Supplementary Material

Long-Range Exchange Limit and Dispersion in Pure Silica Zeolites

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Table S1 Differences ΔE, of the calculated interaction energies with respect to the reference values, in kcal/mol, for lsPBE and lsRPBE exchange families using PBE correlation.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
001_H_2O-NH_3_A24	-0.353	-0.533	-0.573	0.767	0.527	0.287	0.217	1.517
002_H_2O-H_2O_A24	-0.546	-0.616	-0.606	0.224	0.124	-0.026	-0.066	0.874
003_HCN-HCN_A24	-0.365	-0.325	-0.295	-0.045	-0.075	-0.145	-0.165	0.355
004_HF-HF_A24	-0.291	-0.311	-0.291	0.349	0.299	0.169	0.139	0.969
005_NH_3-NH_3_A24	-0.477	-0.437	-0.397	-0.067	-0.077	-0.167	-0.187	0.463
006_HF-CH_4_A24	-0.144	-0.114	-0.084	0.216	0.176	0.086	0.056	0.666
007_NH_3-CH_4_A24	0.025	0.105	0.145	0.005	0.035	0.025	0.035	0.185
008_H_2O-CH_4_A24	-0.013	0.107	0.157	-0.153	-0.073	-0.053	-0.043	-0.013
009_CH_2O-CH_2O_A24	-1.204	-1.274	-1.264	-0.084	-0.194	-0.434	-0.494	0.946
010_H_2O-C_2H_4_A24	-0.317	-0.287	-0.257	0.063	0.053	-0.037	-0.067	0.553
011_CH_2O-C_2H_4_A24	-0.701	-0.571	-0.501	-0.591	-0.511	-0.551	-0.551	-0.141
012_C_2H_2-C_2H_2_A24	-0.174	-0.074	-0.034	-0.154	-0.114	-0.144	-0.144	0.096
013_NH_3-C_2H_4_A24	-0.234	-0.134	-0.084	-0.184	-0.134	-0.164	-0.164	0.116
014_C_2H_4-C_2H_4_A24	-0.560	-0.400	-0.330	-0.590	-0.480	-0.500	-0.490	-0.210
015_CH_4-C_2H_4_A24	-0.042	0.058	0.108	-0.162	-0.122	-0.112	-0.112	-0.062
016_BH_3-CH_4_A24	-0.685	-0.745	-0.735	0.095	-0.035	-0.225	-0.285	0.825
017_CH_4-C_2H_6_A24	-0.527	-0.327	-0.237	-0.727	-0.597	-0.577	-0.567	-0.437
018_CH_4-C_2H_6_A24	-0.297	-0.127	-0.057	-0.527	-0.427	-0.397	-0.387	-0.337
019_CH_4-CH_4_A24	-0.213	-0.033	0.037	-0.453	-0.353	-0.333	-0.313	-0.293
020_Ar-CH_4_A24	-0.015	0.125	0.185	-0.265	-0.195	-0.175	-0.155	-0.185
021_Ar-C_2H_4_A24	0.006	0.126	0.166	-0.204	-0.164	-0.144	-0.124	-0.154
022_C_2H_4-C_2H_2_A24	-0.819	-0.709	-0.649	-0.729	-0.659	-0.689	-0.689	-0.359
023_C_2H_4-C_2H_4_A24	-0.966	-0.866	-0.816	-0.846	-0.776	-0.816	-0.826	-0.436
024_C_2H_2-C_2H_2_A24	-0.695	-0.575	-0.515	-0.665	-0.565	-0.585	-0.585	-0.315
025_NH_3-NH_3_S26	-0.460	-0.460	-0.430	0.050	-0.010	-0.130	-0.150	0.600
026_H_2O-H_2O_S26	-0.560	-0.670	-0.680	0.350	0.170	-0.010	-0.060	1.010
027_CH_4O-CH_4O_S26	-1.020	-1.190	-1.210	0.100	-0.180	-0.420	-0.490	0.880
028_CH_4O-CH_2O_S26	-1.390	-1.570	-1.600	-0.080	-0.350	-0.630	-0.710	0.850
029_C_2H_5NO-C_2H_5NO_S26	-1.470	-1.450	-1.410	-0.750	-0.810	-0.960	-1.000	0.020
030_C_2H_5NO-C_2H_5NO_S26	-4.600	-4.940	-5.010	-2.630	-3.010	-3.390	-3.500	-1.360
031_CH_2O_2-CH_2O_2_S26	-2.680	-3.720	-4.030	1.390	0.210	-0.660	-0.940	3.350
032_CH_3NO-CH_3NO_S26	-2.980	-3.590	-3.750	-0.030	-0.700	-1.300	-1.480	1.680
033_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S26	-4.430	-5.160	-5.360	-1.110	-1.990	-2.700	-2.920	0.700
034_C_5H_5NOa-$C_5H_6N_2$_S26	-2.990	-3.650	-3.830	0.080	-0.690	-1.350	-1.550	1.820
035_$C_5H_5N_5$-$C_5H_6N_2O_2$_S26	-3.540	-4.110	-4.260	-0.600	-1.230	-1.850	-2.040	1.240
036_CH_4-CH_4_S26	-0.100	0.060	0.130	-0.380	-0.300	-0.260	-0.250	-0.280
037_C_2H_4-C_2H_4_S26	-1.160	-0.970	-0.870	-1.070	-0.920	-0.960	-0.960	-0.500
038_C_6H_6-CH_4_S26	-1.580	-1.460	-1.390	-1.360	-1.280	-1.330	-1.340	-0.850
039_C_6H_6-C_6H_6_S26	-5.170	-5.110	-5.040	-4.090	-4.060	-4.290	-4.340	-2.810

Table S1 Continued.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
040_$C_4H_4N_2$-$C_4H_4N_2$_S26	-5.840	-5.830	-5.770	-4.520	-4.520	-4.800	-4.880	-3.070
041_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S26	-8.290	-8.310	-8.240	-6.380	-6.390	-6.780	-6.890	-4.330
042_C_8H_7N-C_6H_6_S26	-8.500	-8.570	-8.520	-6.560	-6.630	-7.030	-7.140	-4.660
043_$C_5H_5N_5$-$C_5H_6N_2O_2$_S26	-12.470	-12.620	-12.560	-9.540	-9.540	-10.12	-10.27	-6.650
044_C_2H_4-C_2H_2_S26	-0.230	-0.140	-0.090	-0.200	-0.160	-0.180	-0.180	0.050
045_C_6H_6-H_2O_S26	-1.440	-1.410	-1.370	-0.940	-0.980	-1.100	-1.130	-0.350
046_C_6H_6-NH_3_S26	-1.470	-1.380	-1.320	-1.160	-1.130	-1.210	-1.230	-0.630
047_C_6H_6-HCN_S26	-1.900	-1.930	-1.920	-1.120	-1.220	-1.410	-1.460	-0.370
048_C_6H_6-C_6H_6_S26	-2.480	-2.410	-2.350	-1.910	-1.920	-2.050	-2.090	-1.160
049_C_8H_7N-C_6H_6_S26	-3.980	-4.010	-3.980	-2.940	-3.030	-3.280	-3.360	-1.850
050_C_6H_6O-C_6H_6O_S26	-3.900	-3.980	-3.950	-2.490	-2.580	-2.850	-2.920	-1.190
051_H_2O-H_2O_S66	-0.570	-0.640	-0.640	0.210	0.100	-0.060	-0.100	0.860
052_H_2O-CH_4O_S66	-1.030	-1.120	-1.130	-0.090	-0.240	-0.430	-0.490	0.680
053_H_2O-CH_5N_S66	-0.520	-0.750	-0.800	0.710	0.410	0.140	0.060	1.500
054_H_2O-C_3H_7NO_S66	-1.710	-1.890	-1.910	-0.330	-0.560	-0.850	-0.930	0.740
055_CH_4O-CH_4O_S66	-1.290	-1.440	-1.470	-0.200	-0.450	-0.690	-0.760	0.590
056_CH_4O-CH_5N_S66	-1.220	-1.500	-1.570	0.240	-0.160	-0.510	-0.630	1.200
057_CH_4O-C_3H_7NO_S66	-2.220	-2.430	-2.470	-0.740	-1.040	-1.360	-1.460	0.370
058_CH_4O-H_2O_S66	-0.760	-0.880	-0.900	0.150	-0.050	-0.250	-0.310	0.820
059_CH_5N-CH_4O_S66	-0.960	-0.880	-0.830	-0.600	-0.600	-0.700	-0.720	-0.030
060_CH_5N-CH_5N_S66	-1.570	-1.590	-1.570	-0.750	-0.820	-1.010	-1.070	0.130
061_CH_5N-C_3H_7NO_S66	-2.750	-2.710	-2.650	-1.860	-1.850	-2.040	-2.080	-0.770
062_CH_5N-H_2O_S66	-0.960	-1.180	-1.230	0.370	0.070	-0.220	-0.310	1.280
063_C_3H_7NO-CH_4O_S66	-2.270	-2.210	-2.150	-1.570	-1.560	-1.700	-1.730	-0.680
064_C_3H_7NO-CH_5N_S66	-2.200	-2.280	-2.270	-1.170	-1.320	-1.560	-1.630	-0.210
065_C_3H_7NO-C_3H_7NO_S66	-3.050	-3.160	-3.150	-1.750	-1.910	-2.200	-2.280	-0.570
066_C_3H_7NO-H_2O_S66	-1.100	-1.090	-1.060	-0.510	-0.550	-0.680	-0.710	0.150
067_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S66	-3.590	-4.200	-4.350	-0.650	-1.330	-1.940	-2.130	1.100
068_H_2O-C_5H_5N_S66	-0.700	-0.870	-0.910	0.420	0.170	-0.070	-0.140	1.190
069_CH_4O-C_5H_5N_S66	-1.260	-1.520	-1.580	0.110	-0.280	-0.600	-0.700	0.960
070_$C_2H_4O_2$-$C_2H_4O_2$_S66	-2.960	-3.970	-4.270	1.030	-0.100	-0.970	-1.250	3.000
071_C_2H_5NO-C_2H_5NO_S66	-3.170	-3.770	-3.930	-0.280	-0.920	-1.520	-1.710	1.440
072_$C_2H_4O_2$-$C_4H_4N_2O_2$_S66	-3.610	-4.430	-4.670	-0.100	-1.010	-1.760	-2.000	1.790
073_C_2H_5NO-$C_4H_4N_2O_2$_S66	-3.800	-4.480	-4.660	-0.710	-1.450	-2.110	-2.320	1.070
074_C_6H_6-C_6H_6_S66	-4.110	-3.960	-3.860	-3.600	-3.450	-3.580	-3.610	-2.590
075_C_5H_5N-C_5H_5N_S66	-4.500	-4.400	-4.320	-3.790	-3.680	-3.860	-3.910	-2.670
076_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S66	-7.980	-7.950	-7.860	-6.210	-6.040	-6.400	-6.490	-4.070
077_C_6H_6-C_5H_5N_S66	-4.400	-4.290	-4.200	-3.740	-3.620	-3.790	-3.830	-2.650
078_C_6H_6-$C_4H_4N_2O_2$_S66	-6.300	-6.230	-6.150	-5.050	-4.900	-5.170	-5.230	-3.410
079_C_5H_5N-$C_4H_4N_2O_2$_S66	-6.340	-6.260	-6.170	-5.070	-4.910	-5.180	-5.240	-3.400

Table S1 Continued.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
080_C_6H_6-C_2H_4_S66	-2.170	-2.020	-1.940	-1.890	-1.770	-1.840	-1.850	-1.190
081_$C_4H_4N_2O_2$-C_2H_4_S66	-2.830	-2.680	-2.590	-2.310	-2.140	-2.250	-2.270	-1.340
082_$C_4H_4N_2O_2$-C_2H_2_S66	-2.610	-2.480	-2.390	-2.090	-1.950	-2.050	-2.070	-1.180
083_C_5H_5N-C_2H_4_S66	-2.350	-2.230	-2.160	-1.960	-1.860	-1.960	-1.990	-1.200
084_C_5H_{12}n-C_5H_{12}n_S66	-4.610	-4.270	-4.090	-3.940	-3.560	-3.720	-3.740	-2.300
085_C_5H_{12}-C_5H_{12}n_S66	-2.950	-2.690	-2.560	-2.590	-2.340	-2.430	-2.440	-1.510
086_C_5H_{12}-C_5H_{12}_S66	-1.730	-1.480	-1.350	-1.710	-1.480	-1.500	-1.500	-1.000
087_C_5H_{10}-C_5H_{12}_S66	-2.780	-2.530	-2.400	-2.420	-2.180	-2.270	-2.280	-1.400
088_C_5H_{10}-C_5H_{10}_S66	-3.420	-3.170	-3.030	-2.920	-2.650	-2.770	-2.790	-1.670
089_C_6H_6-C_5H_{10}_S66	-4.200	-4.070	-3.980	-3.410	-3.290	-3.480	-3.520	-2.190
090_C_6H_6-C_5H_{12}_S66	-3.090	-2.940	-2.850	-2.640	-2.500	-2.620	-2.650	-1.710
091_$C_4H_4N_2O_2$-C_5H_{12}n_S66	-5.520	-5.300	-5.160	-4.490	-4.190	-4.410	-4.450	-2.750
092_$C_4H_4N_2O_2$-C_5H_{10}_S66	-4.650	-4.420	-4.280	-3.900	-3.600	-3.760	-3.790	-2.430
093_$C_4H_4N_2O_2$-C_5H_{12}_S66	-3.610	-3.380	-3.250	-3.100	-2.840	-2.950	-2.970	-1.930
094_C_2H_4-C_5H_{12}n_S66	-2.080	-1.840	-1.730	-1.860	-1.650	-1.720	-1.720	-1.010
095_C_2H_2-C_5H_{12}n_S66	-1.570	-1.370	-1.260	-1.500	-1.330	-1.370	-1.370	-0.860
096_C_3H_7NO-C_5H_{12}n_S66	-4.830	-4.600	-4.450	-3.950	-3.670	-3.870	-3.920	-2.320
097_C_6H_6-C_6H_6_S66	-2.760	-2.660	-2.590	-2.330	-2.260	-2.380	-2.410	-1.560
098_C_5H_5N-C_5H_5N_S66	-2.960	-2.880	-2.820	-2.390	-2.330	-2.480	-2.510	-1.510
099_C_6H_6-C_5H_5N_S66	-2.830	-2.750	-2.690	-2.310	-2.270	-2.410	-2.450	-1.510
100_C_6H_6-C_2H_2_S66	-1.690	-1.630	-1.580	-1.320	-1.300	-1.410	-1.440	-0.720
101_C_2H_2-C_2H_2_S66	-0.160	-0.060	-0.020	-0.140	-0.090	-0.110	-0.120	0.120
102_C_6H_6-$C_2H_4O_2$_S66	-1.810	-1.830	-1.800	-1.030	-1.030	-1.220	-1.270	-0.150
103_C_6H_6-C_2H_5NO_S66	-2.030	-1.980	-1.930	-1.410	-1.350	-1.490	-1.530	-0.550
104_C_6H_6-H_2O_S66	-1.620	-1.610	-1.580	-1.080	-1.100	-1.240	-1.270	-0.430
105_C_6H_6-CH_4O_S66	-2.720	-2.740	-2.720	-1.860	-1.930	-2.150	-2.220	-0.910
106_C_6H_6-CH_5N_S66	-2.700	-2.640	-2.580	-2.100	-2.070	-2.230	-2.270	-1.220
107_C_6H_6-C_3H_7NO_S66	-3.990	-3.970	-3.920	-3.070	-3.060	-3.300	-3.360	-1.920
108_C_5H_5N-C_5H_5N_S66	-1.990	-1.950	-1.900	-1.380	-1.360	-1.500	-1.530	-0.600
109_C_2H_2-H_2O_S66	-0.320	-0.260	-0.210	-0.120	-0.100	-0.150	-0.160	0.260
110_C_2H_2-$C_2H_4O_2$_S66	-0.320	-0.370	-0.360	0.520	0.480	0.300	0.250	1.350
111_C_5H_{12}n-$C_2H_4O_2$_S66	-2.030	-1.710	-1.550	-1.830	-1.470	-1.510	-1.510	-0.760
112_C_5H_{12}n-C_2H_5NO_S66	-3.300	-3.040	-2.900	-2.730	-2.430	-2.550	-2.570	-1.420
113_C_6H_6-$C_2H_4O_2$_S66	-2.500	-2.350	-2.260	-1.980	-1.800	-1.920	-1.940	-0.980
114_C_3H_7NO-C_2H_4_S66	-2.160	-1.970	-1.870	-1.840	-1.680	-1.770	-1.780	-1.000
115_C_5H_5N-C_2H_2_S66	-0.540	-0.550	-0.530	-0.070	-0.150	-0.270	-0.300	0.400
116_CH_5N-C_5H_5N_S66	-2.640	-2.590	-2.540	-1.870	-1.870	-2.050	-2.100	-0.900
117_CH_4-F_2_X40	0.270	0.430	0.500	0.050	0.130	0.160	0.170	0.180
118_CH_4-Cl_2_X40	-0.490	-0.350	-0.270	-0.460	-0.360	-0.390	-0.390	-0.060
119_CH_4-Br_2_X40	8.300	8.240	8.240	9.060	9.060	8.890	8.850	9.780

Table S1 Continued.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
120_CH_4-I_2_X40	8.140	8.270	8.350	8.330	8.440	8.380	8.370	8.920
121_CH_3F-CH_4_X40	-0.330	-0.130	-0.040	-0.560	-0.440	-0.410	-0.400	-0.320
122_CH_3Cl-CH_4_X40	-0.680	-0.480	-0.390	-0.810	-0.670	-0.670	-0.660	-0.460
123_CHF_3-CH_4_X40	-0.240	-0.030	0.060	-0.550	-0.430	-0.400	-0.380	-0.370
124_$CHCl_3$-CH_4_X40	-1.050	-0.830	-0.730	-1.140	-0.990	-0.990	-0.980	-0.700
125_CH_3F-CH_3F_X40	-0.400	-0.180	-0.080	-0.660	-0.490	-0.440	-0.420	-0.430
126_CH_3Cl-CH_3Cl_X40	-0.610	-0.430	-0.350	-0.740	-0.610	-0.600	-0.590	-0.430
127_$C_6H_3F_3$-C_6H_6_X40	-5.500	-5.410	-5.320	-4.430	-4.400	-4.630	-4.690	-3.090
128_C_6F_6-C_6H_6_X40	-6.350	-6.300	-6.220	-5.040	-5.090	-5.380	-5.450	-3.560
129_CH_3Cl-CH_2O_X40	-0.650	-0.500	-0.420	-0.570	-0.460	-0.490	-0.490	-0.130
130_CH_3Br-CH_2O_X40	7.770	7.640	7.800	8.530	8.450	8.300	8.260	9.260
131_CH_3I-CH_2O_X40	5.650	5.550	5.760	6.070	6.110	5.990	5.960	6.730
132_CF_3Cl-CH_2O_X40	-1.060	-0.950	-0.880	-0.770	-0.690	-0.740	-0.750	-0.210
133_CF_3Br-CH_2O_X40	7.360	7.180	7.330	8.260	8.150	7.970	7.930	9.040
134_CF_3I-CH_2O_X40	6.860	6.680	6.860	7.540	7.490	7.330	7.290	8.270
135_C_6H_5Cl-C_3H_6O_X40	-1.180	-1.020	-0.940	-1.040	-0.910	-0.950	-0.950	-0.510
136_C_6H_5Br-C_3H_6O_X40	3.420	3.040	3.380	4.360	4.210	4.000	3.940	5.170
137_C_6H_5I-C_3H_6O_X40	2.850	4.290	4.650	5.480	5.320	5.090	3.020	6.220
138_C_6H_5Cl-C_3H_9N_X40	-1.450	-1.380	-1.330	-1.030	-1.020	-1.110	-1.140	-0.410
139_C_6H_5Br-C_3H_9N_X40	6.290	5.600	5.910	8.000	7.590	7.180	7.060	9.140
140_C_6H_5I-C_3H_9N_X40	4.590	3.760	4.100	6.730	6.090	5.560	5.390	8.090
141_C_6H_5Br-CH_4S_X40	1.170	0.810	0.940	2.350	2.070	1.780	1.680	3.180
142_C_6H_5I-CH_4S_X40	-0.200	-0.560	-0.410	1.050	0.670	0.330	0.230	1.940
143_CH_3Br-C_6H_6_X40	9.540	8.950	9.300	10.84	10.58	10.27	10.18	11.77
144_CH_3I-C_6H_6_X40	6.710	6.060	6.450	8.020	7.590	7.220	7.100	8.940
145_CF_3Br-C_6H_6_X40	8.480	7.760	8.080	10.14	9.780	9.390	9.27	11.19
146_CF_3I-C_6H_6_X40	6.150	5.410	5.770	7.850	7.270	6.810	6.660	8.940
147_$CHOF_3$-H_2O_X40	-1.330	-1.620	-1.690	0.250	-0.140	-0.470	-0.570	1.230
148_$CHOCl_3$-H_2O_X40	-1.460	-1.840	-1.940	0.480	-0.010	-0.440	-0.580	1.660
149_HF-CH_4O_X40	-0.990	-1.260	-1.320	0.540	0.170	-0.130	-0.220	1.450
150_HCl-CH_4O_X40	-0.840	-1.050	-1.100	0.430	0.110	-0.170	-0.250	1.270
151_HBr-CH_4O_X40	-9.750	-10.110	-9.960	-8.320	-8.520	-8.880	-8.990	-7.100
152_HI-CH_4O_X40	-8.830	-9.190	-9.030	-7.600	-7.840	-8.140	-8.230	-6.670
153_HF-CH_5N_X40	-0.530	-1.050	-1.200	1.640	0.970	0.500	0.340	2.720
154_HCl-CH_5N_X40	-0.600	-1.330	-1.570	2.010	1.060	0.390	0.160	3.210
155_CH_4O-CH_3F_X40	-1.040	-0.990	-0.940	-0.540	-0.540	-0.640	-0.660	0.090
156_CH_4O-CH_3Cl_X40	-1.190	-1.170	-1.130	-0.550	-0.590	-0.740	-0.770	0.170

Table S2 Differences ΔE, of the calculated interaction energies with respect to the reference values, in kcal/mol, for lsPBE and lsRPBE exchange families using PW91 correlation.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
001_H_2O-NH_3_A24	-0.313	-0.563	-0.643	0.177	0.567	0.257	0.147	0.927
002_H_2O-H_2O_A24	-0.496	-0.646	-0.676	-0.166	0.174	-0.056	-0.136	0.474
003_HCN-HCN_A24	-0.335	-0.345	-0.335	-0.255	-0.035	-0.165	-0.195	0.145
004_HF-HF_A24	-0.241	-0.341	-0.361	0.029	0.349	0.139	0.079	0.639
005_NH_3-NH_3_A24	-0.437	-0.457	-0.437	-0.337	-0.037	-0.187	-0.227	0.173
006_HF-CH_4_A24	-0.124	-0.134	-0.114	-0.054	0.206	0.066	0.026	0.396
007_NH_3-CH_4_A24	0.045	0.105	0.135	-0.045	0.055	0.025	0.015	0.135
008_H_2O-CH_4_A24	0.007	0.097	0.147	-0.143	-0.053	-0.063	-0.063	-0.003
009_CH_2O-CH_2O_A24	-1.134	-1.314	-1.344	-0.724	-0.124	-0.474	-0.574	0.286
010_H_2O-C_2H_4_A24	-0.287	-0.307	-0.297	-0.217	0.083	-0.057	-0.107	0.263
011_CH_2O-C_2H_4_A24	-0.661	-0.591	-0.541	-0.741	-0.471	-0.561	-0.591	-0.301
012_C_2H_2-C_2H_2_A24	-0.154	-0.084	-0.044	-0.244	-0.094	-0.154	-0.164	-0.004
013_NH_3-C_2H_4_A24	-0.204	-0.144	-0.114	-0.284	-0.114	-0.174	-0.194	0.006
014_C_2H_4-C_2H_4_A24	-0.530	-0.420	-0.360	-0.670	-0.450	-0.510	-0.520	-0.310
015_CH_4-C_2H_4_A24	-0.022	0.058	0.098	-0.162	-0.112	-0.122	-0.122	-0.062
016_BH_3-CH_4_A24	-0.655	-0.765	-0.775	-0.445	-0.005	-0.245	-0.325	0.265
017_CH_4-C_2H_6_A24	-0.497	-0.337	-0.267	-0.737	-0.557	-0.587	-0.587	-0.457
018_CH_4-C_2H_6_A24	-0.277	-0.137	-0.077	-0.507	-0.397	-0.407	-0.407	-0.327
019_CH_4-CH_4_A24	-0.183	-0.043	0.017	-0.423	-0.333	-0.343	-0.333	-0.273
020_Ar-CH_4_A24	-0.005	0.125	0.175	-0.215	-0.185	-0.175	-0.165	-0.145
021_Ar-C_2H_4_A24	0.016	0.116	0.156	-0.164	-0.154	-0.144	-0.134	-0.114
022_C_2H_4-C_2H_2_A24	-0.789	-0.729	-0.689	-0.859	-0.619	-0.709	-0.729	-0.489
023_C_2H_4-C_2H_4_A24	-0.936	-0.886	-0.846	-0.986	-0.736	-0.836	-0.856	-0.596
024_C_2H_2-C_2H_2_A24	-0.665	-0.595	-0.545	-0.745	-0.535	-0.605	-0.615	-0.405
025_NH_3-NH_3_S26	-0.420	-0.480	-0.480	-0.260	0.030	-0.150	-0.200	0.270
026_H_2O-H_2O_S26	-0.510	-0.700	-0.750	-0.100	0.220	-0.050	-0.130	0.550
027_CH_4O-CH_4O_S26	-0.980	-1.220	-1.280	-0.500	-0.130	-0.450	-0.560	0.280
028_CH_4O-CH_2O_S26	-1.340	-1.610	-1.680	-0.780	-0.300	-0.660	-0.790	0.130
029_C_2H_5NO-C_2H_5NO_S26	-1.400	-1.480	-1.480	-1.180	-0.750	-1.000	-1.080	-0.410
030_C_2H_5NO-C_2H_5NO_S26	-4.530	-4.990	-5.130	-3.590	-2.930	-3.440	-3.610	-2.330
031_CH_2O_2-CH_2O_2_S26	-2.630	-3.790	-4.200	-0.610	0.260	-0.730	-1.110	1.340
032_CH_3NO-CH_3NO_S26	-2.900	-3.660	-3.910	-1.490	-0.620	-1.370	-1.640	0.200
033_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S26	-4.370	-5.230	-5.510	-2.800	-1.930	-2.760	-3.070	-1.010
034_C_5H_5NOa-$C_5H_6N_2$_S26	-2.930	-3.710	-3.970	-1.550	-0.640	-1.400	-1.690	0.180
035_$C_5H_5N_5$-$C_5H_6N_2O_2$_S26	-3.470	-4.180	-4.400	-2.180	-1.160	-1.910	-2.180	-0.350
036_CH_4-CH_4_S26	-0.080	0.060	0.120	-0.330	-0.280	-0.270	-0.260	-0.240
037_C_2H_4-C_2H_4_S26	-1.110	-0.990	-0.910	-1.240	-0.880	-0.980	-1.000	-0.690
038_C_6H_6-CH_4_S26	-1.540	-1.480	-1.430	-1.580	-1.240	-1.350	-1.380	-1.080
039_C_6H_6-C_6H_6_S26	-5.090	-5.150	-5.120	-4.820	-3.980	-4.330	-4.430	-3.580

Table S2 Continued.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
040_$C_4H_4N_2$-$C_4H_4N_2$_S26	-5.750	-5.870	-5.860	-5.370	-4.440	-4.850	-4.980	-3.970
041_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S26	-8.170	-8.380	-8.370	-7.570	-6.260	-6.850	-7.030	-5.570
042_C_8H_7N-C_6H_6_S26	-8.400	-8.630	-8.640	-7.790	-6.530	-7.100	-7.270	-5.950
043_$C_5H_5N_5$-$C_5H_6N_2O_2$_S26	-12.31	-12.71	-12.75	-11.39	-9.370	-10.21	-10.47	-8.590
044_C_2H_4-C_2H_2_S26	-0.210	-0.150	-0.110	-0.300	-0.140	-0.200	-0.210	-0.060
045_C_6H_6-H_2O_S26	-1.410	-1.420	-1.410	-1.310	-0.950	-1.120	-1.170	-0.730
046_C_6H_6-NH_3_S26	-1.430	-1.400	-1.360	-1.430	-1.100	-1.230	-1.270	-0.920
047_C_6H_6-HCN_S26	-1.870	-1.950	-1.950	-1.690	-1.200	-1.420	-1.500	-0.960
048_C_6H_6-C_6H_6_S26	-2.440	-2.440	-2.400	-2.370	-1.870	-2.080	-2.140	-1.640
049_C_8H_7N-C_6H_6_S26	-3.950	-4.040	-4.030	-3.720	-3.000	-3.310	-3.410	-2.650
050_C_6H_6O-C_6H_6O_S26	-3.810	-4.030	-4.060	-3.280	-2.490	-2.910	-3.040	-2.010
051_H_2O-H_2O_S66	-0.520	-0.670	-0.700	-0.190	0.150	-0.090	-0.170	0.450
052_H_2O-CH_4O_S66	-0.970	-1.160	-1.200	-0.570	-0.180	-0.470	-0.560	0.190
053_H_2O-CH_5N_S66	-0.490	-0.780	-0.870	0.050	0.450	0.110	-0.010	0.840
054_H_2O-C_3H_7NO_S66	-1.650	-1.930	-2.010	-1.050	-0.490	-0.890	-1.030	0.010
055_CH_4O-CH_4O_S66	-1.250	-1.470	-1.530	-0.780	-0.410	-0.720	-0.830	0.000
056_CH_4O-CH_5N_S66	-1.200	-1.520	-1.630	-0.590	-0.140	-0.540	-0.680	0.360
057_CH_4O-C_3H_7NO_S66	-2.160	-2.470	-2.550	-1.530	-0.980	-1.400	-1.550	-0.440
058_CH_4O-H_2O_S66	-0.720	-0.910	-0.950	-0.340	-0.020	-0.280	-0.370	0.330
059_CH_5N-CH_4O_S66	-0.920	-0.910	-0.880	-0.870	-0.560	-0.720	-0.770	-0.300
060_CH_5N-CH_5N_S66	-1.530	-1.620	-1.630	-1.270	-0.770	-1.040	-1.130	-0.420
061_CH_5N-C_3H_7NO_S66	-2.680	-2.750	-2.730	-2.420	-1.770	-2.080	-2.170	-1.360
062_CH_5N-H_2O_S66	-0.920	-1.220	-1.310	-0.350	0.110	-0.260	-0.390	0.550
063_C_3H_7NO-CH_4O_S66	-2.190	-2.250	-2.230	-1.970	-1.480	-1.740	-1.810	-1.100
064_C_3H_7NO-CH_5N_S66	-2.150	-2.310	-2.340	-1.800	-1.270	-1.590	-1.700	-0.850
065_C_3H_7NO-C_3H_7NO_S66	-2.980	-3.200	-3.240	-2.500	-1.850	-2.240	-2.370	-1.340
066_C_3H_7NO-H_2O_S66	-1.050	-1.120	-1.120	-0.850	-0.500	-0.700	-0.770	-0.210
067_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S66	-3.510	-4.260	-4.510	-2.120	-1.250	-2.010	-2.290	-0.380
068_H_2O-C_5H_5N_S66	-0.650	-0.910	-0.980	-0.160	0.220	-0.100	-0.210	0.610
069_CH_4O-C_5H_5N_S66	-1.230	-1.540	-1.640	-0.640	-0.260	-0.630	-0.760	0.210
070_$C_2H_4O_2$-$C_2H_4O_2$_S66	-2.910	-4.040	-4.430	-0.940	-0.060	-1.030	-1.410	1.030
071_C_2H_5NO-C_2H_5NO_S66	-3.090	-3.840	-4.080	-1.720	-0.850	-1.590	-1.860	-0.020
072_$C_2H_4O_2$-$C_4H_4N_2O_2$_S66	-3.550	-4.510	-4.840	-1.830	-0.950	-1.830	-2.160	0.040
073_C_2H_5NO-$C_4H_4N_2O_2$_S66	-3.740	-4.540	-4.810	-2.260	-1.390	-2.180	-2.470	-0.500
074_C_6H_6-C_6H_6_S66	-4.050	-3.990	-3.930	-4.030	-3.370	-3.610	-3.680	-3.050
075_C_5H_5N-C_5H_5N_S66	-4.440	-4.430	-4.380	-4.350	-3.620	-3.900	-3.980	-3.260
076_$C_4H_4N_2O_2$-$C_4H_4N_2O_2$_S66	-7.850	-8.020	-8.000	-7.320	-5.900	-6.480	-6.650	-5.240
077_C_6H_6-C_5H_5N_S66	-4.340	-4.320	-4.270	-4.260	-3.550	-3.820	-3.900	-3.200
078_C_6H_6-$C_4H_4N_2O_2$_S66	-6.200	-6.290	-6.250	-5.890	-4.790	-5.230	-5.350	-4.290
079_C_5H_5N-$C_4H_4N_2O_2$_S66	-6.230	-6.320	-6.290	-5.900	-4.800	-5.240	-5.360	-4.280

Table S2 Continued.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
080_C_6H_6-C_2H_4_S66	-2.120	-2.050	-1.990	-2.150	-1.710	-1.870	-1.910	-1.480
081_$C_4H_4N_2O_2$-C_2H_4_S66	-2.750	-2.720	-2.670	-2.700	-2.060	-2.290	-2.360	-1.760
082_$C_4H_4N_2O_2$-C_2H_2_S66	-2.530	-2.520	-2.470	-2.470	-1.870	-2.090	-2.160	-1.580
083_C_5H_5N-C_2H_4_S66	-2.300	-2.260	-2.210	-2.290	-1.810	-1.990	-2.040	-1.560
084_C_5H_{12}n-C_5H_{12}n_S66	-4.490	-4.330	-4.200	-4.510	-3.440	-3.780	-3.860	-2.940
085_C_5H_{12}-C_5H_{12}n_S66	-2.870	-2.730	-2.630	-2.950	-2.250	-2.470	-2.520	-1.910
086_C_5H_{12}-C_5H_{12}_S66	-1.680	-1.510	-1.410	-1.880	-1.420	-1.530	-1.550	-1.200
087_C_5H_{10}-C_5H_{12}_S66	-2.700	-2.570	-2.480	-2.760	-2.100	-2.310	-2.360	-1.780
088_C_5H_{10}-C_5H_{10}_S66	-3.330	-3.210	-3.110	-3.360	-2.560	-2.810	-2.880	-2.160
089_C_6H_6-C_5H_{10}_S66	-4.120	-4.110	-4.050	-4.010	-3.220	-3.520	-3.600	-2.830
090_C_6H_6-C_5H_{12}_S66	-3.040	-2.970	-2.910	-3.040	-2.440	-2.650	-2.710	-2.140
091_$C_4H_4N_2O_2$-C_5H_{12}n_S66	-5.400	-5.360	-5.280	-5.240	-4.070	-4.470	-4.580	-3.550
092_$C_4H_4N_2O_2$-C_5H_{10}_S66	-4.550	-4.480	-4.390	-4.470	-3.490	-3.810	-3.900	-3.060
093_$C_4H_4N_2O_2$-C_5H_{12}_S66	-3.520	-3.430	-3.340	-3.530	-2.740	-3.000	-3.060	-2.400
094_C_2H_4-C_5H_{12}n_S66	-2.010	-1.870	-1.780	-2.130	-1.580	-1.750	-1.780	-1.310
095_C_2H_2-C_5H_{12}n_S66	-1.520	-1.390	-1.310	-1.670	-1.280	-1.400	-1.420	-1.060
096_C_3H_7NO-C_5H_{12}n_S66	-4.720	-4.650	-4.550	-4.630	-3.560	-3.930	-4.020	-3.050
097_C_6H_6-C_6H_6_S66	-2.720	-2.680	-2.630	-2.710	-2.210	-2.400	-2.460	-1.960
098_C_5H_5N-C_5H_5N_S66	-2.920	-2.910	-2.870	-2.840	-2.280	-2.500	-2.570	-1.990
099_C_6H_6-C_5H_5N_S66	-2.790	-2.770	-2.730	-2.740	-2.230	-2.440	-2.490	-1.970
100_C_6H_6-C_2H_2_S66	-1.670	-1.640	-1.610	-1.660	-1.280	-1.430	-1.480	-1.080
101_C_2H_2-C_2H_2_S66	-0.140	-0.070	-0.040	-0.230	-0.070	-0.130	-0.140	0.020
102_C_6H_6-$C_2H_4O_2$_S66	-1.770	-1.850	-1.860	-1.590	-0.990	-1.250	-1.330	-0.730
103_C_6H_6-C_2H_5NO_S66	-1.980	-2.010	-1.990	-1.850	-1.300	-1.530	-1.590	-1.020
104_C_6H_6-H_2O_S66	-1.590	-1.630	-1.620	-1.480	-1.070	-1.250	-1.310	-0.840
105_C_6H_6-CH_4O_S66	-2.680	-2.760	-2.760	-2.480	-1.890	-2.170	-2.260	-1.550
106_C_6H_6-CH_5N_S66	-2.660	-2.660	-2.630	-2.570	-2.020	-2.250	-2.320	-1.730
107_C_6H_6-C_3H_7NO_S66	-3.940	-3.990	-3.970	-3.750	-3.010	-3.330	-3.420	-2.630
108_C_5H_5N-C_5H_5N_S66	-1.940	-1.970	-1.950	-1.790	-1.310	-1.530	-1.590	-1.030
109_C_2H_2-H_2O_S66	-0.290	-0.270	-0.250	-0.280	-0.060	-0.160	-0.190	0.090
110_C_2H_2-$C_2H_4O_2$_S66	-0.270	-0.400	-0.430	-0.010	0.530	0.270	0.180	0.810
111_C_5H_{12}n-$C_2H_4O_2$_S66	-1.940	-1.760	-1.640	-2.110	-1.370	-1.560	-1.600	-1.080
112_C_5H_{12}n-C_2H_5NO_S66	-3.200	-3.090	-2.990	-3.200	-2.330	-2.600	-2.670	-1.930
113_C_6H_6-$C_2H_4O_2$_S66	-2.430	-2.390	-2.330	-2.420	-1.730	-1.960	-2.020	-1.460
114_C_3H_7NO-C_2H_4_S66	-2.090	-2.000	-1.930	-2.140	-1.610	-1.800	-1.840	-1.330
115_C_5H_5N-C_2H_2_S66	-0.510	-0.560	-0.570	-0.390	-0.130	-0.290	-0.340	0.080
116_CH_5N-C_5H_5N_S66	-2.580	-2.620	-2.600	-2.390	-1.810	-2.080	-2.160	-1.450
117_CH_4-F_2_X40	0.290	0.420	0.480	0.070	0.150	0.150	0.160	0.210
118_CH_4-Cl_2_X40	-0.460	-0.360	-0.300	-0.580	-0.330	-0.400	-0.420	-0.190
119_CH_4-Br_2_X40	8.340	8.210	8.190	8.530	9.090	8.870	8.800	9.240

Table S2 Continued.

	ΔE							
	lsRPBE				lsPBE			
Code	PBE	MGEA	mol	sol	PBE	MGEA	mol	sol
120_CH_4-I_2_X40	8.180	8.250	8.310	8.130	8.490	8.360	8.330	8.690
121_CH_3F-CH_4_X40	-0.300	-0.140	-0.070	-0.550	-0.410	-0.420	-0.420	-0.320
122_CH_3Cl-CH_4_X40	-0.640	-0.490	-0.420	-0.860	-0.640	-0.680	-0.690	-0.520
123_CHF_3-CH_4_X40	-0.210	-0.040	0.040	-0.510	-0.400	-0.410	-0.400	-0.330
124_$CHCl_3$-CH_4_X40	-1.00	-0.840	-0.760	-1.210	-0.940	-1.000	-1.010	-0.780
125_CH_3F-CH_3F_X40	-0.360	-0.190	-0.110	-0.610	-0.450	-0.460	-0.450	-0.380
126_CH_3Cl-CH_3Cl_X40	-0.580	-0.440	-0.370	-0.760	-0.570	-0.610	-0.610	-0.460
127_$C_6H_3F_3$-C_6H_6_X40	-5.410	-5.450	-5.410	-5.170	-4.310	-4.680	-4.790	-3.880
128_C_6F_6-C_6H_6_X40	-6.260	-6.350	-6.320	-5.920	-4.990	-5.440	-5.570	-4.490
129_CH_3Cl-CH_2O_X40	-0.610	-0.520	-0.460	-0.690	-0.420	-0.510	-0.520	-0.270
130_CH_3Br-CH_2O_X40	7.850	7.600	7.720	8.200	8.520	8.260	8.180	8.920
131_CH_3I-CH_2O_X40	5.700	5.510	5.670	5.610	6.150	5.950	5.870	6.280
132_CF_3Cl-CH_2O_X40	-1.000	-0.970	-0.940	-0.980	-0.630	-0.770	-0.810	-0.430
133_CF_3Br-CH_2O_X40	7.440	7.140	7.240	7.870	8.220	7.930	7.840	8.640
134_CF_3I-CH_2O_X40	6.920	6.620	6.730	6.950	7.560	7.280	7.160	7.710
135_C_6H_5Cl-C_3H_6O_X40	-1.130	-1.040	-0.980	-1.210	-0.870	-0.970	-1.000	-0.690
136_C_6H_5Br-C_3H_6O_X40	3.490	3.000	3.300	3.860	4.270	3.960	3.860	4.660
137_C_6H_5I-C_3H_6O_X40	4.750	4.250	4.550	4.730	5.350	5.050	4.920	5.470
138_C_6H_5Cl-C_3H_9N_X40	-1.410	-1.410	-1.380	-1.360	-0.970	-1.140	-1.190	-0.750
139_C_6H_5Br-C_3H_9N_X40	6.340	5.570	5.830	7.050	7.640	7.150	6.970	8.170
140_C_6H_5I-C_3H_9N_X40	4.630	3.710	3.990	5.460	6.130	5.510	5.260	6.790
141_C_6H_5Br-CH_4S_X40	1.200	0.780	0.880	1.650	2.100	1.750	1.620	2.470
142_C_6H_5I-CH_4S_X40	-0.170	-0.590	-0.480	0.200	0.700	0.300	0.160	1.080
143_CH_3Br-C_6H_6_X40	9.590	8.920	9.230	10.08	10.63	10.24	10.10	11.00
144_CH_3I-C_6H_6_X40	6.720	6.040	6.410	7.090	7.610	7.190	7.040	7.970
145_CF_3Br-C_6H_6_X40	8.520	7.730	8.000	9.210	9.820	9.360	9.190	10.24
146_CF_3I-C_6H_6_X40	6.170	5.380	5.710	6.700	7.300	6.770	6.580	7.750
147_$CHOF_3$-H_2O_X40	-1.270	-1.660	-1.780	-0.520	-0.080	-0.510	-0.670	0.440
148_$CHOCl_3$-H_2O_X40	-1.420	-1.880	-2.030	-0.550	0.030	-0.480	-0.670	0.620
149_HF-CH_4O_X40	-0.920	-1.310	-1.420	-0.150	0.230	-0.180	-0.330	0.750
150_HCl-CH_4O_X40	-0.800	-1.080	-1.170	-0.240	0.150	-0.200	-0.320	0.590
151_HBr-CH_4O_X40	-9.710	-10.14	-10.03	-9.340	-8.480	-8.910	-9.060	-8.140
152_HI-CH_4O_X40	-8.810	-9.210	-9.070	-8.470	-7.840	-8.170	-8.280	-7.560
153_HF-CH_5N_X40	-0.500	-1.080	-1.280	0.550	0.990	0.460	0.260	1.620
154_HCl-CH_5N_X40	-0.660	-1.330	-1.580	0.510	1.000	0.390	0.150	1.700
155_CH_4O-CH_3F_X40	-0.980	-1.020	-1.000	-0.840	-0.480	-0.670	-0.720	-0.220
156_CH_4O-CH_3Cl_X40	-1.140	-1.190	-1.180	-0.970	-0.540	-0.760	-0.830	-0.260

Table S3 Mean absolute deviation MAD, mean signed deviation MSD, percentage of mean absolute relative deviation %MARD, and standard deviation SD, for the calculated molar volumes V, in cm^3/mol, and for the calculated energy ΔE_c, in kJ/mol, per SiO_2 unit considering different DFAs, of silica zeolites relative to α-quartz.

			V				ΔE_c			
X	C	μ_x	MAD	MSD	%MARD	SD	MAD	MSD	%MARD	SD
LDA	VWN	-	1.81	1.72	5.25	2.18	1.81	1.58	21.17	2.04
PW91	PW91	sol	3.15	3.15	9.13	3.50	6.59	-6.59	68.27	6.51
PBE	PBE	PBE	3.41	3.41	9.87	3.56	6.34	-6.34	65.43	6.30
RPBE	PBE	PBE	4.22	4.22	12.28	4.31	9.40	-9.40	98.37	9.20
PBE0	PBE	PBE	2.67	2.67	7.72	2.81	6.60	-6.60	68.75	6.48
RPBE0	PBE	PBE	3.18	3.18	9.29	3.29	8.75	-8.75	92.03	8.53
B3[a]	LYP	-	3.39	3.39	9.89	5.42	8.68	-8.68	91.53	11.60
PBE0-D[a]	PBE	PBE	1.99	1.96	5.72	3.70	2.60	2.59	29.88	3.80
B3-D[a]	LYP	-	2.41	2.37	6.87	4.28	6.84	6.84	74.81	9.20
lsPBE	PBE	sol	2.63	2.63	7.56	2.89	3.89	-3.89	38.76	4.04
		PBE	3.28	3.28	9.50	3.46	5.83	-5.83	59.87	5.81
		MGEA	3.50	3.50	10.14	3.65	6.13	-6.13	63.25	6.08
		mol	3.55	3.55	10.31	3.70	6.18	-6.18	63.85	6.13
lsRPBE	PBE	sol	3.02	3.02	8.73	3.21	6.54	-6.54	67.40	6.49
		PBE	3.97	3.97	11.53	4.07	7.46	-7.46	77.73	7.33
		MGEA	4.24	4.24	12.33	4.34	7.03	-7.03	73.31	6.91
		mol	4.33	4.33	12.57	4.42	6.83	-6.83	71.18	6.72
lsPBE	PW91	sol	3.21	3.21	9.28	3.38	5.32	-5.32	54.62	5.31
		PBE	3.32	3.32	9.60	3.49	5.71	-5.71	58.71	5.70
		MGEA	3.49	3.49	10.11	3.64	6.17	-6.17	63.73	6.13
		mol	3.56	3.56	10.31	3.71	6.27	-6.27	64.74	6.22
lsRPBE	PW91	sol	3.58	3.58	10.40	3.71	7.49	-7.49	78.00	7.35
		PBE	4.01	4.01	11.64	4.11	7.36	-7.36	76.71	7.23
		MGEA	4.25	4.25	12.35	4.34	7.07	-7.07	73.66	6.95
		mol	4.29	4.29	12.48	4.42	6.89	-6.89	71.82	6.78
lsPBE0	PBE	sol	2.22	2.22	6.38	2.43	4.61	-4.61	47.31	4.62
		PBE	2.62	2.62	7.56	2.78	6.18	-6.18	64.32	6.09
		MGEA	2.75	2.75	7.97	2.89	6.43	-6.43	67.08	6.32
		mol	2.79	2.79	8.09	2.93	6.48	-6.48	67.67	6.37
lsRPBE0	PBE	sol	2.49	2.49	7.20	2.65	6.46	-6.46	67.31	6.36
		PBE	3.03	3.03	8.83	3.15	7.23	-7.23	75.85	7.07
		MGEA	3.20	3.20	9.33	3.31	6.97	-6.97	73.17	6.81
		mol	3.26	3.26	9.50	3.37	6.80	-6.80	71.42	6.65
lsPBE-D	PBE	sol	1.96	1.74	5.72	2.44	7.57	7.57	84.30	7.54
		PBE	2.51	2.51	7.19	2.93	4.59	4.59	51.92	4.76
		MGEA	2.76	2.76	7.92	3.11	4.10	4.10	46.48	4.31
		mol	2.84	2.84	8.16	3.17	4.10	4.10	46.49	4.27
lsRPBE-D	PBE	sol	2.23	2.20	6.42	2.71	3.97	3.97	45.45	4.20
		PBE	3.27	3.17	9.43	3.52	1.87	1.66	21.52	2.28
		MGEA	3.58	3.58	10.31	3.79	2.14	2.05	24.60	2.56
		mol	3.64	3.64	10.50	3.85	2.18	2.11	25.00	2.60

[a]Roman-Roman EI, Zicovich-Wilson CM (2015) Chem Phys Lett 619:109-114.

Table S4 Experimental and calculated molar volumes, in cm^3/mol per SiO_2 unit, for the silica zeolites of framework code FCode, considered using different DFAs. Here qua refers to α-quartz.

			FCode	AFI	AST	CFI	CHA	FAU	FER	IFR	ISV	ITE	MEL	MFI	MTW	MWW	STT	qua
X	C	μ_x	Expt.	33.83	34.83	32.94	39.10	44.77	32.67	35.36	39.21	37.04	33.83	33.51	31.06	36.47	35.78	22.71
LDA	VWN	-		36.09	39.07	36.95	40.90	46.76	35.08	35.49	40.65	37.77	35.22	33.66	34.02	38.61	36.59	22.03
PW91	PW91	sol		37.69	40.16	38.17	42.22	48.11	36.11	37.65	42.43	39.66	36.98	35.94	35.60	36.84	38.44	24.29
PBE	PBE	PBE		37.74	40.30	38.25	42.37	48.18	36.20	37.69	42.52	39.71	37.02	35.89	35.64	39.95	38.47	24.38
RPBE	PBE	PBE		38.44	40.85	38.86	42.98	48.93	36.73	38.84	43.32	40.65	37.67	37.00	36.46	40.57	39.35	25.73
PBE0	PBE	PBE		37.04	39.27	37.32	41.30	47.31	35.32	37.37	41.61	39.09	36.28	35.51	34.95	39.04	37.84	23.84
RPBE0	PBE	PBE		37.46	39.66	37.74	41.73	47.80	35.68	37.86	42.08	39.63	36.73	36.35	35.45	39.45	38.42	24.83
lsPBE	PBE	sol		37.02	39.79	37.72	40.71	47.61	35.74	36.82	41.67	38.84	36.39	34.93	34.95	39.37	37.67	23.27
		PBE		37.69	40.27	38.22	41.21	48.14	36.17	37.62	42.46	39.61	36.98	35.79	35.55	39.90	38.39	24.27
		MGEA		37.86	40.41	38.37	41.75	48.34	36.31	37.84	42.70	39.84	37.14	36.04	35.74	40.06	38.64	24.53
		mol		37.93	40.46	38.42	41.67	48.42	36.35	37.93	42.76	39.95	37.18	36.11	35.81	40.11	38.71	24.61
lsRPBE	PBE	sol		37.44	40.00	37.98	40.96	47.88	35.96	37.30	42.14	39.25	36.75	35.57	35.36	39.66	38.10	23.99
		PBE		38.25	40.71	38.71	42.70	48.73	36.59	38.37	43.10	40.35	37.51	36.61	36.11	40.41	39.14	25.32
		MGEA		38.47	40.96	38.94	43.07	49.01	36.82	38.86	43.41	40.68	37.72	36.86	36.33	40.65	39.40	25.59
		mol		38.54	41.04	39.04	43.16	49.13	36.88	38.94	43.51	40.76	37.79	36.93	36.39	40.76	39.45	25.67
lsPBE	PW91	sol		37.53	40.08	38.08	42.11	48.03	36.02	37.48	42.31	39.53	36.84	35.72	35.45	39.76	38.29	24.10
		PBE		37.69	40.27	38.22	41.41	48.18	36.17	37.65	42.49	39.63	36.98	35.89	35.62	39.92	38.44	24.28
		MGEA		37.86	40.41	38.37	41.70	48.34	36.31	37.84	42.67	39.82	37.14	36.02	35.74	40.06	38.64	24.53
		mol		37.93	40.46	38.44	41.67	48.42	36.37	37.91	42.76	39.90	37.18	36.11	35.81	40.14	38.71	24.64
lsRPBE	PW91	sol		37.88	40.33	38.32	42.37	48.34	36.24	37.91	42.64	40.00	37.16	36.31	35.85	40.00	38.74	24.78
		PBE		38.25	40.71	38.71	42.73	48.77	36.61	38.64	43.13	40.41	37.53	36.66	36.13	40.43	39.19	25.32
		MGEA		38.47	40.99	38.97	43.07	49.01	36.82	38.84	43.41	40.68	37.72	36.86	36.33	40.68	39.40	25.60
		mol		38.54	41.07	39.04	43.20	49.13	36.88	38.94	43.51	40.76	37.79	36.91	36.39	40.76	39.48	25.68
lsPBE0	PBE	sol		36.73	38.94	36.98	40.90	46.90	34.99	36.93	41.10	38.54	35.94	34.87	34.55	38.64	37.30	23.07
		PBE		37.00	39.25	37.30	41.27	47.27	35.30	37.34	41.58	39.04	36.26	35.45	34.91	38.99	37.77	23.64
		MGEA		37.14	39.35	37.41	41.38	47.42	35.39	37.44	41.70	39.17	36.35	35.60	35.03	39.12	37.93	23.95
		mol		37.14	39.40	37.44	41.44	47.42	35.43	37.48	41.78	39.22	36.39	35.66	35.01	39.14	37.98	24.04
lsRPBE0	PBE	sol		36.98	39.09	37.16	41.10	47.13	35.16	37.18	41.38	38.94	36.11	35.36	34.83	38.84	37.58	23.60
		PBE		37.32	39.58	37.65	41.61	47.65	35.60	37.72	41.99	39.48	36.59	36.02	35.34	39.35	38.25	24.47
		MGEA		37.46	39.74	37.79	41.81	47.88	35.74	37.88	42.16	39.63	36.73	36.17	35.49	39.53	38.42	24.74
		mol		37.48	39.79	37.84	41.87	47.95	35.79	37.96	42.22	39.71	36.79	36.24	35.53	39.58	38.49	24.79
lsPBE-D	PBE	sol		36.44	39.71	37.48	38.59	46.98	35.62	35.08	40.99	37.69	35.74	33.34	34.12	39.12	36.31	21.98
		PBE		37.09	40.19	38.00	39.71	47.69	36.04	36.42	41.75	38.57	36.39	34.37	34.81	39.66	37.18	22.86
		MGEA		37.30	40.33	38.17	40.30	47.95	36.17	36.75	41.99	38.84	36.59	34.65	35.01	39.84	37.46	23.15
		mol		37.37	40.38	38.22	40.52	47.99	36.22	36.84	42.08	38.94	36.66	34.73	35.08	39.90	37.55	23.23
lsRPBE-D	PBE	sol		36.82	39.92	37.77	39.07	47.39	35.83	35.98	41.41	38.22	36.17	34.08	34.63	39.40	36.86	22.51
		PBE		37.77	40.63	38.52	40.96	48.34	36.48	37.39	42.52	39.66	37.00	35.32	35.49	40.19	38.05	23.85
		MGEA		38.00	40.87	38.74	41.55	48.69	36.68	37.96	42.83	39.95	37.25	35.60	35.70	40.43	38.37	24.14
		mol		38.08	40.96	38.81	41.67	48.73	36.75	37.84	42.95	39.79	37.32	35.70	35.79	40.54	38.47	24.27
lsPBE-D*	PBE	sol		36.39	39.71	37.48	38.44	46.94	35.62	34.91	40.87	37.60	35.70	33.23	34.06	39.09	36.22	21.88
		PBE		37.09	40.16	23.95	39.63	47.69	36.04	36.42	41.73	38.54	36.44	34.41	34.83	39.66	37.14	22.83
		MGEA		37.30	40.33	38.17	40.11	47.88	36.17	36.88	41.99	38.81	36.59	34.67	34.99	39.82	37.41	23.11
		mol		37.37	40.38	38.22	40.19	47.95	36.22	36.95	42.05	38.89	36.66	34.79	35.03	39.90	37.51	23.19
lsRPBE-D*	PBE	sol		36.82	39.92	37.77	39.07	47.39	35.83	36.02	41.38	38.22	36.20	34.06	34.61	39.40	36.88	22.51
		PBE		37.74	40.65	38.49	40.49	48.30	36.48	37.65	42.49	39.43	36.95	35.32	35.49	40.19	38.03	23.84
		MGEA		38.03	40.87	38.76	40.82	48.65	36.68	38.00	42.83	39.76	37.27	35.66	35.72	40.43	38.37	24.19
		mol		38.12	40.96	38.84	41.27	48.73	36.75	38.12	42.98	39.90	37.34	35.76	35.81	40.52	38.49	24.29

Table S5 Experimental enthalpy of transition ΔH_x, and calculated energy ΔE_c, in kJ/mol per SiO_2 unit, of silica zeolites of framework code FCode, relative to α-quartz using different DFAs.

			FCode	AFI	AST	CFI	CHA	FAU	FER	IFR	ISV	ITE	MEL	MFI	MTW	MWW	STT
X	C	μ_x	Expt.	7.20	10.90	8.80	11.40	13.60	6.60	10.00	14.40	10.10	8.20	6.80	8.70	10.40	9.20
LDA	VWN	-		10.92	13.87	11.61	12.93	13.92	10.35	10.59	12.83	10.65	9.86	8.85	9.74	11.42	10.90
PW91	PW91	sol		2.59	4.89	3.45	3.72	4.61	2.24	3.20	5.12	2.55	1.84	1.32	1.84	3.49	3.16
PBE	PBE	PBE		3.01	5.29	3.94	3.85	4.62	2.54	3.26	5.27	2.71	2.12	1.53	2.29	3.70	3.35
RPBE	PBE	PBE		-0.18	1.92	0.77	0.43	1.24	-0.50	0.54	2.52	-0.32	-0.98	-1.32	-0.73	0.83	0.52
PBE0	PBE	PBE		2.51	4.71	3.05	3.89	5.23	1.91	3.53	5.30	2.57	1.68	1.25	1.55	3.48	3.27
RPBE0	PBE	PBE		0.13	2.36	0.87	1.55	2.90	-0.20	1.60	3.42	0.43	-0.53	-0.84	-0.63	1.48	1.30
lsPBE	PBE	sol		5.64	7.91	6.46	6.37	7.35	5.09	5.48	7.42	5.12	4.73	3.89	4.77	6.05	5.62
		PBE		3.53	5.86	4.46	4.41	5.23	3.05	3.72	5.80	3.25	2.61	1.99	2.76	4.22	3.86
		MGEA		3.15	5.60	4.10	4.15	4.95	2.68	3.48	5.60	2.95	2.23	1.64	2.42	3.95	3.62
		mol		3.07	5.55	4.03	4.14	4.92	2.60	3.43	5.59	2.90	2.15	1.58	2.35	3.91	3.58
lsRPBE	PBE	sol		2.85	4.95	3.69	3.50	4.45	2.43	3.13	4.92	2.52	2.08	1.49	2.12	3.47	3.11
		PBE		1.62	4.18	2.65	2.78	3.51	1.33	2.27	4.50	1.68	0.82	0.38	1.01	2.74	2.42
		MGEA		2.02	4.71	3.03	3.35	4.06	1.66	2.64	5.07	2.13	1.10	0.65	1.36	3.21	2.89
		mol		2.19	4.96	3.26	3.60	4.32	1.83	2.84	5.34	2.34	1.26	0.79	1.53	3.43	3.06
lsPBE	PW91	sol		3.94	6.36	4.75	5.17	6.10	3.39	4.35	6.34	3.82	3.05	2.43	3.10	4.69	4.39
		PBE		3.61	5.97	4.52	4.57	5.42	3.13	3.86	5.94	3.37	2.70	2.08	2.83	4.34	3.99
		MGEA		3.12	5.55	4.08	4.09	4.87	2.65	3.41	5.55	2.89	2.20	1.60	2.39	3.90	3.56
		mol		3.01	5.48	3.99	4.00	4.74	2.55	3.30	5.48	2.80	2.08	1.51	2.32	3.83	3.48
lsRPBE	PW91	sol		1.62	3.92	2.51	2.76	3.72	1.28	2.44	4.33	1.66	0.90	0.46	0.93	2.63	2.34
		PBE		1.70	4.28	2.71	2.92	3.69	1.40	2.38	4.63	1.79	0.90	0.45	1.07	2.84	2.54
		MGEA		2.00	4.68	3.02	3.29	3.98	1.64	2.58	5.03	2.09	1.08	0.63	1.34	3.17	2.85
		mol		2.15	4.91	3.24	3.50	4.15	1.79	2.74	5.25	2.26	1.21	0.74	1.51	3.37	3.02
lsPBE0	PBE	sol		4.61	6.84	5.00	6.07	7.43	3.87	5.38	7.08	4.57	3.73	3.18	3.48	5.34	5.12
		PBE		2.93	5.17	3.44	4.37	5.70	2.30	3.90	5.72	3.00	2.08	1.63	1.93	3.88	3.67
		MGEA		2.61	4.92	3.19	4.13	5.47	2.04	3.67	5.55	2.76	1.77	1.34	1.65	3.67	3.47
		mol		2.54	4.86	3.14	4.08	5.43	1.96	3.63	5.53	2.71	1.70	1.28	1.60	3.63	3.43
lsRPBE0	PBE	sol		2.52	4.78	3.10	4.09	5.44	2.08	3.73	5.39	2.74	1.89	1.46	1.61	3.59	3.38
		PBE		1.63	4.10	2.32	3.36	4.68	1.23	2.95	4.94	1.99	0.89	0.52	0.74	2.95	2.77
		MGEA		1.83	4.44	2.61	3.70	5.02	1.40	3.17	5.33	2.27	1.05	0.67	0.95	3.25	3.06
		mol		1.97	4.66	2.77	3.89	5.23	1.54	3.33	5.53	2.44	1.17	0.79	1.10	3.44	3.24
lsPBE-D	PBE	sol		16.75	20.98	18.31	18.37	19.79	16.56	14.85	18.60	16.26	15.75	13.73	15.53	17.43	19.38
		PBE		13.61	17.73	15.12	15.51	16.51	13.24	12.51	15.90	13.43	12.52	10.93	12.45	14.40	16.73
		MGEA		13.04	17.20	14.54	15.15	16.02	12.64	12.12	15.51	12.99	11.90	10.44	11.89	13.91	16.36
		mol		12.97	17.16	14.47	15.18	16.00	12.56	12.10	15.51	12.97	11.83	10.83	11.81	13.88	16.37
lsRPBE-D	PBE	sol		13.04	16.87	14.46	14.53	15.82	12.78	12.02	15.10	12.80	12.13	10.58	11.95	13.77	15.97
		PBE		10.41	14.54	11.89	12.74	13.32	10.08	9.96	13.27	10.82	9.35	8.19	9.37	11.51	14.12
		MGEA		10.73	15.04	12.22	13.40	13.83	10.31	10.29	13.82	11.24	9.56	8.40	9.63	11.92	14.67
		mol		10.77	15.15	12.26	13.56	13.93	10.33	10.34	13.95	11.18	9.56	8.42	9.67	11.99	14.74
lsPBE-D*	PBE	sol		17.65	22.03	19.29	19.32	20.81	17.50	15.59	19.50	17.15	16.65	14.51	16.39	18.36	20.44
		PBE		13.84	18.02	15.38	15.77	16.78	13.49	12.67	16.14	13.67	12.75	11.14	12.68	14.64	17.04
		MGEA		13.13	17.31	14.64	15.24	16.12	12.73	12.14	15.60	13.08	11.99	10.52	11.97	14.00	16.47
		mol		12.95	17.13	14.45	15.13	15.98	12.54	12.04	15.49	12.95	11.81	10.36	11.80	13.86	16.35
lsRPBE-D*	PBE	sol		13.05	16.87	14.46	14.51	15.81	12.78	11.96	15.10	12.79	12.12	10.59	11.95	13.77	15.97
		PBE		10.47	14.63	11.96	12.80	13.40	10.15	10.00	13.34	10.74	9.42	8.26	9.43	11.57	14.20
		MGEA		10.44	14.71	11.92	13.15	13.51	10.03	10.04	13.54	10.83	9.28	8.15	9.37	11.63	14.31
		mol		10.52	14.86	12.01	13.33	13.66	10.09	10.13	13.71	10.95	9.32	8.20	9.44	11.74	14.43

Table S6 Mean absolute deviation MAD, mean signed deviation MSD, percentage of mean absolute relative deviation %MARD, and standard deviation SD, for the calculated molar volumes V, in cm³/mol, and for the calculated energy ΔE_c, in kJ/mol, per SiO_2 unit considering a mean value of s_6=0.7, of silica zeolites relative to α-quartz.

			V				ΔE_c			
X	C	μ_x	MAD	MSD	%MARD	SD	MAD	MSD	%MARD	SD
lsPBE-D*	PBE	sol	1.96	1.67	5.74	2.43	8.49	8.49	94.20	8.42
		PBE	2.76	1.56	7.97	3.50	4.84	4.84	54.54	4.98
		MGEA	2.74	2.74	7.87	3.10	4.19	4.19	47.43	4.39
		mol	2.81	2.81	8.08	3.16	4.04	4.04	45.76	4.25
lsRPBE-D*	PBE	sol	2.23	2.20	6.42	2.71	3.96	3.96	45.39	4.19
		PBE	3.23	3.23	9.32	3.50	1.90	1.72	20.68	2.33
		MGEA	3.53	3.53	10.20	3.76	1.89	1.76	20.84	2.34
		mol	3.65	3.65	10.55	3.86	1.96	1.86	21.90	2.41

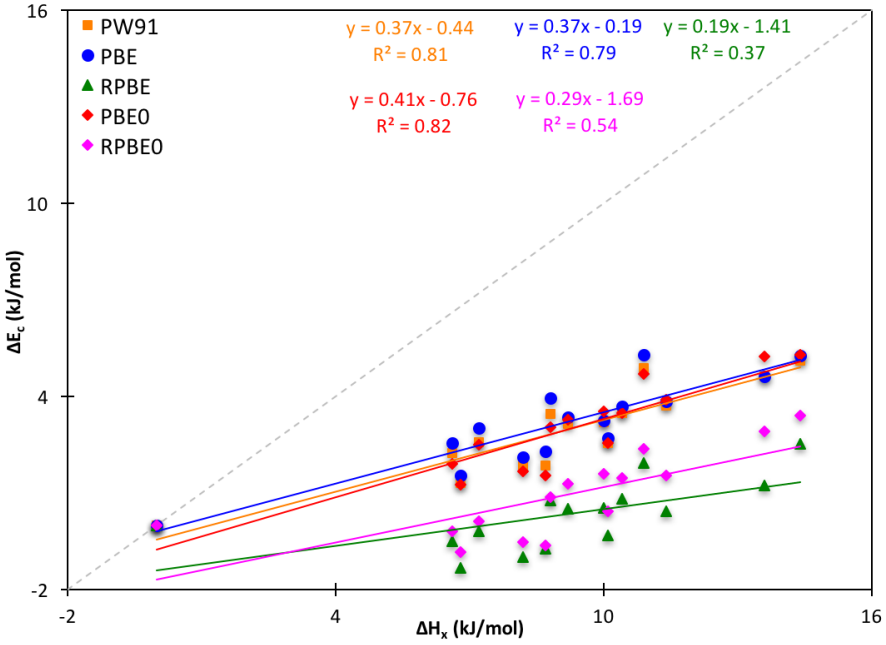

Fig. S1 Linear regression and correlation coefficients for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for various GGAs and hybrid DFAs.

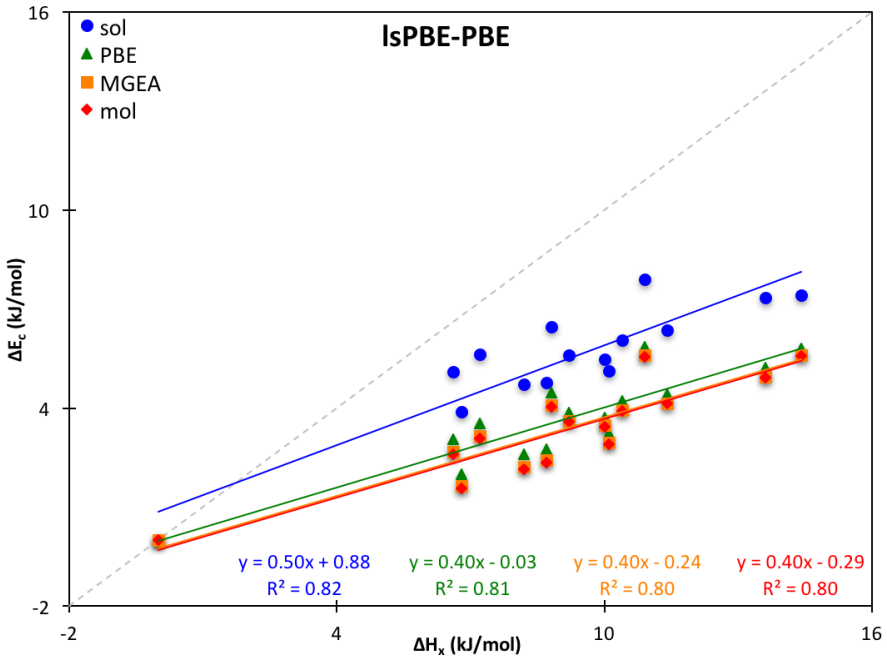

Fig. S2 Linear regression and correlation coefficient for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for the lsPBE exchange family with PBE correlation.

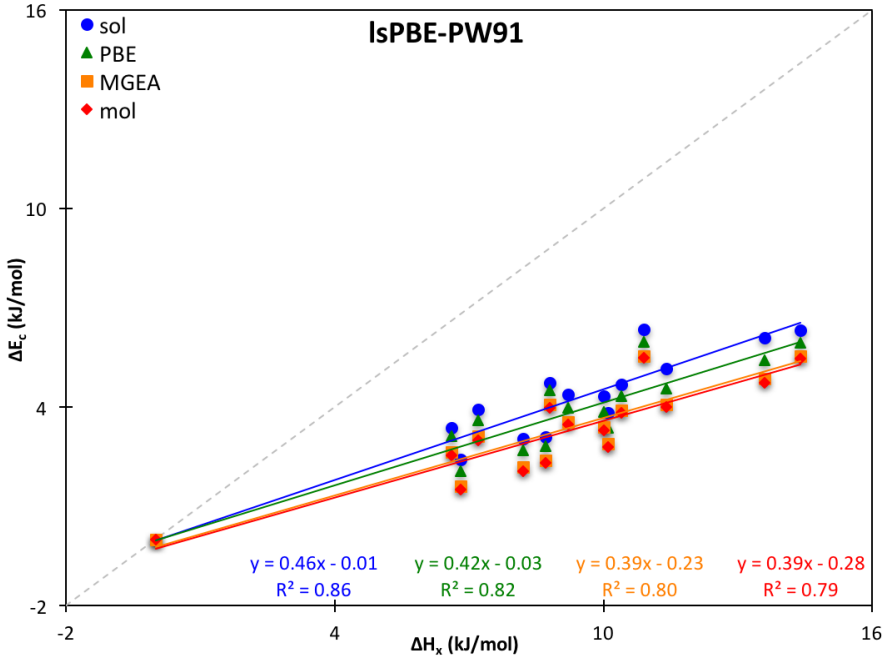

Fig. S3 Linear regression and correlation coefficient for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for the lsPBE exchange family with PW91 correlation.

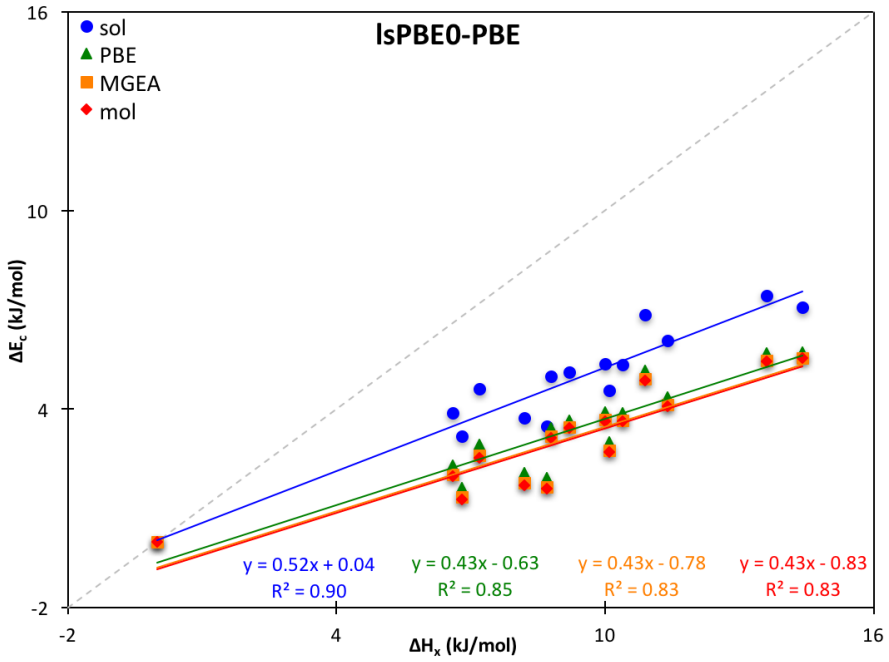

Fig. S4 Linear regression and correlation coefficient for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for the hybrid lsPBE0 family with PBE correlation.

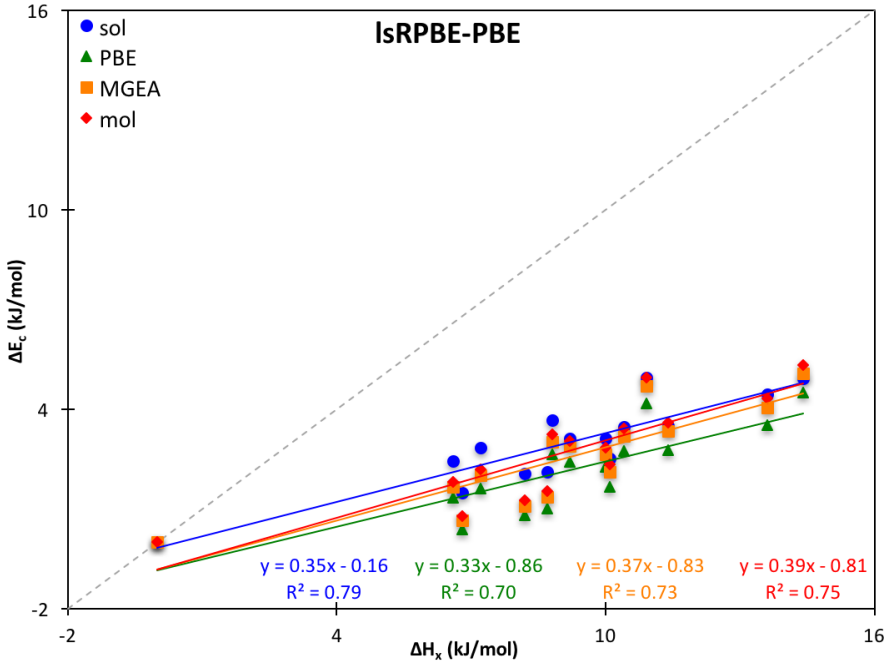

Fig. S5 Linear regression and correlation coefficient for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for the lsRPBE exchange family with PBE correlation.

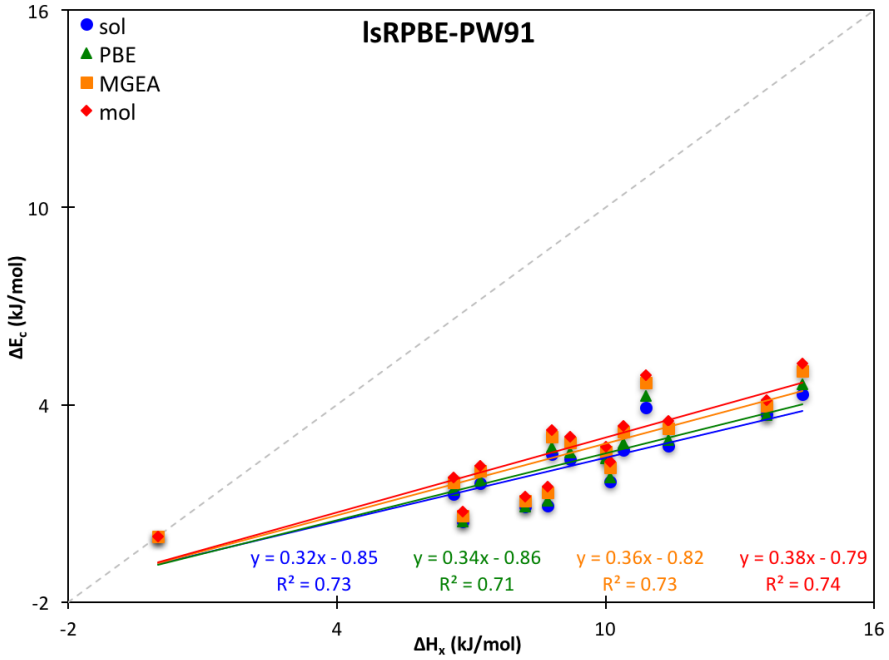

Fig. S6 Linear regression and correlation coefficient for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for the lsRPBE exchange family with PW91 correlation.

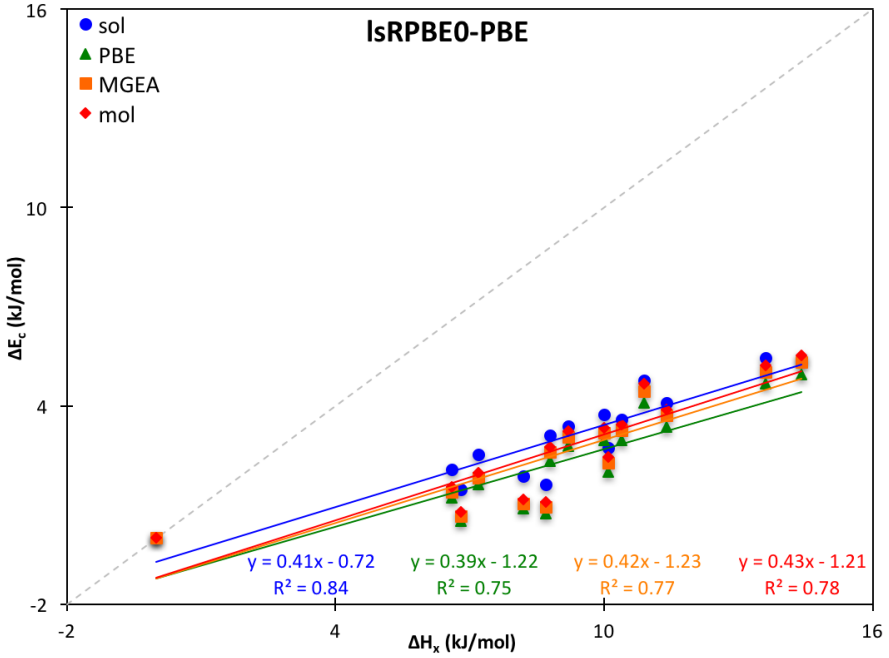

Fig. S7 Linear regression and correlation coefficient for the calculated energy differences ΔE_c, in kJ/mol per SiO_2 unit and transition enthalpies ΔH_x, for the hybrid lsRPBE0 family with PBE correlation.