Electronic Supplementary Material for PCCP

Supporting Information

Table 1: Basis set dependence of interaction energies for the benzene dimer (in kcal mol^{-1}) using the AVnZ basis sets[a]. Density fitting was used in all cases. The DF-SCS-LMP2 structures of Table 1 were used.

		PD(B)			S			T		
Method	n	ΔE	ΔE_{CP}	BSSE	ΔE	ΔE_{CP}	BSSE	ΔE	ΔE_{CP}	BSSE
HF	2	2.275	3.557	-1.283	2.697	3.637	-0.939	-0.321	0.780	-1.102
	3	3.310	3.524	-0.214	3.310	3.490	-0.179	0.610	0.794	-0.184
	4	3.461	3.517	-0.056	3.430	3.479	-0.048	0.751	0.793	-0.042
MP2	2	-7.308	-4.049	-3.259	-5.138	-2.800	-2.338	-6.037	-3.032	-3.005
	3	-5.699	-4.365	-1.334	-4.085	-3.065	-1.021	-4.503	-3.297	-1.207
	4	-4.967	-4.468	-0.499	-3.533	-3.142	-0.391	-3.802	-3.373	-0.429
LMP2	2	-4.551	-3.519	-1.031	-3.335	-2.570	-0.765	-3.604	-2.619	-0.985
	3	-4.265	-4.059	-0.206	-3.068	-2.892	-0.176	-3.300	-3.108	-0.192
	4	-4.302	-4.266	-0.037	-3.041	-3.009	-0.032	-3.283	-3.254	-0.029
SCS-MP2	2	-5.758	-2.444	-3.314	-3.910	-1.529	-2.382	-5.143	-2.095	-3.048
	3	-4.130	-2.705	-1.425	-2.850	-1.758	-1.092	-3.617	-2.329	-1.288
	4	-3.348	-2.798	-0.550	-2.256	-1.826	-0.430	-2.877	-2.404	-0.473
SCS-LMP2	2	-3.070	-2.038	-1.033	-2.146	-1.379	-0.767	-2.746	-1.761	-0.986
	3	-2.667	-2.457	-0.210	-1.809	-1.630	-0.179	-2.371	-2.175	-0.196
	4	-2.667	-2.629	-0.038	-1.753	-1.721	-0.033	-2.334	-2.304	-0.030