7	-4.1	-4.1	-8.6	-11.2
TPSSH	48.1	47.0	44.6	41.8	38.8	32.8	27.6	-1.2	-1.7	-2.7	-4.1	-5.4	-8.6	-11.2
ωB97	39.6	38.0	36.7	33.7	31.5	27.3	24.4	-0.5	-1.1	-2.4	-4.1	-0.4	-8.3	-10.2
ωB97X	40.2	38.6	38.4	35.5	32.8	28.1	24.7	-0.6	-1.3	-2.5	-4.2	-1.3	-8.2	-10.1
ωB97X-D	43.5	40.9	41.6	37.9	34.4	29.0	25.5	1.0	-1.4	-2.6	-4.2	-2.3	-8.2	-10.2

Table S22: The values of hydrogen bond length (in au) obtained for the HF$\cdots$HF and HCN$\cdots$HCN complexes at different ω values employing various DFT functionals as well as the HF, MP2, CCSD and CCSD(T) methods. All data were obtained using the aug-cc-pVTZ basis set. The ω values are given in au.

	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$	$\omega = 0.0$	$\omega = 0.1$	$\omega = 0.2$	$\omega = 0.3$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.8$
method	**HF$\cdots$HF**							**HCN$\cdots$HCN**						
CCSD(T)	1.9089	1.8934	1.8557	1.8014	1.7316	1.5972	1.5284	2.2044	2.1933	2.1698	2.1514	2.1442	2.1381	2.1051
CCSD	1.9234	1.9073	1.8683	1.8122	1.7407	1.6039	1.5336	2.2258	2.2141	2.1895	2.1700	2.1619	2.1536	2.1173
MP2	1.9153	1.8976	1.8560	1.7982	1.7255	1.5884	1.5197	2.1876	2.1766	2.1535	2.1360	2.1301	2.1278	2.0986
HF	2.0058	1.9898	1.9493	1.8904	1.8158	1.6709	1.5919	2.3363	2.3225	2.2936	2.2702	2.2595	2.2431	2.1907
B2PLYP	1.8988	1.8811	1.8410	1.7870	1.7190	1.5875	1.5193	2.2075	2.1939	2.1660	2.1443	2.1356	2.1313	2.1038
B2LYPD3	1.8947	1.8774	1.8379	1.7845	1.7171	1.5866	1.5188	2.1900	2.1770	2.1503	2.1293	2.1205	2.1164	2.0913
B3LYP	1.9044	1.8856	1.8437	1.7885	1.7193	1.5859	1.5171	2.2252	2.2097	2.1781	2.1535	2.1433	2.1391	2.1120
B3PW91	1.9626	1.9390	1.8858	1.8171	1.7352	1.5895	1.5207	2.2323	2.2148	2.1802	2.1540	2.1436	2.1365	2.1026
B97-2	2.0162	1.9915	1.9384	1.8666	1.7801	1.6214	1.5441	2.2691	2.2506	2.2149	2.1880	2.1761	2.1612	2.1158
B97D	2.1847	2.1356	2.0065	1.9160	1.8198	1.6561	1.5611	2.3390	2.3172	2.2694	2.2296	2.2133	2.1943	2.1411
BLYP	1.9442	1.9215	1.8733	1.8141	1.7409	1.5971	1.5231	2.2549	2.2371	2.2014	2.1740	2.1634	2.1602	2.1311
BMK	1.8553	1.8470	1.8013	1.7652	1.7175	1.5941	1.5215	2.1864	2.1788	2.1639	2.1523	2.1500	2.1565	2.1330
CAM-B3LYP	1.8447	1.8284	1.7914	1.7415	1.6786	1.5571	1.4937	2.1899	2.1752	2.1451	2.1207	2.1097	2.1052	2.0833
HCTH	2.0965	2.0751	2.0231	1.9513	1.8622	1.6591	1.5588	2.3668	2.3471	2.3017	2.2590	2.2364	2.2032	2.1411
HISS	1.8820	1.8648	1.8246	1.7696	1.7011	1.5749	1.5116	2.1755	2.1627	2.1364	2.1163	2.1086	2.1069	2.0840
HSE06	1.8921	1.8727	1.8291	1.7718	1.7016	1.5732	1.5091	2.1787	2.1639	2.1341	2.1113	2.1017	2.0970	2.0719
LC-BLYP	1.7803	1.7661	1.7330	1.6876	1.6302	1.5180	1.4590	2.1536	2.1402	2.1119	2.0881	2.0763	2.0721	2.0567
LC-HCTH	1.8127	1.8019	1.7761	1.7371	1.6836	1.5654	1.4964	2.1937	2.1838	2.1618	2.1422	2.1318	2.1235	2.0985
LC-revTPSS	1.8371	1.8198	1.7800	1.7256	1.6589	1.5373	1.4780	2.1737	2.1593	2.1300	2.1064	2.0956	2.0895	2.0641
LC-τHCTH	1.6863	1.6798	1.6623	1.6328	1.5904	1.4994	1.4503	2.0714	2.0663	2.0544	2.0441	2.0397	2.0440	2.0404
LSDA	1.6677	1.6569	1.6297	1.5897	1.5385	1.4442	1.4007	1.9864	1.9769	1.9566	1.9401	1.9339	1.9412	1.9419
M06	1.8832	1.8655	1.8248	1.7714	1.7089	1.5979	1.5423	2.1632	2.1566	2.1423	2.1335	2.1362	2.1480	2.1259
M06-2X	1.8583	1.8462	1.8176	1.7745	1.7155	1.5955	1.5310	2.2135	2.2029	2.1812	2.1658	2.1658	2.1753	2.1353
M06-HF	1.8982	1.8808	1.8414	1.7896	1.7156	1.5854	1.5159	2.2141	2.2001	2.1699	2.1498	2.1529	2.1623	2.1203
M06L	1.8774	1.8607	1.8214	1.7653	1.6992	1.5833	1.5270	2.1509	2.1450	2.1294	2.1138	2.1077	2.1153	2.0890
M11	1.8783	1.8626	1.8247	1.7733	1.7122	1.5995	1.5401	2.1953	2.1840	2.1599	2.1392	2.1310	2.1385	2.1267
M11-L	1.9886	1.9711	1.9203	1.8406	1.7402	1.6005	1.5453	2.1811	2.1769	2.1670	2.1633	2.1739	2.1888	2.1429
MN12-L	1.9616	1.9459	1.9073	1.8534	1.7832	1.6327	1.5514	2.2331	2.2271	2.2139	2.2064	2.2117	2.2245	2.1949
MN12-SX	1.9213	1.9081	1.8739	1.8236	1.7565	1.6171	1.5431	2.2292	2.2230	2.2099	2.2028	2.2106	2.2320	2.2035
mPW1PW91	1.9332	1.9113	1.8623	1.7989	1.7225	1.5847	1.5173	2.2105	2.1939	2.1605	2.1347	2.1238	2.1168	2.0858
N12	1.8540	1.8329	1.7771	1.7251	1.6512	1.5324	1.4727	2.1871	2.1638	2.1255	2.0983	2.0852	2.0785	2.0639
N12-SX	1.8562	1.8422	1.8070	1.7549	1.6892	1.5612	1.4979	2.1748	2.1615	2.1346	2.1137	2.1054	2.1073	2.0935
PBE	1.9153	1.8936	1.8472	1.7888	1.7153	1.5753	1.5056	2.1934	2.1766	2.1428	2.1168	2.1059	2.1003	2.0736
PBE0	1.9031	1.8842	1.8411	1.7835	1.7115	1.5774	1.5106	2.1902	2.1748	2.1436	2.1191	2.1082	2.1008	2.0716
revTPSS	1.9436	1.9188	1.8660	1.8018	1.7251	1.5886	1.5227	2.2202	2.2045	2.1738	2.1515	2.1438	2.1394	2.1086
SOGGA11-X	1.8474	1.8349	1.8047	1.7603	1.7025	1.5908	1.5286	2.1755	2.1667	2.1471	2.1306	2.1233	2.1152	2.0839
τHCTH	2.0596	2.0238	1.9509	1.8573	1.7576	1.5950	1.5234	2.2320	2.2126	2.1780	2.1527	2.1422	2.1305	2.0901
τHCTHHYB	1.9416	1.9180	1.8692	1.8014	1.7231	1.5851	1.5169	2.2037	2.1852	2.1535	2.1318	2.1245	2.1235	2.0974
TPSSH	1.9547	1.9289	1.8725	1.8036	1.7218	1.5815	1.5155	2.2093	2.1916	2.1569	2.1312	2.1210	2.1155	2.0871
ωB97	1.8419	1.8295	1.8006	1.7603	1.7061	1.5924	1.5306	2.1682	2.1602	2.1428	2.1287	2.1236	2.1207	2.0931
ωB97X	1.8529	1.8401	1.8087	1.7633	1.7068	1.5906	1.5314	2.1721	2.1625	2.1428	2.1278	2.1230	2.1219	2.0947
ωB97X-D	1.9128	1.8971	1.8594	1.8002	1.7298	1.6016	1.5405	2.1995	2.1863	2.1594	2.1417	2.1369	2.1362	2.1071

Table S23: Structural parameters obtained for the HF$\cdots$HF complex using the CCSD(T) method as well as B2PLYP, B3LYP and ωB97X-D functionals. The % error was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVTZ basis set. The bond lengths are given in au.

	ω	CCSD(T)	B2PLYP	% error	B3LYP	% error	ωB97X-D	% error
	0.0	0.9220	0.9235	0.16	0.9254	0.37	0.9195	-0.27
	0.1	0.9183	0.9198	0.16	0.9218	0.38	0.9160	-0.25
	0.2	0.9086	0.9101	0.16	0.9125	0.42	0.9068	-0.20
H-F(1)	0.3	0.8949	0.8965	0.17	0.8992	0.48	0.8937	-0.14
	0.4	0.8787	0.8804	0.20	0.8835	0.55	0.8781	-0.07
	0.5	0.8439	0.8460	0.25	0.8495	0.67	0.8450	0.14
	0.8	0.8130	0.8153	0.28	0.8190	0.73	0.8158	0.35
	0.0	1.9089	1.8988	-0.53	1.9044	-0.24	1.9128	0.20
	0.1	1.8934	1.8811	-0.64	1.8856	-0.41	1.8971	0.20
	0.2	1.8557	1.8410	-0.79	1.8437	-0.65	1.8594	0.20
HF$\cdots$H	0.3	1.8014	1.7870	-0.80	1.7885	-0.72	1.8002	-0.07
	0.4	1.7316	1.7190	-0.73	1.7193	-0.71	1.7298	-0.10
	0.5	1.5972	1.5875	-0.61	1.5859	-0.71	1.6016	0.28
	0.8	1.5284	1.5193	-0.59	1.5171	-0.74	1.5405	0.79
	0.0	0.9238	0.9257	0.21	0.9279	0.44	0.9225	-0.14
	0.1	0.9202	0.9221	0.21	0.9244	0.46	0.9191	-0.12
	0.2	0.9107	0.9126	0.22	0.9154	0.52	0.9101	-0.06
H-F(2)	0.3	0.8975	0.8996	0.24	0.9027	0.59	0.8977	0.02
	0.4	0.8822	0.8845	0.27	0.8881	0.67	0.8832	0.12
	0.5	0.8501	0.8530	0.34	0.8572	0.83	0.8529	0.33
	0.8	0.8206	0.8238	0.39	0.8283	0.94	0.8250	0.53

Table S24: Structural parameters obtained for the HCN$\cdots$HCN complex using the CCSD(T) method as well as B2PLYP, B3LYP and ωB97X-D functionals. The % error was calculated with respect to the CCSD(T) results. All data were obtained using the aug-cc-pVTZ basis set. The bond lengths are given in au.

	ω [au]	CCSD(T)	B2PLYP	% error	B3LYP	% error	ωB97X-D	% error
	0.0	1.0684	1.0652	-0.31	1.0665	-0.18	1.0670	-0.13
	0.1	1.0620	1.0588	-0.30	1.0603	-0.16	1.0608	-0.11
	0.2	1.0459	1.0430	-0.28	1.0448	-0.11	1.0452	-0.06
H-C(1)	0.3	1.0255	1.0230	-0.25	1.0250	-0.05	1.0254	-0.01
	0.4	1.0044	1.0022	-0.22	1.0044	0.00	1.0049	0.05
	0.5	0.9648	0.9632	-0.17	0.9657	0.09	0.9661	0.14
	0.8	0.9304	0.9292	-0.12	0.9318	0.16	0.9320	0.18
	0.0	1.1584	1.1523	-0.52	1.1444	-1.20	1.1416	-1.45
	0.1	1.1525	1.1466	-0.52	1.1388	-1.19	1.1360	-1.43
	0.2	1.1381	1.1323	-0.50	1.1248	-1.16	1.1223	-1.38
C-N(1)	0.3	1.1195	1.1141	-0.49	1.1070	-1.12	1.1047	-1.33
	0.4	1.0997	1.0946	-0.47	1.0880	-1.07	1.0858	-1.26
	0.5	1.0611	1.0566	-0.43	1.0507	-0.98	1.0488	-1.16
	0.8	1.0259	1.0219	-0.38	1.0168	-0.89	1.0148	-1.08
	0.0	2.2044	2.2075	0.14	2.2252	0.94	2.1995	-0.22
	0.1	2.1933	2.1939	0.03	2.2097	0.75	2.1863	-0.32
	0.2	2.1698	2.1660	-0.18	2.1781	0.38	2.1594	-0.48
N$\cdots$HC	0.3	2.1514	2.1443	-0.33	2.1535	0.10	2.1417	-0.45
	0.4	2.1442	2.1356	-0.40	2.1433	-0.04	2.1369	-0.34
	0.5	2.1381	2.1313	-0.32	2.1391	0.04	2.1362	-0.09
	0.8	2.1051	2.1038	-0.06	2.1120	0.33	2.1071	0.09
	0.0	1.0729	1.0707	-0.21	1.0723	-0.06	1.0739	0.08
	0.1	1.0666	1.0646	-0.19	1.0664	-0.02	1.0679	0.11
	0.2	1.0508	1.0492	-0.16	1.0513	0.05	1.0526	0.17
H-C(2)	0.3	1.0306	1.0293	-0.13	1.0318	0.11	1.0327	0.20
	0.4	1.0094	1.0083	-0.11	1.0110	0.16	1.0117	0.23
	0.5	0.9692	0.9685	-0.07	0.9714	0.23	0.9720	0.29
	0.8	0.9350	0.9345	-0.05	0.9376	0.28	0.9379	0.31
	0.0	1.1606	1.1545	-0.52	1.1467	-1.20	1.1440	-1.43
	0.1	1.1545	1.1486	-0.52	1.1408	-1.19	1.1383	-1.41
	0.2	1.1397	1.1340	-0.50	1.1266	-1.15	1.1242	-1.36
C-N(2)	0.3	1.1208	1.1154	-0.48	1.1085	-1.10	1.1063	-1.30
	0.4	1.1006	1.0955	-0.46	1.0891	-1.05	1.0870	-1.23
	0.5	1.0614	1.0569	-0.42	1.0513	-0.95	1.0494	-1.13
	0.8	1.0265	1.0226	-0.38	1.0176	-0.87	1.0158	-1.05

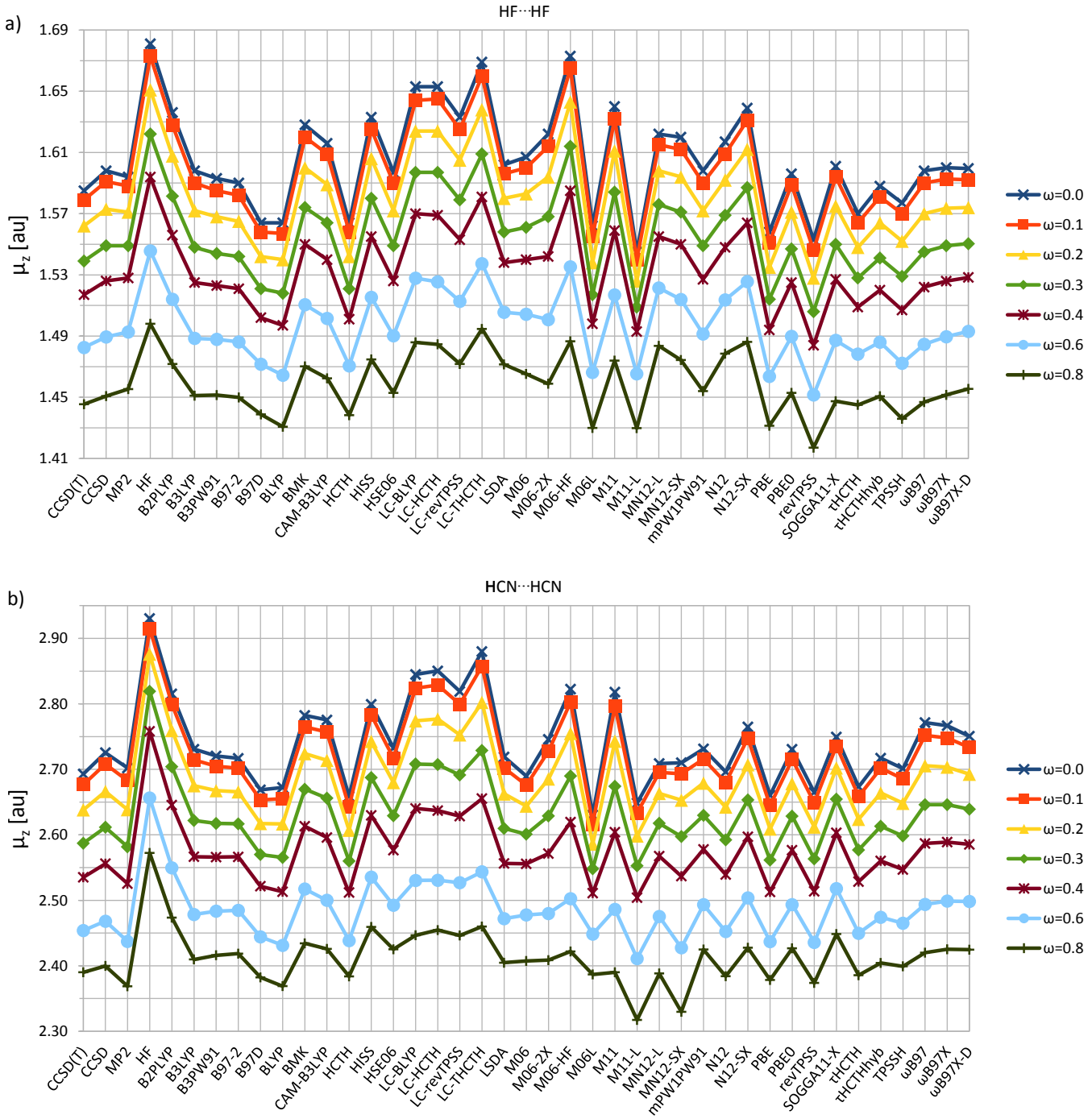

Figure S2: Dipole moment (μ_z) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVQZ basis set. The ω values are given in au. Lines are drawn to guide the eye.

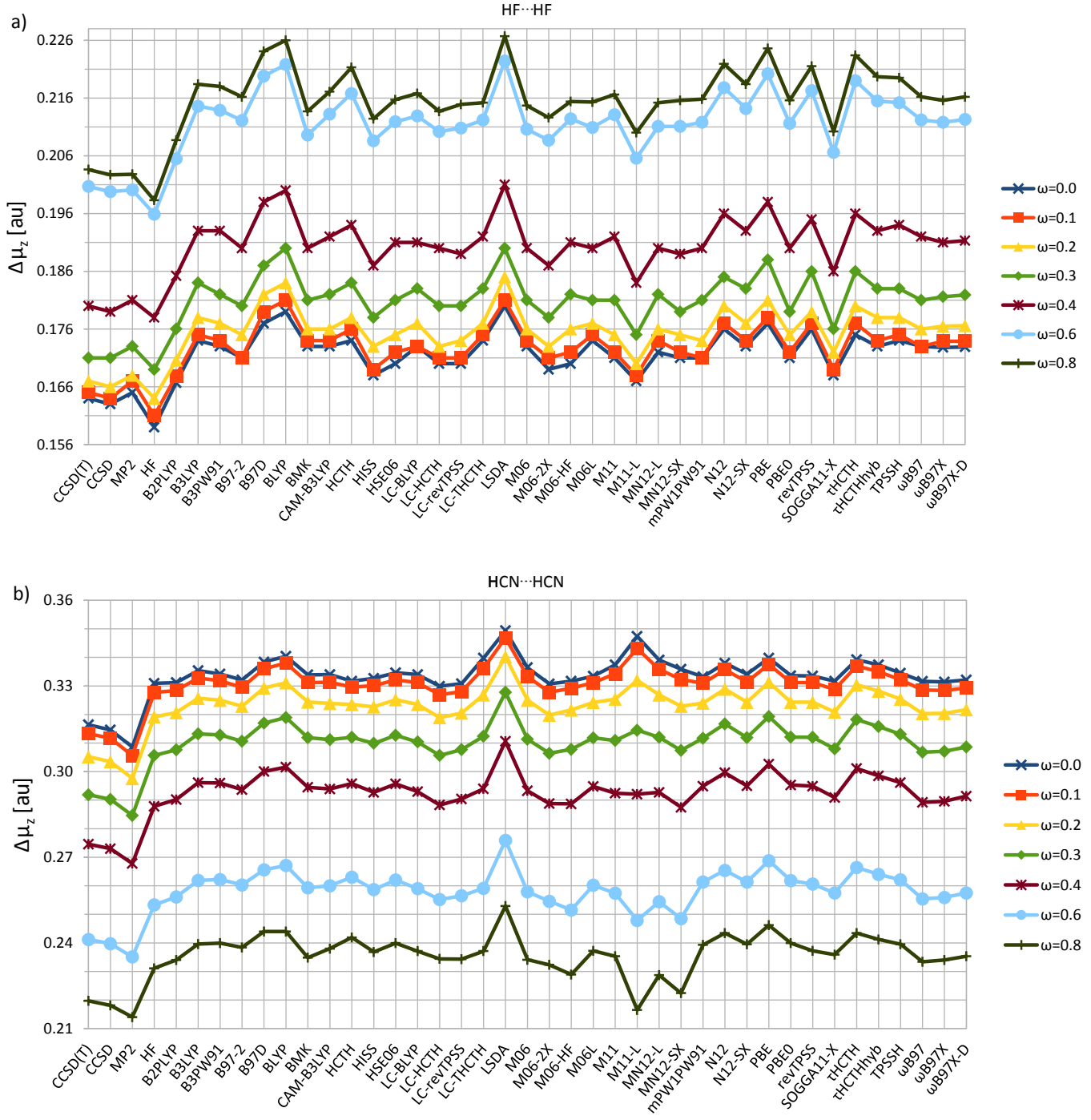

Figure S3: Interaction-induced dipole moment ($\Delta\mu_z$) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVQZ basis set. The ω values are given in au. Lines are drawn to guide the eye.

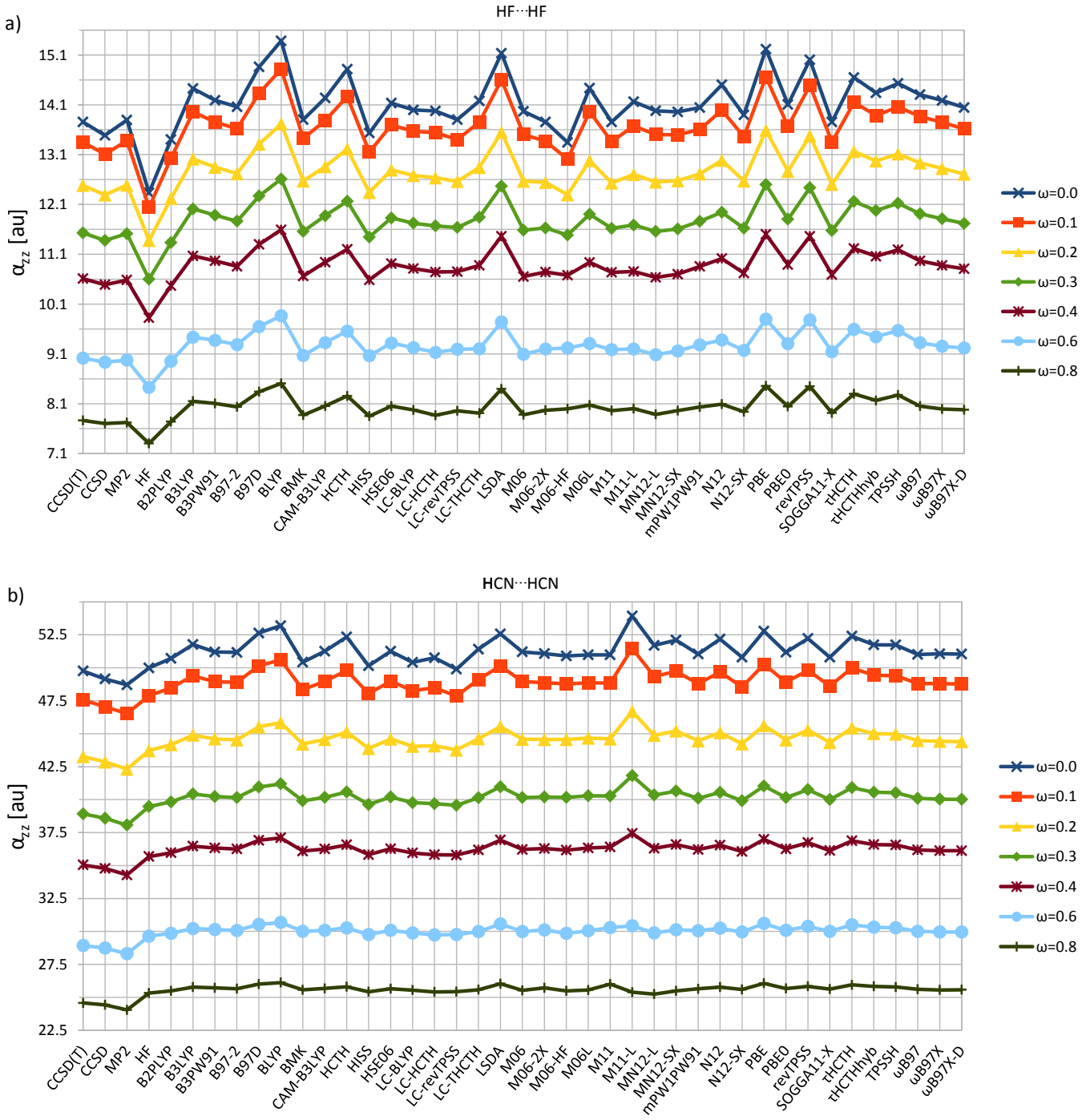

Figure S4: Polarizability (α_{zz}) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVQZ basis set. The ω values are given in au. Lines are drawn to guide the eye.

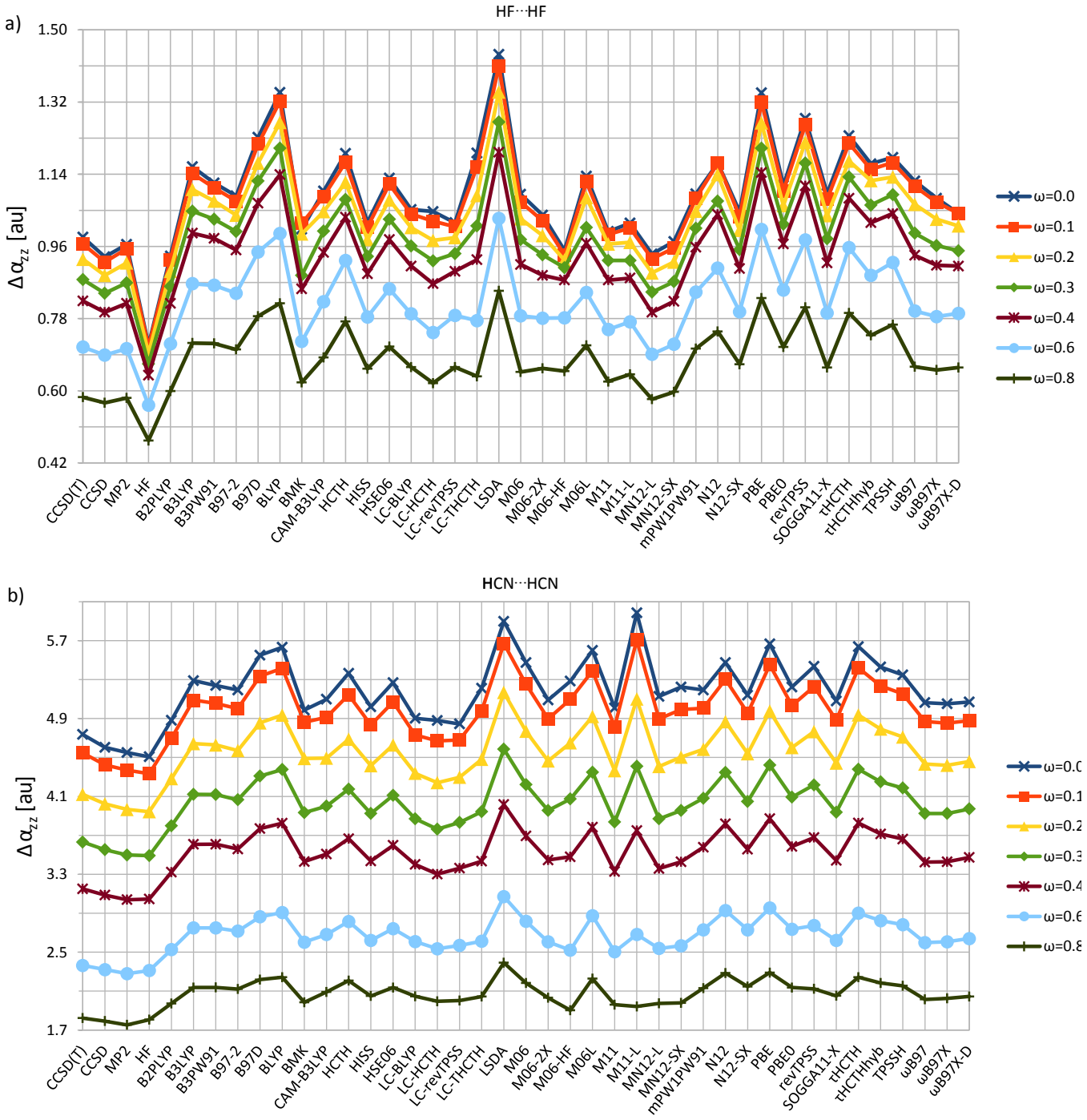

Figure S5: Interaction-induced polarizability ($\Delta\alpha_{zz}$) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVQZ basis set. The ω values are given in au. Lines are drawn to guide the eye.

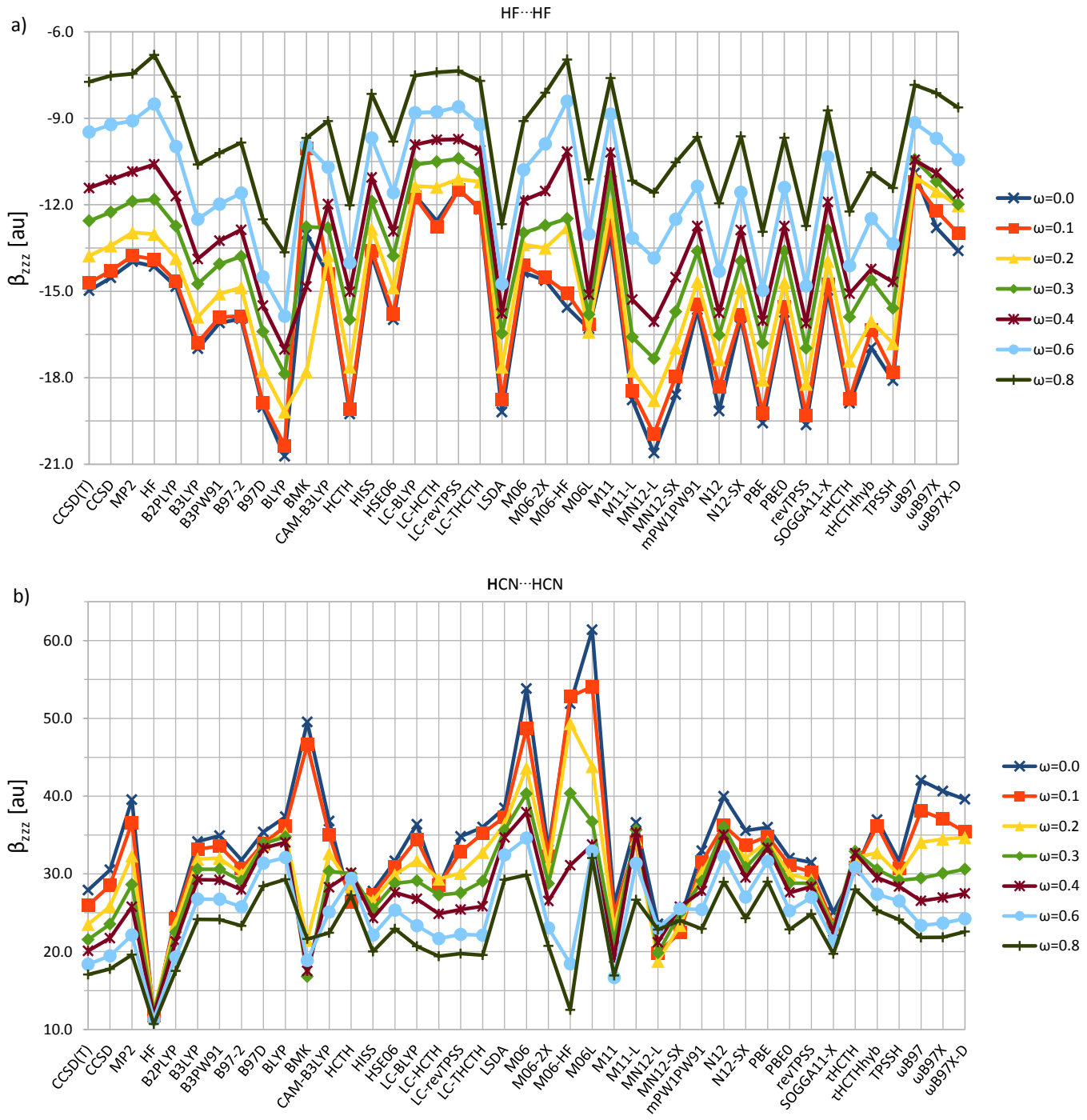

Figure S6: First hyperpolarizability (β_{zzz}) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVQZ basis set. The ω values are given in au. Lines are drawn to guide the eye.

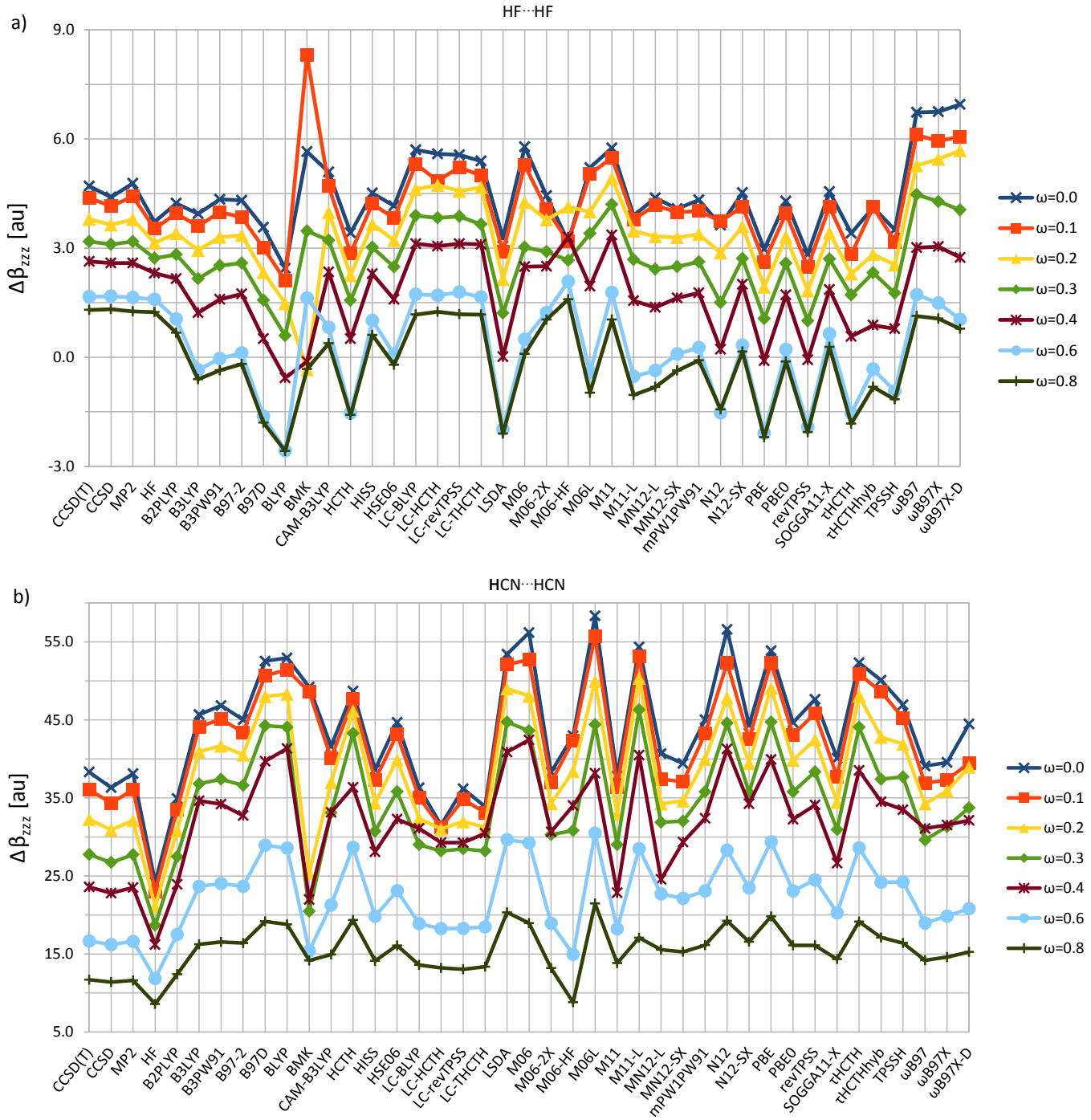

Figure S7: Interaction-induced first hyperpolarizability ($\Delta\beta_{zzz}$) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVQZ basis set. The ω values are given in au. Lines are drawn to guide the eye.

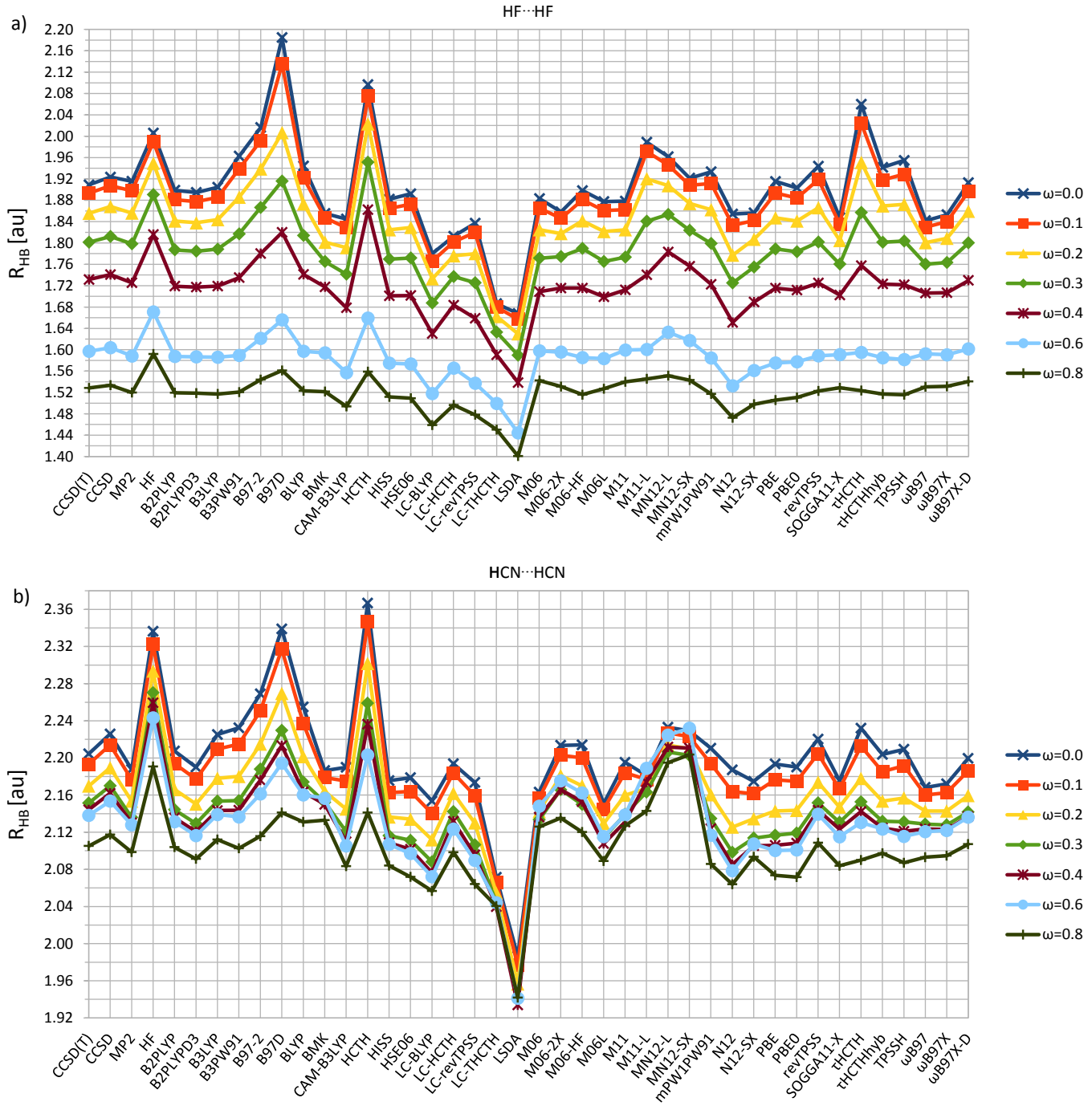

Figure S8: Hydrogen bond length (R_{HB}) of the isolated and spatially confined a)HF$\cdots$HF and b)HCN$\cdots$HCN dimers calculated using various exchange-correlation functionals as well as HF, MP2, CCSD and CCSD(T) methods. All data were computed employing the aug-cc-pVTZ basis set. The ω values are given in au. Lines are drawn to guide the eye.