Supporting information for:

Frozen Density Embedding with External Orthogonality in Delocalized Covalent Systems

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1 System Geometries

Table S1: Water dimer geometry (in Å).

	subsystem I				subsystem II		
atom	x	y	z	atom	x	y	z
O	-1.4626	0.0000	0.0000	O	1.4626	0.0000	0.0000
H	-1.7312	0.9302	0.0000	H	1.9309	0.3579	0.7697
H	-0.4844	0.0275	0.0000	H	1.9309	0.3579	-0.7697

Table S2: FHF^- geometry (in Å).

	FH subsystem				F^- subsystem		
atom	x	y	z	atom	x	y	z
F	0.0000	0.0000	1.1587	F	0.0000	0.0000	-1.1587
H	0.0000	0.0000	0.0000				

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Table S3: BH_3NH_3 geometry (in Å).

BH_3 subsystem				NH_3 subsystem			
atom	x	y	z	atom	x	y	z
B	0.0000	0.0000	0.8382	N	0.0000	0.0000	-0.8158
H	-0.5864	-1.0157	1.1548	H	0.4765	-0.8252	-1.1862
H	-0.5864	1.0157	1.1548	H	0.4765	0.8252	-1.1862
H	1.1728	0.0000	1.1548	H	-0.9529	0.0000	-1.1862

Table S4: C_2H_6 geometry (in Å).

CH_3^+ subsystem				CH_3^- subsystem			
atom	x	y	z	atom	x	y	z
C	0.0000	0.0000	0.7651	C	0.0000	0.0000	-0.7651
H	0.0000	-1.0222	1.1666	H	0.8853	-0.5111	-1.1666
H	-0.8853	0.5111	1.1666	H	0.0000	1.0222	-1.1666
H	0.8853	0.5111	1.1666	H	-0.8853	-0.5111	-1.1666

Table S5: C_6H_{12} geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-3.1595	-0.3535	0.0351	C	0.6165	0.2594	-0.0400
H	-3.1754	-1.1510	-0.7229	H	0.7222	1.3357	-0.2323
H	-4.0780	0.2386	-0.0819	C	1.9083	-0.5197	0.1097
H	-3.1945	-0.8346	1.0241	H	1.9381	-1.3285	-0.6388
C	-1.9086	0.5199	-0.1096	H	1.9250	-1.0195	1.0921
H	-1.9408	1.3297	0.6377	C	3.1600	0.3521	-0.0367
H	-1.9241	1.0183	-1.0928	H	4.0779	-0.2418	0.0744
C	-0.6166	-0.2579	0.0421	H	3.1807	1.1466	0.7245
H	-0.7219	-1.3344	0.2335	H	3.1915	0.8372	-1.0239

Table S6: C_8H_{16} geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-0.5764	-0.0196	-4.2325	C	0.6473	-0.3793	0.5416
H	-1.4640	0.3376	-4.7742	H	0.6756	-1.4674	0.3942
H	-0.5526	-1.1169	-4.3182	C	0.6194	0.0918	1.9688
H	0.3123	0.3729	-4.7505	H	0.6127	1.1936	1.9948
C	-0.6019	0.4206	-2.7654	H	1.5461	-0.2279	2.4798
H	-1.5144	0.0423	-2.2761	C	-0.5819	-0.4528	2.7648
H	-0.6578	1.5208	-2.7097	H	-0.5780	-1.5546	2.7114
C	0.6257	-0.0595	-1.9677	H	-1.5127	-0.1257	2.2730
H	1.5348	0.3101	-2.4767	C	-0.5836	-0.0086	4.2309
H	0.6783	-1.1600	-1.9944	H	-1.4521	-0.4117	4.7713
C	0.6257	0.4116	-0.5402	H	-0.6190	1.0886	4.3135
H	0.5927	1.4996	-0.3924	H	0.3236	-0.3513	4.7521

Table S7: $C_{10}H_{20}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	0.0855	0.7963	-5.0878	C	0.6551	-0.3168	0.5133
H	1.1425	0.6724	-4.8099	H	0.8182	-1.3865	0.3246
H	-0.1514	1.8703	-5.0274	C	0.5973	0.0963	1.9579
H	-0.0142	0.4921	-6.1401	H	1.5590	-0.1463	2.4425
C	-0.8452	-0.0226	-4.1845	H	0.4764	1.1898	2.0253
H	-1.8796	0.0812	-4.5506	C	-0.5445	-0.5967	2.7292
H	-0.5976	-1.0945	-4.2743	H	-0.4254	-1.6914	2.6431
C	-0.8134	0.3794	-2.7005	H	-1.4963	-0.3522	2.2300
H	-1.6203	-0.1476	-2.1655	C	-0.6397	-0.2132	4.2150
H	-1.0386	1.4570	-2.6108	H	-1.5758	-0.6287	4.6225
C	0.5180	0.0813	-1.9814	H	-0.7327	0.8834	4.3007
H	1.3356	0.6078	-2.5036	C	0.5342	-0.6972	5.0755
H	0.7407	-0.9960	-2.0508	H	1.4888	-0.2535	4.7565
C	0.5039	0.5014	-0.5377	H	0.6399	-1.7920	5.0177
H	0.3363	1.5704	-0.3490	H	0.3870	-0.4324	6.1328

Table S8: $C_{12}H_{24}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-0.0185	1.9689	-5.3535	C	0.5329	-0.3242	0.5389
H	0.7078	2.3769	-6.0718	H	0.6786	-1.4049	0.4054
H	0.0983	2.5311	-4.4149	C	0.4734	0.1618	1.9608
H	-1.0273	2.1795	-5.7429	H	1.4386	-0.0496	2.4538
C	0.1907	0.4628	-5.1500	H	0.3485	1.2569	1.9725
H	0.1421	-0.0403	-6.1298	C	-0.6596	-0.4973	2.7728
H	1.2107	0.2810	-4.7724	H	-0.5347	-1.5930	2.7429
C	-0.8384	-0.2018	-4.2170	H	-1.6162	-0.2904	2.2656
H	-0.6756	-1.2933	-4.2288	C	-0.7606	-0.0187	4.2321
H	-1.8466	-0.0407	-4.6364	H	-1.6753	-0.4474	4.6771
C	-0.8374	0.2806	-2.7555	H	-0.9053	1.0754	4.2356
H	-1.6875	-0.1833	-2.2290	C	0.4333	-0.3632	5.1415
H	-1.0182	1.3683	-2.7174	H	0.2707	0.1181	6.1200
C	0.4524	-0.0438	-1.9753	H	1.3544	0.0884	4.7370
H	1.3109	0.4211	-2.4912	C	0.6527	-1.8662	5.3570
H	0.6297	-1.1316	-1.9890	H	1.4814	-2.0495	6.0565
C	0.4131	0.4437	-0.5533	H	0.8961	-2.3854	4.4179
H	0.2638	1.5238	-0.4192	H	-0.2486	-2.3421	5.7752

Table S9: $C_{14}H_{28}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	0.6824	2.2735	-6.4294	C	0.5178	-0.3216	0.5731
H	1.7278	2.2052	-6.0905	H	0.6394	-1.4122	0.5234
H	0.4567	3.3362	-6.5997	C	0.5068	0.2784	1.9520
H	0.6152	1.7576	-7.3998	H	1.4752	0.0726	2.4408
C	-0.2723	1.6525	-5.4035	H	0.4193	1.3748	1.8779
H	-0.2055	2.2196	-4.4603	C	-0.6291	-0.2715	2.8375
H	-1.3137	1.7638	-5.7535	H	-0.5512	-1.3712	2.8820
C	0.0115	0.1666	-5.1401	H	-1.5903	-0.0587	2.3413
H	-0.0306	-0.3753	-6.1009	C	-0.6676	0.3107	4.2617
H	1.0495	0.0540	-4.7814	H	-1.5858	-0.0430	4.7586
C	-0.9609	-0.5106	-4.1576	H	-0.7703	1.4075	4.1934
H	-0.7491	-1.5934	-4.1374	C	0.5484	-0.0078	5.1537
H	-1.9860	-0.4102	-4.5531	H	0.4107	0.5069	6.1207
C	-0.9412	0.0234	-2.7138	H	1.4550	0.4339	4.7081
H	-1.7663	-0.4416	-2.1500	C	0.8087	-1.5012	5.4252
H	-1.1495	1.1065	-2.7116	H	1.7426	-1.5883	6.0048
C	0.3743	-0.2385	-1.9532	H	0.9986	-2.0260	4.4738
H	1.2136	0.1865	-2.5312	C	-0.3173	-2.2150	6.1845
H	0.5550	-1.3239	-1.8895	H	-0.0503	-3.2603	6.3992
C	0.3817	0.3591	-0.5734	H	-1.2560	-2.2279	5.6108
H	0.2548	1.4490	-0.5220	H	-0.5229	-1.7191	7.1466

Table S10: C_6H_8 geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-3.0670	-0.3214	-0.0670	C	0.5943	0.3283	0.0291
H	-4.0109	0.2224	-0.0697	H	0.5913	1.4238	0.0304
H	-3.1172	-1.4114	-0.1095	C	1.8844	-0.3239	0.0331
C	-1.8842	0.3233	-0.0025	H	1.8786	-1.4183	0.0662
H	-1.8776	1.4175	0.0391	C	3.0673	0.3233	-0.0025
C	-0.5947	-0.3299	0.0151	H	3.1159	1.4135	-0.0379
H	-0.5919	-1.4255	0.0088	H	4.0122	-0.2187	0.0088

Table S11: C_8H_{12} geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-4.4159	0.3378	0.0131	C	0.5969	0.3298	-0.0130
H	-4.3294	1.4325	0.0247	H	0.5956	1.4252	-0.0124
H	-4.9997	0.0306	0.8963	C	1.8847	-0.3224	-0.0036
H	-5.0147	0.0496	-0.8665	H	1.8804	-1.4188	-0.0018
C	-3.0719	-0.3224	-0.0036	C	3.0739	0.3214	0.0049
H	-3.0636	-1.4184	-0.0046	H	3.0711	1.4174	0.0004
C	-1.8855	0.3265	-0.0106	C	4.4144	-0.3461	0.0209
H	-1.8851	1.4230	-0.0095	H	5.0130	-0.0636	-0.8607
C	-0.5963	-0.3228	-0.0157	H	4.3219	-1.4402	0.0358
H	-0.5939	-1.4182	-0.0137	H	5.0016	-0.0403	0.9023

Table S12: $C_{10}H_{12}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-5.5488	-0.2968	0.0080	C	0.6003	0.3120	-0.0192
H	-6.4845	0.2609	0.0127	H	0.5937	1.4070	-0.0160
H	-5.6162	-1.3867	0.0227	C	1.8776	-0.3314	-0.0154
C	-4.3525	0.3311	-0.0094	H	1.8868	-1.4266	-0.0116
H	-4.3293	1.4260	-0.0203	C	3.0716	0.3311	-0.0094
C	-3.0762	-0.3389	-0.0147	H	3.0632	1.4265	-0.0123
H	-3.0869	-1.4340	-0.0223	C	4.3597	-0.3139	0.0196
C	-1.8731	0.3068	-0.0099	H	4.3592	-1.4090	0.0154
H	-1.8708	1.4021	0.0058	C	5.5419	0.3397	0.0609
C	-0.5998	-0.3448	-0.0195	H	5.5851	1.4308	0.0706
H	-0.5965	-1.4394	-0.0270	H	6.4892	-0.1975	0.0876

Table S13: $C_{12}H_{16}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-6.8885	0.3419	-0.0728	C	0.6022	0.3258	0.0897
H	-6.7995	1.4363	-0.0737	H	0.5997	1.4208	0.0908
H	-7.5116	0.0473	0.7876	C	1.8769	-0.3224	0.0686
H	-7.4495	0.0431	-0.9736	H	1.8794	-1.4177	0.0714
C	-5.5482	-0.3224	-0.0249	C	3.0765	0.3298	0.0271
H	-5.5434	-1.4184	-0.0241	H	3.0752	1.4249	0.0216
C	-4.3582	0.3232	0.0145	C	4.3585	-0.3224	-0.0249
H	-4.3546	1.4197	0.0148	H	4.3552	-1.4188	-0.0166
C	-3.0757	-0.3291	0.0515	C	5.5475	0.3229	-0.0922
H	-3.0747	-1.4242	0.0484	H	5.5427	1.4188	-0.1023
C	-1.8755	0.3225	0.0785	C	6.8860	-0.3431	-0.1607
H	-1.8771	1.4178	0.0798	H	7.4280	-0.0548	-1.0765
C	-0.6010	-0.3263	0.0903	H	6.7961	-1.4373	-0.1479
H	-0.5991	-1.4213	0.0871	H	7.5274	-0.0395	0.6831

Table S14: $C_{14}H_{16}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-8.0253	-0.2506	0.0699	C	0.6022	0.2962	-0.1200
H	-8.1149	-1.3381	0.0308	H	0.5907	1.3911	-0.1146
H	-8.9487	0.3255	0.1139	C	1.8755	-0.3407	-0.0986
C	-6.8164	0.3542	0.0654	H	1.8897	-1.4359	-0.0947
H	-6.7729	1.4477	0.1064	C	3.0732	0.3271	-0.0592
C	-5.5529	-0.3348	0.0076	H	3.0583	1.4218	-0.0605
H	-5.5795	-1.4291	-0.0212	C	4.3496	-0.3085	0.0046
C	-4.3402	0.2958	-0.0161	H	4.3615	-1.4036	0.0148
H	-4.3249	1.3907	0.0093	C	5.5439	0.3542	0.0654
C	-3.0774	-0.3675	-0.0706	H	5.5395	1.4493	0.0547
H	-3.0834	-1.4621	-0.0853	C	6.8256	-0.2976	0.1464
C	-1.8693	0.2818	-0.0961	H	6.8159	-1.3924	0.1682
H	-1.8707	1.3767	-0.0834	C	8.0135	0.3456	0.1949
C	-0.6011	-0.3651	-0.1221	H	8.0685	1.4359	0.1754
H	-0.5940	-1.4597	-0.1265	H	8.9542	-0.2006	0.2523

Table S15: $C_{16}H_{20}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-9.2739	-0.3141	0.5769	C	0.6156	-0.3666	-0.5073
H	-9.6805	-0.0164	1.5577	H	0.6172	-1.4616	-0.4963
H	-9.1981	-1.4092	0.5584	C	1.8778	0.2893	-0.4390
H	-10.0232	-0.0062	-0.1707	H	1.8726	1.3844	-0.4526
C	-7.9513	0.3380	0.3230	C	3.0836	-0.3516	-0.3041
H	-7.9327	1.4336	0.3380	H	3.0905	-1.4463	-0.2790
C	-6.7888	-0.3194	0.0923	C	4.3356	0.3134	-0.1383
H	-6.7986	-1.4155	0.0777	H	4.3254	1.4084	-0.1649
C	-5.5170	0.3208	-0.1095	C	5.5261	-0.3194	0.0923
H	-5.5033	1.4158	-0.0938	H	5.5380	-1.4139	0.1247
C	-4.3332	-0.3422	-0.2836	C	6.7726	0.3561	0.3342
H	-4.3460	-1.4373	-0.2962	H	6.7551	1.4519	0.3010
C	-3.0630	0.2963	-0.4097	C	7.9421	-0.2664	0.6191
H	-3.0515	1.3912	-0.3970	H	7.9520	-1.3618	0.6511
C	-1.8626	-0.3629	-0.4958	C	9.2368	0.4255	0.9096
H	-1.8689	-1.4581	-0.4976	H	9.6140	0.1569	1.9103
C	-0.5941	0.2833	-0.5294	H	9.1327	1.5177	0.8674
H	-0.5922	1.3785	-0.5293	H	10.0216	0.1246	0.1963

Table S16: $C_{18}H_{20}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-10.4842	0.2977	-0.2389	C	0.6032	-0.3477	0.2105
H	-11.4160	-0.2626	-0.3026	H	0.5890	-1.4422	0.2122
H	-10.5549	1.3873	-0.2340	C	1.8718	0.2885	0.1794
C	-9.2872	-0.3277	-0.1683	H	1.8836	1.3838	0.1770
H	-9.2614	-1.4226	-0.1738	C	3.0765	-0.3738	0.1330
C	-8.0167	0.3437	-0.0835	H	3.0690	-1.4685	0.1325
H	-8.0288	1.4389	-0.0807	C	4.3406	0.2730	0.0721
C	-6.8124	-0.3001	-0.0061	H	4.3407	1.3683	0.0738
H	-6.8081	-1.3954	-0.0057	C	5.5498	-0.3737	-0.0013
C	-5.5472	0.3537	0.0707	H	5.5582	-1.4682	-0.0055
H	-5.5465	1.4484	0.0749	C	6.8067	0.2952	-0.0845
C	-4.3417	-0.3011	0.1300	H	6.7859	1.3902	-0.0878
H	-4.3464	-1.3960	0.1241	C	8.0216	-0.3277	-0.1683
C	-3.0750	0.3426	0.1797	H	8.0561	-1.4225	-0.1685
H	-3.0660	1.4371	0.1788	C	9.2761	0.3722	-0.2625
C	-1.8698	-0.3194	0.2090	H	9.2227	1.4662	-0.2724
H	-1.8815	-1.4144	0.2090	C	10.4887	-0.2217	-0.3354
C	-0.6009	0.3183	0.2198	H	10.5880	-1.3090	-0.3312
H	-0.5873	1.4134	0.2209	H	11.4048	0.3630	-0.4028

Table S17: $C_{20}H_{24}$ geometry (in Å).

subsystem I				subsystem II			
atom	x	y	z	atom	x	y	z
C	-10.2566	-0.1748	-3.1129	C	0.5891	-0.2332	2.1222
H	-10.0833	0.0411	-4.1805	H	0.5318	-1.3270	2.1221
H	-11.2821	0.1660	-2.8952	C	1.8798	0.3468	1.9709
H	-10.2181	-1.2635	-2.9764	H	1.9426	1.4401	1.9681
C	-9.2521	0.5277	-2.2536	C	3.0186	-0.3732	1.6858
H	-9.2055	1.6187	-2.3451	H	2.9429	-1.4654	1.6617
C	-8.3897	-0.0834	-1.4044	C	4.2567	0.1963	1.2729
H	-8.4265	-1.1758	-1.3177	H	4.3384	1.2881	1.2883
C	-7.3770	0.5939	-0.6388	C	5.2966	-0.5265	0.7373
H	-7.3376	1.6852	-0.7218	H	5.2009	-1.6168	0.6987
C	-6.4258	-0.0404	0.1145	C	6.4415	0.0456	0.1047
H	-6.4641	-1.1332	0.1815	H	6.5363	1.1362	0.1345
C	-5.3167	0.6091	0.7362	C	7.3603	-0.6664	-0.6190
H	-5.2722	1.7008	0.6644	H	7.2586	-1.7559	-0.6638
C	-4.2528	-0.0525	1.3023	C	8.4120	-0.0796	-1.4057
H	-4.2947	-1.1459	1.3504	H	8.5123	1.0114	-1.3646
C	-3.0338	0.5680	1.6992	C	9.2367	-0.7764	-2.2259
H	-2.9868	1.6608	1.6459	H	9.1253	-1.8658	-2.2696
C	-1.8789	-0.1206	1.9974	C	10.2815	-0.1748	-3.1129
H	-1.9260	-1.2144	2.0250	H	10.0903	-0.4214	-4.1708
C	-0.5928	0.4753	2.1195	H	11.2834	-0.5728	-2.8833
H	-0.5405	1.5690	2.0927	H	10.3141	0.9187	-3.0199

2 Energy, Density, and Dipole Differences

Table S18: Energy difference (ΔE, in mE_h) between the KS-DFT and FDE(EO,5ft) methods with different levels of basis set overlap.

System n	d	m	e1	e2	e3	e4	e5	e6	e7	e8	e9	e10
6	1	-2784	-517	-12	2							
	3	-1173	-851	-63	1							
8	1	-2703	-636	-152	-7	1						
	3	-2234	-600	-144	-52	3						
10	1	-2827	-757	-313	-65	-3	2					
	5	5354†	-623	-220	-84	-45	1					
12	1	-2882	-749	-376	-112	-5	2	2				
	5	5409†	-654	-358	-150	-55	-22	4				
14	1	-2951	-782	-405	-201	-1	2	2	2			
	7	121986†	-723	-332	-165	-83	-40	-10	2			
16	7	202558†	-689	-349	-233	-154	-77	-36	-38	-4		
18	9	529592†	-678	-338	-249	-559	-86	-51	-24	-2	6	
20	9	-2157.706	-654	-342	-250	-147	-143	-127	-45	-28	-4	8

n - number of carbon atoms; d - number of conjugated double bonds.

†One or more SCF cycles failed to converge during the freeze-and-thaw iterations.

Table S19: Integrated absolute density difference (Δ^{abs}, in e) for the FDE(EO,5ft) method with different levels of basis set overlap.

System n	d	m	e1	e2	e3	e4	e5	e6	e7	e8	e9	e10
6	1	4.74	2.23	0.11	0.00							
	3	6.98	2.54	0.61	0.00							
8	1	5.65	2.29	0.93	0.08	0.00						
	3	6.56	2.40	1.17	0.58	0.00						
10	1	6.00	2.72	2.00	0.66	0.06	0.00					
	5	16.00†	2.54	1.66	0.95	0.44	0.00					
12	1	6.65	2.65	2.21	0.87	0.10	0.00	0.00				
	5	18.26†	2.72	2.44	1.47	0.69	0.37	0.00				
14	1	6.82	2.77	2.23	1.47	0.12	0.01	0.00	0.00			
	7	44.99†	2.76	2.47	1.66	1.05	0.64	0.26	0.00			
16	7	54.41†	2.86	2.54	2.45	1.76	1.04	0.46	0.55	0.01		
18	9	67.99†	2.92	2.56	2.54	3.14	1.27	0.83	0.50	0.20	0.00	
20	9	6.37	2.98	2.61	2.59	1.91	1.88	1.59	0.80	0.40	0.20	0.00

n - number of carbon atoms; d - number of conjugated double bonds.

†One or more SCF cycles failed to converge during the freeze-and-thaw iterations.

Table S20: Absolute dipole difference ($|\Delta\mu|$, in D) for the FDE(EO,5ft) method with different levels of basis set overlap.

System n	d	m	e1	e2	e3	e4	e5	e6	e7	e8	e9	e10
6	1	17.32	9.14	0.06	0.00							
	3	39.09	7.80	3.08	0.00							
8	1	26.34	9.27	2.16	0.20	0.00						
	3	46.78	16.14	6.18	3.35	0.00						
10	1	30.73	11.94	7.28	1.76	0.14	0.00					
	5	106.17†	22.49	12.19	7.23	0.08	0.01					
12	1	43.31	12.41	9.49	1.16	0.21	0.00	0.00				
	5	121.73†	26.32	22.88	11.34	5.20	3.10	0.01				
14	1	46.25	13.60	9.75	3.34	0.23	0.00	0.00	0.00			
	7	272.74†	33.11	29.84	16.62	10.39	6.54	2.70	0.00			
16	7	311.68†	35.45	31.80	30.20	18.65	10.21	4.06	5.88	0.05		
18	9	407.66†	43.75	38.98	38.28	10.28	15.44	10.15	6.25	2.60	0.01	
20	9	64.86	41.79	37.43	36.98	23.31	23.19	18.78	8.87	3.72	2.54	0.04

n - number of carbon atoms; d - number of conjugated double bonds.

†One or more SCF cycles failed to converge during the freeze-and-thaw iterations.

3 Extended Monomer Truncation

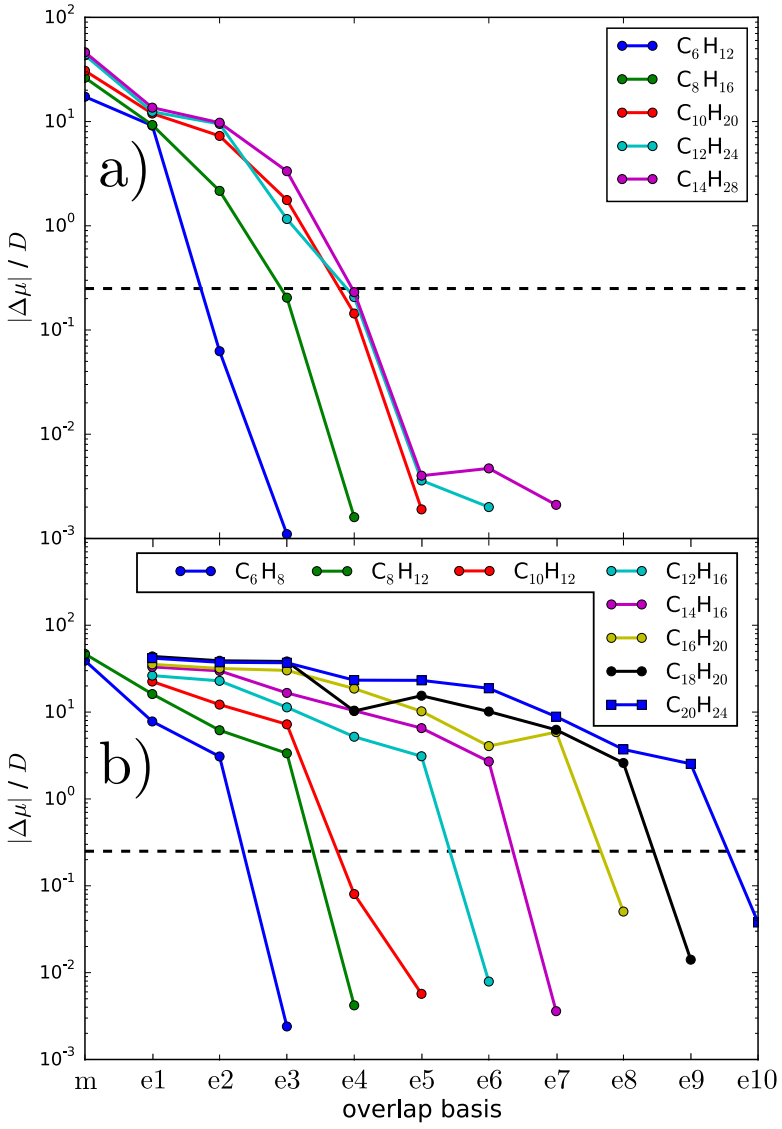

Figure S1: $|\Delta\mu|$ for the FDE(EO,5ft) method with different levels of basis set overlap for (a) alkane-like systems, and (b) conjugated alkenes. The dashed line is the dipole difference threshold of 0.25 D.

4 DZP-Truncated Basis Data

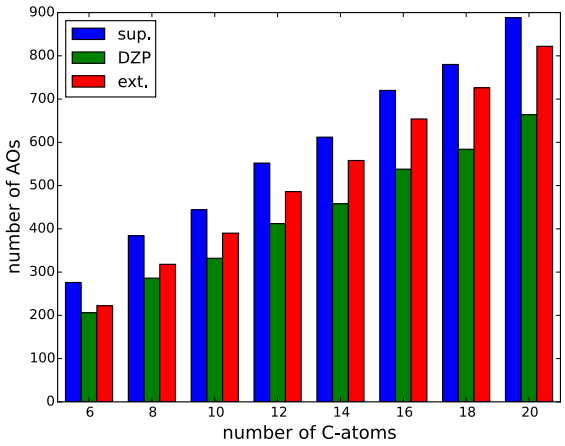

Figure S2: Number of basis functions for the fragments of the conjugated alkenes in the supermolecular basis (sup.), the DZP truncated basis (DZP), and the largest extended monomer basis truncation (exp.).

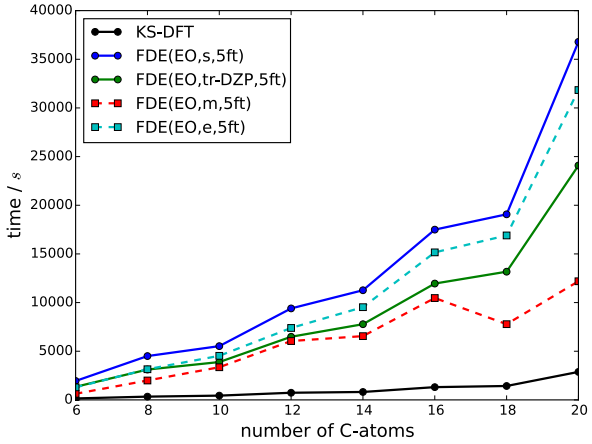

Figure S3: Computation time (on 8 processors) for the KS-DFT method, and various levels of basis set truncations of the FDE(EO) method. FDE(EO,e) represents the largest extended monomer basis truncation.