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Supporting Information

Computational Investigation of The Structures and Energies of Microporous Materials

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	2Å	3Å	4Å	5Å	6Å	7Å	8Å	9Å	
Quartz Energy for Reference	-17453.42	-16498.63	-16620.56	-16756.95	-16818.48	-16848.92	-16871.17	-16882.45	
Energy Difference from Quartz for Different Cut-offs / kJ									
Structure	2Å	3Å	4Å	5Å	6Å	7Å	8Å	9Å	EXP /kJ
AST-FW	1.58	1.38	19.07	37.99	42.59	46.77	50.15	51.55	10.9
BEA-FW	3.74	5.48	13.73	30.03	37.44	41.56	46.12	47.93	9.3
CIT-5	-1.43	-3.37	16.85	25.47	30.32	32.69	36.90	38.58	8.8
CHA	5.66	8.48	19.53	37.98	49.04	53.33	57.61	59.52	11.4
ITQ-4	4.95	8.32	15.51	31.49	37.48	41.64	45.35	46.96	10
ITQ-7	4.80	8.14	17.59	34.46	41.37	45.76	50.31	52.20	14.4
ITQ-3	3.09	3.89	14.98	32.53	40.61	44.21	48.46	50.25	10.1
ZSM-11	-0.09	-1.51	13.56	22.51	29.87	32.70	36.68	37.92	8.2
ZSM-5	-0.96	-3.02	12.79	22.20	28.50	31.38	35.26	36.46	6.8
ITQ-1	3.49	4.88	17.52	27.65	36.65	39.78	43.74	45.27	10.4
SSZ-23	2.66	3.91	16.28	30.59	38.91	42.63	46.68	48.29	9.2
AFI-FW	-0.61	-1.93	23.85	28.97	29.38	32.02	36.78	38.05	7.2
EMT-FW	8.34	13.34	18.32	43.40	53.06	57.17	61.38	63.63	10.5
FER-FW	0.19	-0.79	15.38	21.56	30.08	32.59	36.46	37.20	6.6
ZSM-18	8.40	13.57	22.19	40.46	49.27	54.24	58.74	60.82	13.9
ZSM-12	-2.06	-4.89	11.96	21.99	26.00	28.58	32.24	33.45	8.7

Table S1. Van Beest Cut-Off Parameter Benchmarks

Structure	Normalised Lattice Energy /kJ	Normalised ΔE Quartz /kJ	Structure	Normalised Lattice Energy /kJ	Normalised ΔE Quartz /kJ	Structure	Normalised Lattice Energy /kJ	Normalised ΔE Quartz /kJ	Structure	Normalised Lattice Energy /kJ	Normalised ΔE Quartz /kJ
Quartz	-12418.0	0	JSW-FW	-12401.5	16.5	GME-FW	-12401.5	16.5	LTJ-FW	-12403.3	14.8
ITQ-33	-12398.2	19.8	ABW-FW	-12405.5	11.9	LOS-FW	-12404.1	13.9	LTL-FW	-12399.9	18.1
CIT-5	-12405.4	12.7	ANA-FW	-12404.3	13.7	FRA-FW	-12404.4	13.6	MAR-FW	-12404.2	13.1
CIT-7	-12401.3	15.2	DON-FW	-12407.8	10.2	LTF-FW	-12401.1	19.3	MEP-FW	-12405.8	12.2
EDI-FW	-12395.2	22.8	BIK-FW	-12406.7	7.2	MAPO-39-FW	-12405.3	12.7	MER-FW	-12401.8	16.3
ITQ-12	-12403.1	14.9	LOV-FW	-12393.1	24.9	STA-6-FW	-12402.1	15.9	MON-FW	-12403.2	14.9
AEN-FW	-12405.8	12.2	MOZ-FW	-12400.3	17.7	STA-15-FW	-12407.6	10.4	MOR-FW	-12405.7	12.3
SAPO-40-FW	-12401.2	16.8	MWW-FW	-12403.6	14.4	SIZ-7-FW	-12402.6	15.4	MSO-FW	-12406.0	12.0
ACO-FW	-12399.5	18.5	SAPO-31-FW	-12407.9	10.1	DAC-FW	-12405.7	12.3	BEA-FW	-12403.6	14.4
ITQ-13-FW	-12405.5	12.5	SAPO-56-FW	-12401.6	16.4	EPI-FW	-12404.5	13.5	BRE-FW	-12404.3	13.3
ITQ-22	-12404.1	13.9	VFI-FW	-12398.4	19.5	DOH-FW	-12407.4	10.6	CAN-FW	-12404.1	13.9
ITQ-24-FW	-12402.4	15.6	ZSM-12	-12409.8	8.2	EAB-FW	-12401.6	16.4	CAS-FW	-12407.1	11.0
ITQ-3	-12403.9	14.1	AEL-FW	-12407.9	11.0	EMT-FW	-12397.9	20.1	NAT-FW	-12395.6	22.4
ITQ-34-FW	-12405.5	12.5	AHT-FW	-12397.2	20.8	EON-FW	-12403.0	13.0	NES-FW	-12402.2	15.9
ITQ-38-FW	-12403.8	14.2	ITQ-33-FW	-12398.2	19.8	ERI-FW	-12401.6	16.4	OFF	-12401.2	16.8
ITQ-4	-12403.0	15.0	ITQ-39-FW	-12383.1	36.2	ERS-7	-12404.5	13.5	PHI-FW	-12402.3	15.7

ITQ-49-FW	-12400.5	17.6	ITQ-44-FW	-12393.2	24.8	ETR-FW	-12396.9	21.1	PST-21	-12402.0	16.0
ITQ-50	-12398.7	19.3	GOO-FW	-12398.9	19.1	FAR-FW	-12404.3	13.7	PST-22	-12403.0	15.0
ITQ-52	-12404.2	13.8	GUS-1	-12406.2	9.1	HEU-FW	-12405.5	12.5	RHO-FW	-12399.7	18.3
ITQ-7	-12401.6	16.4	FER-FW	-12404.1	11.8	JBW-FW	-12407.0	11.0	ITQ-26-FW	-12400.5	15.2
ZSM-5	-12408.3	9.7	AFG-FW	-12399.0	13.9	JOZ-FW	-12384.4	33.6	AFY-FW	-12390.7	27.3
ZON-FW	-12401.5	16.6	AFS-FW	-12404.0	19.0	KFI-FW	-12400.8	17.3	ZSM-18	-12399.2	18.9
MAPO-36	-12405.1	12.9	BOG-FW	-12398.8	14.0	LAU-FW	-12403.8	14.2	ZSM-11	-12407.3	10.8
WEI-FW	-12383.4	34.6	BPH-FW	-12403.0	19.2	LEV-FW	-12402.0	16.0	EWS-FW	-12401.4	16.6
JNT-FW	-12399.2	18.8	GIS-FW	-12404.2	15.0	LIO-FW	-12404.1	13.9	NAB-FW	-12385.2	32.8
DFT-FW	-12403.2	14.8	GIU-FW	-12398.9	13.8	LTA-FW	-12398.7	19.3	LTJ-FW	-12403.3	14.8
AST-FW	-12399.9	18.1	CHA	-12401.9	16.1	SSZ-23	-12403.3	14.7	AFI-FW	-12406.1	11.9

Table S2. Zeolite Lattice Energies: Shell Model Potentials

Framework	Normalised Energy /kJmol-1	ΔE Berlinite /kJ
Berlinite	-12938.8	0
ITQ-51	-12929.1	9.8
ALPO-C	-12929.8	9.0
ALPO-12	-12929.1	9.8
ALPO-5	-12932.1	6.8
ALPO-11	-12929.7	9.1
ALPO-18	-12928.0	10.8
VPI-5	-12926.2	12.6
ALPO-41	-12933.1	5.7
ALPO-8	-12928.1	10.8
ALPO-D	-12931.0	7.8
SAPO-56	-12928.2	10.6
STA-20	-12927.9	11.0
UiO-6	-12933.4	5.4
STA-1	-12924.9	13.9
PST-14	-12925.5	13.3
ALPO-16	-12926.5	12.4
SAPO-42	-12925.9	12.9

Table S3. Interatomic Potential ALPO Lattice Energies

Structure	Normalised Cohesive Energy /kJ	Normalised ΔE Quartz /kJ	Structure	Normalised Cohesive Energy /kJ	Normalised ΔE Quartz /kJ	Structure	Normalised Cohesive Energy /kJ	Normalised ΔE Quartz /kJ	Structure	Normalised Cohesive Energy /kJ	Normalised ΔE Quartz /kJ
Quartz	-2314.9	0	JSW-FW	-2303.7	11.2	GME-FW	-2302.7	10.9	LTJ-FW	-2303.5	11.4
ITQ-33	-2300.3	14.5	ABW-FW	-2304.6	10.3	LOS-FW	-2303.8	10.9	LTL-FW	-2304.0	10.8
CIT-5	-2303.0	11.9	ANA-FW	-2305.0	9.9	FRA-FW	-2304.0	9.6	MAR-FW	-2304.0	10.9
CIT-7	-2303.2	11.7	DON-FW	-2305.8	9.1	LTF-FW	-2303.9	11.0	MEP-FW	-2305.2	9.6
EDI-FW	-2298.7	16.1	BIK-FW	-2305.2	9.6	MAPO-39-FW	-2305.3	9.5	MER-FW	-2303.2	11.6
ITQ-12	-2304.1	10.7	LOV-FW	-2299.7	15.1	STA-6-FW	-2303.6	11.2	MON-FW	-2305.1	9.7
AEN-FW	-2304.1	10.8	MOZ-FW	-2303.9	11.0	STA-15-FW	-2307.1	7.8	MOR-FW	-2305.1	8.2
SAPO-40-FW	-2302.7	12.1	MWW-FW	-2303.7	11.1	SIZ-7-FW	-2303.3	11.5	MSO-FW	-2306.7	11.0
ACO-FW	-2301.8	13.1	SAPO-31-FW	-2306.7	8.2	DAC-FW	-2304.9	10.0	BEA-FW	-2303.9	10.8
ITQ-13-FW	-2305.2	9.7	SAPO-56-FW	-2302.7	12.2	EPI-FW	-2304.5	10.4	BRE-FW	-2304.7	10.2
ITQ-22	-2304.0	10.8	VFI-FW	-2297.9	16.9	DOH-FW	-2303.9	11.1	CAN-FW	-2303.8	11.0
ITQ-24-FW	-2303.5	11.4	ZSM-12	-12409.8	8.2	EAB-FW	-2303.4	11.0	CAS-FW	-2305.5	9.4
ITQ-3	-2304.2	10.7	AEL-FW	-2306.5	8.4	EMT-FW	-2301.9	11.5	NAT-FW	-2298.7	16.2
ITQ-34-FW	-2305.2	9.7	AHT-FW	-2298.6	16.3	EON-FW	-2304.4	12.9	NES-FW	-2301.0	13.9
ITQ-38-FW	-2303.6	11.2	ITQ-33-FW	-2303.6	14.5	ERI-FW	-2303.4	10.5	OFF	-2303.4	11.5
ITQ-4	-2304.6	10.3	ITQ-39-FW	-2304.6	8.8	ERS-7	-2304.6	10.3	PHI-FW	-2303.3	11.6
ITQ-49-FW	-2302.7	12.2	ITQ-44-FW	-2302.7	16.6	ETR-FW	-2301.5	13.3	PST-21	-2303.0	11.8
ITQ-50	-2301.3	13.6	GOO-FW	-2300.2	14.6	FAR-FW	-2304.9	10.0	PST-22	-2303.9	11.0
ITQ-52	-2304.1	10.8	GUS-1	-2307.5	7.4	HEU-FW	-2305.1	9.8	RHO-FW	-2302.3	12.6

ITQ-7	-2301.5	11.7	FER-FW	-2305.3	9.6	JBW-FW	-2305.8	9.1	ITQ-26-FW	-2301.6	13.3
ZSM-5	-2306.7	8.2	AFG-FW	-2303.9	11.0	JOZ-FW	-2296.2	18.6	AFY-FW	-2295.8	19.0
ZON-FW	-2303.2	11.6	AFS-FW	-2302.1	12.9	KFI-FW	-2302.7	12.2	ZSM-18	-2301.9	13.0
MAPO-36	-2305.0	9.8	BOG-FW	-2304.5	10.40	LAU-FW	-2304.9	10.0	ZSM-11	-2305.7	9.1
WEI-FW	-2295.9	18.9	BPH-FW	-2301.9	13.0	LEV-FW	-2303.4	11.5	EWS-FW	-2302.3	12.5
JNT-FW	-2301.9	12.9	GIS-FW	-2303.4	11.5	LIO-FW	-2303.5	11.3	NAB-FW	-2296.6	18.2
DFT-FW	-2303.7	11.2	GIU-FW	-2304.1	10.8	LTA-FW	-2301.6	13.3	LTJ-FW	-2303.5	11.4
AST-FW	-2302.2	12.7	CHA	-2302.7	12.2	SSZ-23	-2303.5	11.4	AFI-FW	-2305.0	10.0

Table S4. DFT Zeolite Cohesive Energies

Framework	Normalised Energy /kJmol-1	ΔE Berlinite /kJ
Berlinite	-2192.5	0
ITQ-51	-2182.2	10.3
ALPO-C	-2181.2	11.3
ALPO-12	-2180.1	12.4
ALPO-5	-2181.6	10.8
ALPO-11	-2181.6	10.9
ALPO-18	-2179.1	13.3
VPI-5	-2178.0	14.5
ALPO-41	-2183.0	9.5
ALPO-8	-2182.1	10.4
ALPO-D	-2183.0	9.5
SAPO-56	-2179.3	13.1
STA-20	-2180.1	12.4
UiO-6	-2184.1	8.3
STA-1	-2177.9	14.6
PST-14	-2178.5	14.0
ALPO-16	-2178.3	14.2
SAPO-42	-2178.6	13.9

Table S5. DFT ALPO Cohesive Energies