Identifying Zeolite Topologies for Storage and Release of Hydrogen

ELECTRONIC SUPPORTING INFORMATION

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Table S1: Weight percentage of hydrogen of zeolites at moderate conditions (77K and 1 MPa) and extreme conditions (25 K and 100 MPa)

Zeolite	H_2 %wt 77 K and 1 MPa	H_2 %wt 25 K and 100 MPa	Zeolite	H_2 %wt 77 K and 1 MPa	H_2 %wt 25 K and 100 MPa
ABW	1.6412	1.64988	CAN	1.56669	2.18781
ACO	2.16743	2.45457	CAS	0.571303	0.611972
AEI	2.19823	3.24281	CDO	1.15984	1.45476
AEL	0.704187	0.790348	CFI	1.54456	1.86825
AEN	1.03762	1.106	CGF	0.796896	1.28051
AET	0.740532	1.17158	CGS	1.46336	1.89564
AFG	1.59156	1.91958	CHA	2.24534	2.97677
AFI	1.02042	1.64896	CHI	0.660154	0.732177
AFN	1.32771	1.67671	CLO	2.2404	4.57877
AFO	0.693878	0.964568	CON	1.56981	2.39521
AFR	1.83591	2.60774	CZP	0.830196	0.831803
AFS	1.92693	3.03339	DAC	1.40453	1.65552
AFT	2.24593	2.97175	DDR	1.24014	1.66095
AFV	1.85406	2.84953	DFO	1.79741	2.8158
AFX	2.34875	3.10689	DFT	1.47188	1.79155
AFY	2.07002	3.83092	DOH	1.35203	1.79055
AHT	1.09997	1.106	DON	0.91385	1.49957
ANA	1.10437	1.106	EAB	1.77635	2.69513
APC	1.26464	1.64988	EDI	2.20894	2.79232
APD	0.916286	1.31861	EEI	1.17433	1.39587
AST	1.76695	2.00297	EMT	1.8119	3.51459
ASV	0.88453	0.996505	EON	1.52453	1.87167
ATN	1.52962	1.65953	EPI	1.38217	1.75908
ATO	0.615051	1.19743	ERI	1.64389	2.18781
ATS	1.48408	2.06819	ESV	1.32127	1.6395
ATT	1.75668	1.93916	ETR	1.5277	2.59498
ATV	0.603841	0.712152	EUO	1.46911	1.88338
AVL	2.04962	2.88873	EZT	1.15378	1.7308
AWO	0.938312	1.26489	FAR	1.47316	1.79771
AWW	1.46311	1.77896	FAU	1.84855	3.44954
BCT	1.00521	1.50217	FER	1.13145	1.49076
BEA	1.59772	2.50268	FRA	1.60045	2.1878
BEC	1.64483	2.45457	GIS	2.03721	2.45433
BIK	1.09787	1.106	GIU	1.50841	1.98979
BOF	1.11579	1.53409	GME	2.38159	3.14775
BOG	1.47677	2.06268	GON	0.737002	0.914192
BOZ	2.53437	3.86117	GOO	1.25489	1.64988
BPH	1.97927	3.07829	HEU	1.53383	2.17973
BRE	1.34567	1.65146	IFO	1.1851	1.8459
BSV	1.1771	1.27291	IFR	1.31712	1.82835

Zeolite	H_2 %wt 77 K and 1 MPa	H_2 %wt 25 K and 100 MPa	Zeolite	H_2 %wt 77 K and 1 MPa	H_2 %wt 25 K and 100 MPa
IFW	1.50191	2.16233	MEL	1.11431	1.54405
IFY	1.61064	1.90095	MEP	1.36667	1.43777
IHW	1.16576	1.41753	MER	1.99563	2.42786
IMF	1.14673	1.6511	MFI	1.01551	1.49649
IRN	1.81526	2.66709	MFS	1.38701	1.743
IRR	1.67954	4.52688	MON	1.63922	1.64988
IRY	1.90392	4.98817	MOR	1.36358	1.66775
ISV	1.73522	2.52648	MOZ	1.37433	2.00871
ITE	1.59541	2.14297	MRE	0.564573	0.853789
ITG	1.41001	2.1923	MSE	1.4925	2.00795
ITH	1.14254	1.65552	MSO	1.03445	1.53882
ITN	1.4571	2.34477	MTF	0.761559	0.906736
ITR	1.19134	1.48654	MTN	1.24026	1.74085
ITT	1.52245	3.65553	MTT	0.998785	1.62127
ITV	1.7681	5.00959	MTW	1.20358	1.42444
ITW	1.2639	1.57792	MVY	0.967639	1.106
IWR	1.64538	2.60898	MWW	1.50645	2.2851
IWS	1.69239	2.81243	NAB	2.12289	2.49045
IWV	1.57686	2.51392	NAT	1.8912	2.41069
IWW	1.47856	2.25277	NES	1.55551	1.97962
JBW	1.10037	1.106	NON	1.5121	1.9489
JOZ	1.87605	2.61369	NPO	0.78694	0.884077
JRY	1.19259	1.64988	NPT	2.82646	4.24436
JSN	1.23677	1.64988	NSI	1.10208	1.106
JSR	2.26672	4.07687	OBW	2.59795	4.47601
JST	2.18765	2.78064	OFF	1.65276	2.33298
JSW	1.14298	1.38543	OKO	1.34184	1.74524
KFI	2.26318	3.13355	OSI	1.03809	1.43099
LAU	1.13418	1.37869	OSO	2.36812	3.24429
LEV	1.90681	2.71989	OWE	1.58945	1.92545
LIO	1.20696	1.64988	PAR	0.777234	0.805224
LIT	0.187585	0.531729	PAU	2.1914	2.65366
LOS	1.56937	2.09247	PCR	0.977012	1.2604
LOV	1.53904	1.80646	PHI	2.20093	2.45457
LTA	2.03983	2.87729	PON	1.00192	1.55783
LTF	1.54177	1.93074	POS	1.54033	2.39032
LTJ	1.02532	1.64277	PUN	2.01666	2.96036
LTL	1.27622	2.00971	RHO	2.07812	3.00452
LTN	1.37688	2.02844	RON	0.765222	1.09436
MAR	1.25119	1.64567	RRO	1.4731	1.5466
MAZ	1.57928	2.11249	RSN	1.67977	1.89811
MEI	1.9879	3.05609	RTE	1.51289	1.64988

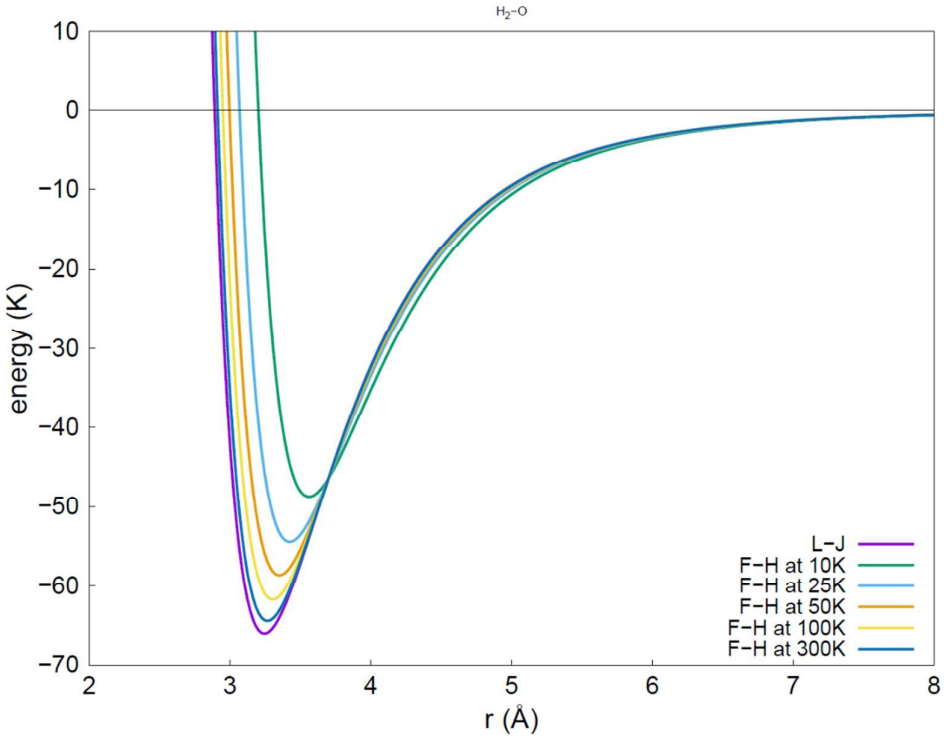
Zeolite	H_2 %wt 77 K and 1 MPa	H_2 %wt 25 K and 100 MPa	Zeolite	H_2 %wt 77 K and 1 MPa	H_2 %wt 25 K and 100 MPa
RTH	1.59437	2.21543	STF	1.43215	1.989
RUT	1.34441	1.65572	STI	1.69511	2.04898
RWR	0.844455	0.83783	STO	0.790236	1.22637
RWY	2.65738	7.17642	STT	1.4188	1.97398
SAF	0.700404	0.969093	STW	1.70421	2.28787
SAO	1.99481	3.23951	SVR	1.0759	1.51324
SAS	1.89799	3.22936	SVV	1.36521	1.77011
SAT	1.67442	2.18781	SZR	1.47792	2.03172
SAV	2.33244	3.28654	TER	1.26591	1.84674
SBE	1.94669	3.44545	THO	2.28736	2.74678
SBN	1.52593	2.35693	TOL	1.19537	1.47518
SBS	2.00009	3.18175	TON	1.05747	1.64988
SBT	2.00406	3.33977	TSC	1.95341	3.32114
SEW	1.24405	1.99243	TUN	1.16742	1.68637
SFE	1.19141	1.88106	UEI	1.22669	1.78915
SFF	1.29286	1.85229	UFI	1.84554	2.58251
SFG	0.91507	1.42999	UOS	1.1595	1.57254
SFH	1.63811	2.2562	UOV	1.44995	2.30329
SFN	1.41178	2.24999	UOZ	0.971961	1.16066
SFO	1.83866	2.75669	USI	1.65193	2.44329
SFS	1.28977	1.88628	UTL	1.408	2.54136
SFV	1.10649	1.5945	UWY	1.30148	1.93901
SFW	2.28446	3.11689	VET	0.743406	0.783256
SGT	1.62826	2.05388	VFI	1.54238	3.01168
SIV	2.13067	2.45457	VNI	1.41093	1.75776
SOD	1.36003	1.83399	VSV	1.85145	2.15187
SOF	1.70224	2.08798	WEI	1.93908	2.5708
SOS	1.50511	1.97793	WEN	1.55624	2.11351
SSF	1.28968	1.99064	YUG	1.7571	2.05379
SSO	1.21494	1.8117	ZON	1.37484	1.74674
SSY	1.23649	1.80542			

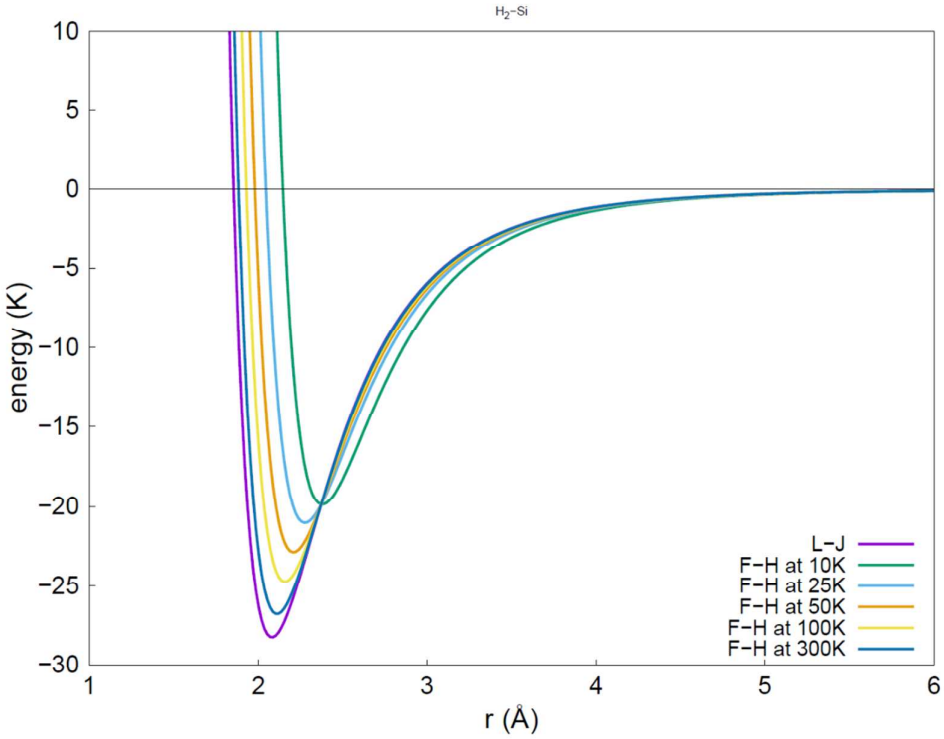
Table S2: Adsorption of hydrogen in zeolites at moderate conditions (77K and 1 MPa). The excess loading was obtained using the method of Duren *et al.*[1]

zeolite	excess (mol/Kg)	absolute (mol/kg)	Δ (mol/kg)	zeolite	excess (mol/Kg)	absolute (mol/kg)	Δ (mol/kg)
ABW	8.20	8.28	0.08	CAN	7.67	7.90	0.22
ACO	10.82	10.99	0.17	CAS	2.77	2.85	0.09
AEI	10.75	11.15	0.40	CDO	5.65	5.82	0.17
AEL	3.37	3.52	0.15	CFI	7.53	7.78	0.25
AEN	5.14	5.20	0.06	CGF	3.84	3.98	0.14
AET	3.49	3.70	0.21	CGS	7.13	7.37	0.23
AFG	7.78	8.02	0.24	CHA	10.99	11.39	0.40
AFI	4.84	5.11	0.27	CHI	3.27	3.30	0.03
AFN	6.52	6.67	0.16	CLO	10.61	11.37	0.76
AFO	3.31	3.47	0.16	CON	7.50	7.91	0.41
AFR	8.87	9.28	0.40	CZP	4.08	4.15	0.07
AFS	9.30	9.75	0.45	DAC	6.86	7.07	0.21
AFT	11.00	11.40	0.39	DDR	5.98	6.23	0.25
AFV	9.00	9.37	0.37	DFO	8.62	9.08	0.46
AFX	11.54	11.93	0.39	DFT	7.28	7.41	0.14
AFY	10.01	10.49	0.48	DOH	6.50	6.80	0.30
AHT	5.49	5.52	0.03	DON	4.30	4.58	0.27
ANA	5.51	5.54	0.03	EAB	8.62	8.97	0.35
APC	6.28	6.35	0.08	EDI	10.99	11.21	0.22
APD	4.46	4.59	0.13	EEI	5.70	5.89	0.20
AST	8.52	8.92	0.40	EMT	8.55	9.15	0.60
ASV	4.27	4.43	0.15	EON	7.42	7.68	0.26
ATN	7.54	7.71	0.17	EPI	6.75	6.95	0.20
ATO	2.92	3.07	0.15	ERI	7.94	8.29	0.35
ATS	7.16	7.47	0.31	ESV	6.42	6.64	0.22
ATT	8.67	8.87	0.20	ETR	7.33	7.70	0.36
ATV	2.93	3.01	0.08	EUO	7.14	7.40	0.26
AVL	10.04	10.38	0.34	EZT	5.50	5.79	0.29
AWO	4.59	4.70	0.11	FAR	7.17	7.42	0.25
AWW	7.07	7.37	0.29	FAU	8.74	9.34	0.60
BCT	5.03	5.04	0.00	FER	5.44	5.68	0.24
BEA	7.61	8.05	0.45	FRA	7.74	8.07	0.32
BEC	7.84	8.30	0.46	GIS	10.13	10.32	0.19
BIK	5.45	5.51	0.06	GIU	7.36	7.60	0.24
BOF	5.38	5.60	0.21	GME	11.73	12.10	0.37
BOG	7.06	7.44	0.37	GON	3.52	3.68	0.17
BOZ	12.39	12.90	0.51	GOO	6.22	6.30	0.08
BPH	9.57	10.02	0.45	HEU	7.51	7.73	0.21
BRE	6.61	6.77	0.16	IFO	5.65	5.95	0.30
BSV	5.77	5.91	0.14	IFR	6.28	6.62	0.34

zeolite	excess (mol/Kg)	absolute (mol/kg)	Δ (mol/kg)	zeolite	excess (mol/Kg)	absolute (mol/kg)	Δ (mol/kg)
IFW	7.19	7.56	0.37	MEL	5.31	5.59	0.28
IFY	7.88	8.12	0.24	MEP	6.64	6.87	0.23
IHW	5.64	5.85	0.21	MER	9.88	10.10	0.22
IMF	5.49	5.75	0.27	MFI	4.88	5.09	0.21
IRN	8.76	9.17	0.41	MFS	6.75	6.98	0.23
IRR	7.71	8.47	0.76	MON	8.18	8.27	0.09
IRY	8.76	9.63	0.87	MOR	6.60	6.86	0.26
ISV	8.30	8.76	0.46	MOZ	6.65	6.91	0.27
ITE	7.67	8.04	0.37	MRE	2.67	2.82	0.14
ITG	6.77	7.09	0.33	MSE	7.16	7.52	0.35
ITH	5.49	5.73	0.25	MSO	4.95	5.19	0.23
ITN	6.97	7.33	0.36	MTF	3.67	3.81	0.14
ITR	5.73	5.98	0.25	MTN	5.93	6.23	0.30
ITT	7.03	7.67	0.64	MTT	4.84	5.00	0.17
ITV	8.11	8.93	0.82	MTW	5.85	6.04	0.19
ITW	6.18	6.35	0.17	MVY	4.84	4.85	0.01
IWR	7.88	8.30	0.42	MWW	7.21	7.59	0.38
IWS	8.06	8.54	0.48	NAB	10.66	10.76	0.09
IWV	7.51	7.95	0.43	NAT	9.37	9.56	0.19
IWW	7.13	7.44	0.32	NES	7.52	7.84	0.31
JBW	5.45	5.52	0.07	NON	7.42	7.62	0.20
JOZ	9.34	9.48	0.14	NPO	3.89	3.93	0.04
JRY	5.83	5.99	0.15	NPT	14.00	14.43	0.43
JSN	6.02	6.21	0.19	NSI	5.48	5.53	0.04
JSR	10.83	11.50	0.67	OBW	12.71	13.23	0.52
JST	10.78	11.09	0.31	OFF	7.99	8.34	0.34
JSW	5.58	5.74	0.15	OKO	6.45	6.75	0.30
KFI	11.10	11.49	0.39	OSI	5.02	5.20	0.19
LAU	5.47	5.69	0.22	OSO	11.57	12.03	0.46
LEV	9.29	9.64	0.36	OWE	7.77	8.01	0.24
LIO	5.85	6.06	0.21	PAR	3.84	3.89	0.05
LIT	0.93	0.93	0.00	PAU	10.84	11.11	0.27
LOS	7.64	7.91	0.27	PCR	4.74	4.89	0.16
LOV	7.60	7.75	0.15	PHI	10.95	11.16	0.21
LTA	9.80	10.33	0.53	PON	4.87	5.02	0.15
LTF	7.52	7.77	0.25	POS	7.34	7.76	0.42
LTJ	5.09	5.14	0.05	PUN	9.87	10.21	0.34
LTL	6.14	6.41	0.27	RHO	10.07	10.53	0.46
LTN	6.65	6.93	0.27	RON	3.68	3.83	0.14
MAR	6.07	6.29	0.22	RRO	7.30	7.42	0.12
MAZ	7.69	7.96	0.27	RSN	8.35	8.47	0.13
MEI	9.61	10.06	0.45	RTE	7.34	7.62	0.28

zeolite	excess (mol/Kg)	absolute (mol/kg)	Δ (mol/kg)	zeolite	excess (mol/Kg)	absolute (mol/kg)	Δ (mol/kg)
RTH	7.67	8.04	0.36	STF	6.88	7.21	0.33
RUT	6.55	6.76	0.21	STI	8.25	8.55	0.31
RWR	4.15	4.22	0.08	STO	3.76	3.95	0.19
RWY	12.31	13.54	1.24	STT	6.83	7.14	0.31
SAF	3.32	3.50	0.18	STW	8.27	8.60	0.33
SAO	9.55	10.10	0.55	SVR	5.15	5.40	0.24
SAS	9.18	9.60	0.42	SVV	6.64	6.87	0.22
SAT	8.15	8.45	0.30	SZR	7.25	7.44	0.19
SAV	11.44	11.85	0.40	TER	6.08	6.36	0.28
SBE	9.33	9.85	0.51	THO	11.39	11.61	0.22
SBN	7.49	7.69	0.20	TOL	5.80	6.00	0.20
SBS	9.58	10.12	0.55	TON	5.13	5.30	0.17
SBT	9.60	10.14	0.55	TSC	9.32	9.88	0.56
SEW	5.94	6.25	0.31	TUN	5.59	5.86	0.27
SFE	5.73	5.98	0.25	UEI	6.03	6.16	0.13
SFF	6.20	6.50	0.29	UFI	8.88	9.33	0.44
SFG	4.35	4.58	0.23	UOS	5.63	5.82	0.19
SFH	7.97	8.26	0.29	UOV	6.93	7.30	0.37
SFN	6.82	7.10	0.29	UOZ	4.71	4.87	0.16
SFO	8.89	9.29	0.40	USI	7.96	8.33	0.37
SFS	6.15	6.48	0.33	UTL	6.66	7.08	0.42
SFV	5.28	5.55	0.27	UWY	6.20	6.54	0.34
SFW	11.22	11.60	0.38	VET	3.57	3.72	0.14
SGT	7.92	8.21	0.29	VFI	7.35	7.77	0.43
SIV	10.60	10.80	0.20	VNI	7.02	7.10	0.08
SOD	6.54	6.84	0.30	VSV	9.25	9.36	0.11
SOF	8.32	8.59	0.28	WEI	9.69	9.81	0.12
SOS	7.42	7.58	0.16	WEN	7.58	7.84	0.26
SSF	6.17	6.48	0.31	YUG	8.77	8.87	0.10
SSO	5.84	6.10	0.26	ZON	6.72	6.92	0.20
SSY	5.95	6.21	0.26				


H2-O
energy (K)
r (Å)
L-J
F-H at 10K
F-H at 25K
F-H at 50K
F-H at 100K
F-H at 300K


H2-Si
energy (K)
r (Å)
L-J
F-H at 10K
F-H at 25K
F-H at 50K
F-H at 100K
F-H at 300K

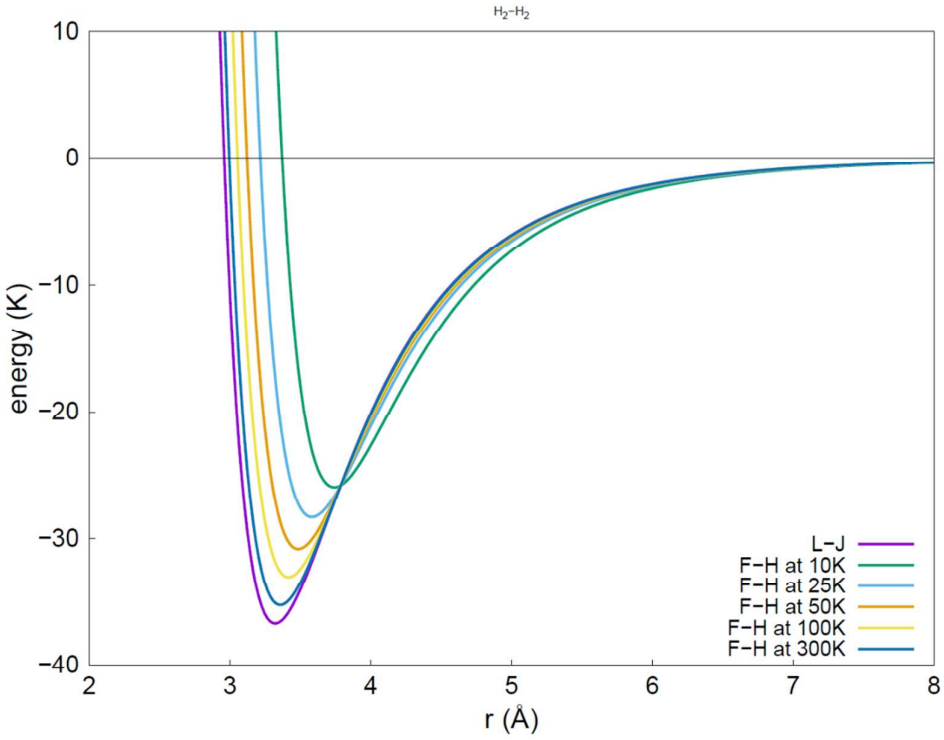


Figure S1: Comparison of the Lennard- Jones potential with and without Feynman-Hibbs quantum correction for the interactions Ozeo-H_2 (top), Si-H_2 (center), and H_2-H_2 (bottom).

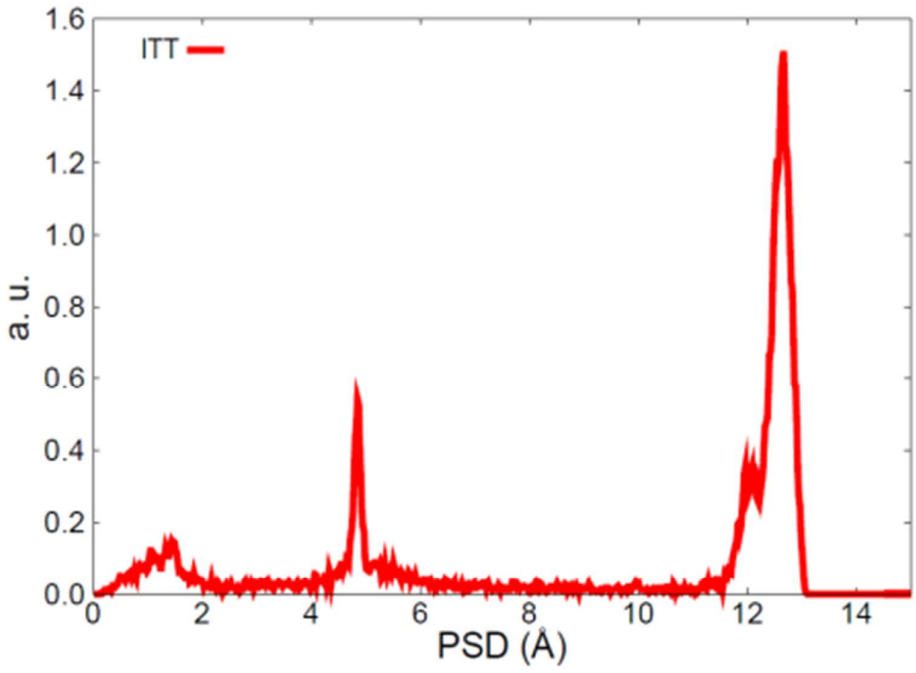


Figure S2: Computed pore size distribution of ITT.

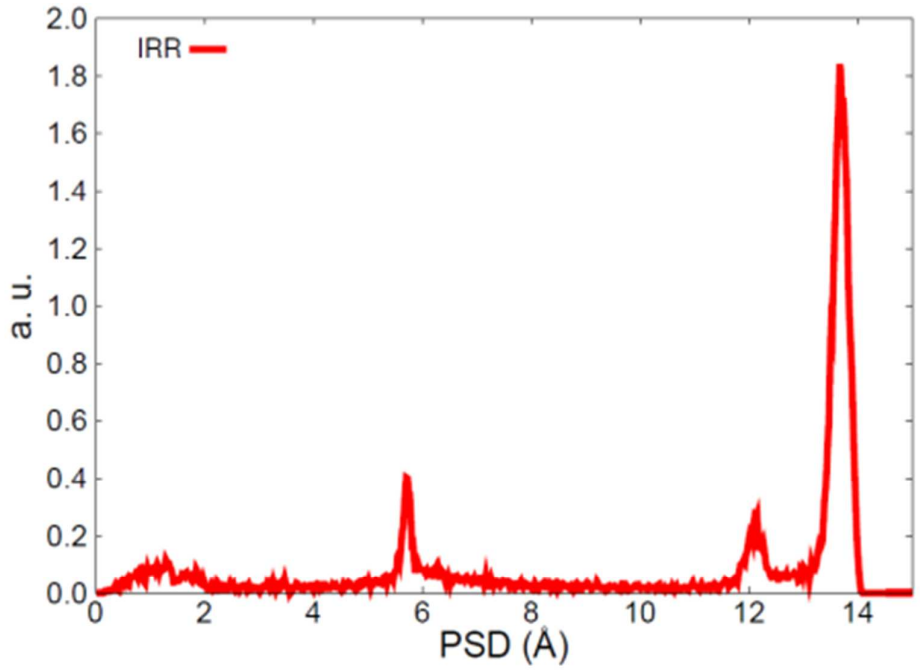


Figure S3: Computed pore size distribution of IRR.

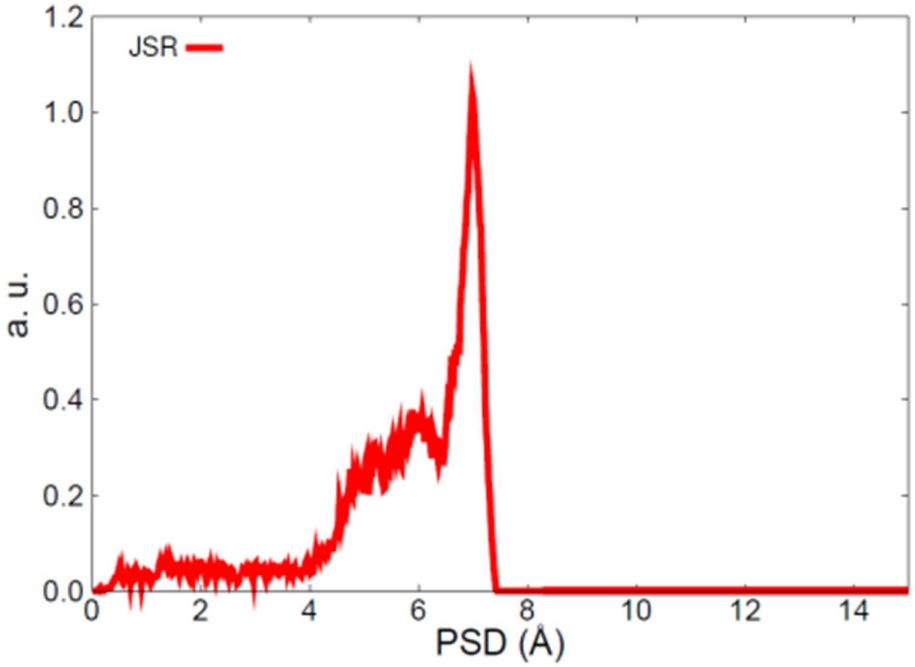


Figure S4: Computed pore size distribution of JSR.

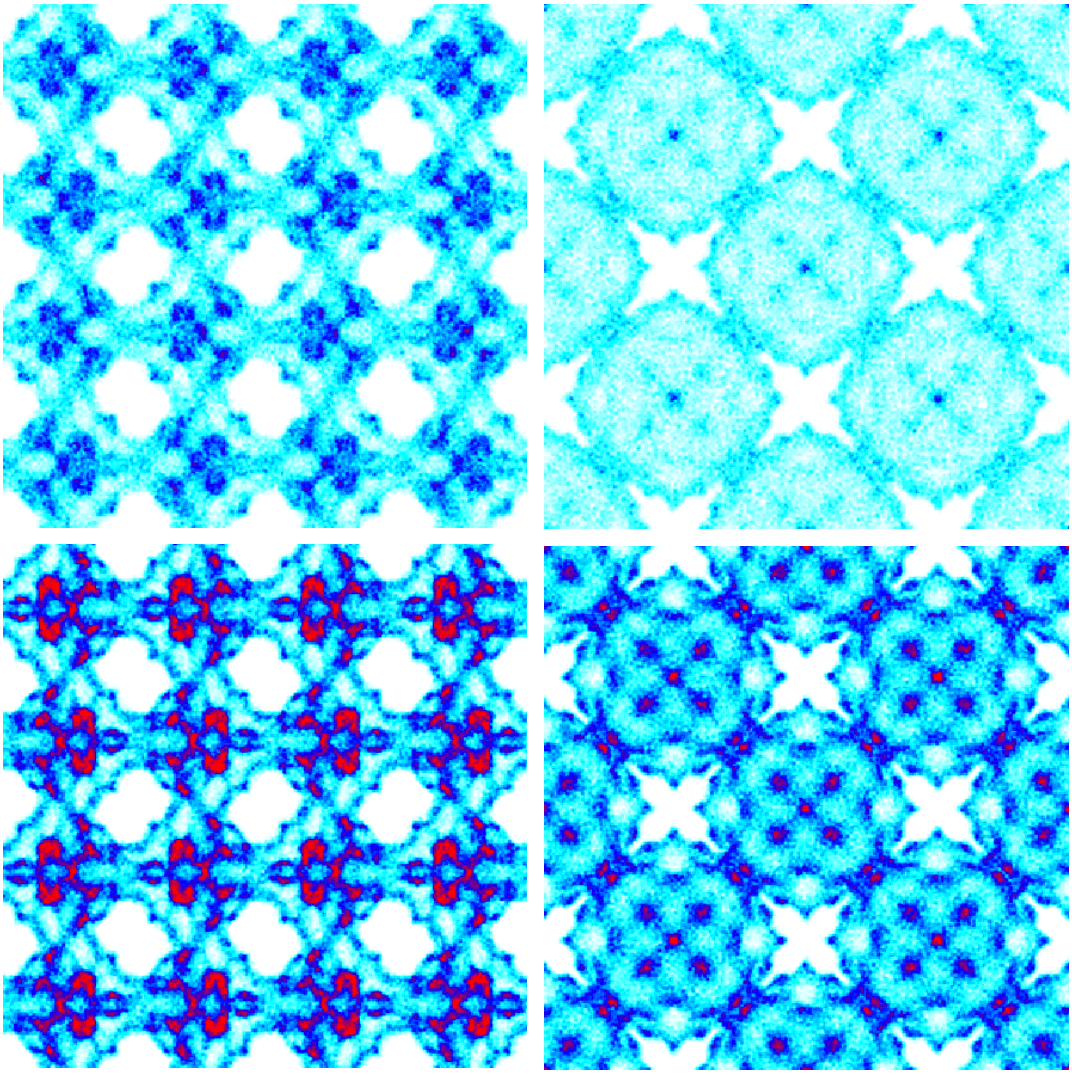


Figure S5: Average density profiles of hydrogen at 77 K and 1 MPa (top) and 100 MPa (bottom) on JSR (left) and RWY (right). The color gradation indicates the occupational density (white-cyan-blue-red).

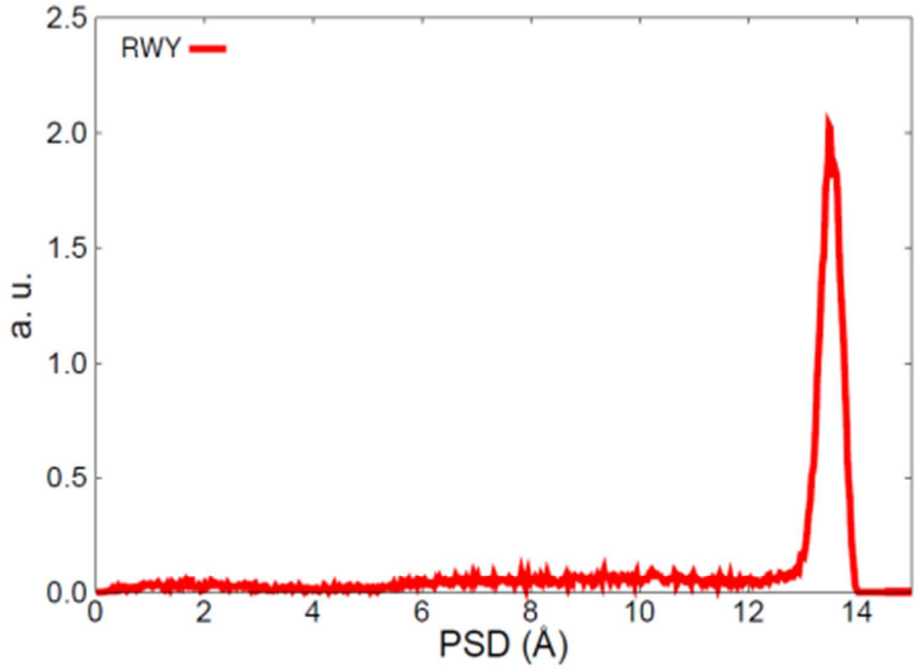


Figure S6: Computed pore size distribution of RWY.

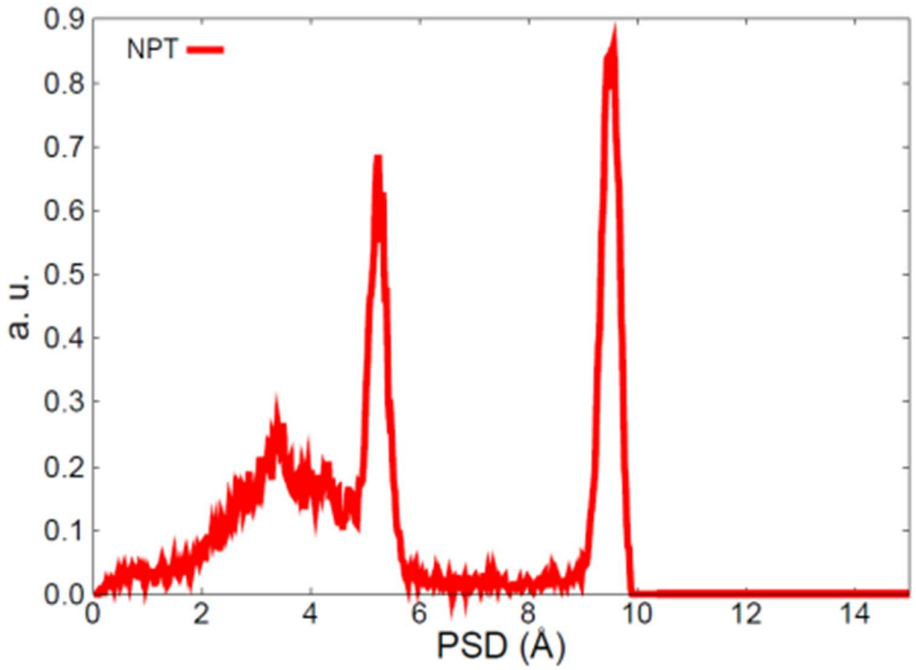


Figure S7: Computed pore size distribution of NPT.

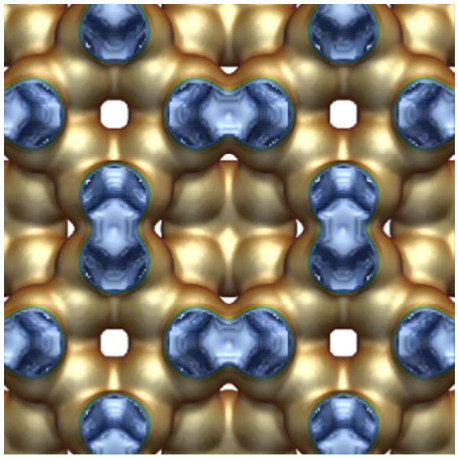


Figure S8: Energy grid profile of NPT. All views are identical. Brown and blue colors represent the accessible and inaccessible surface, respectively.

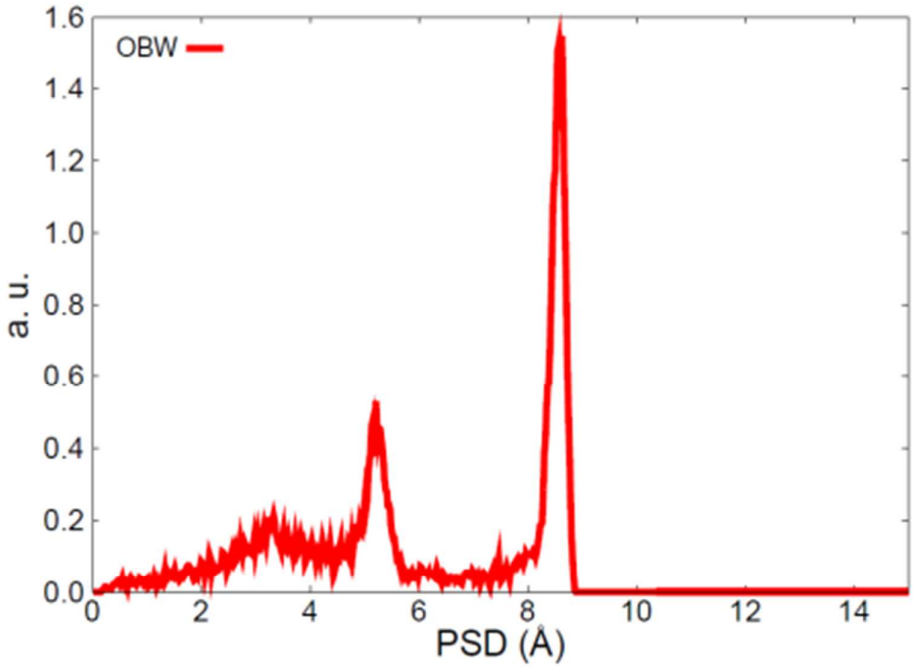


Figure S9: Computed pore size distribution of OBW.

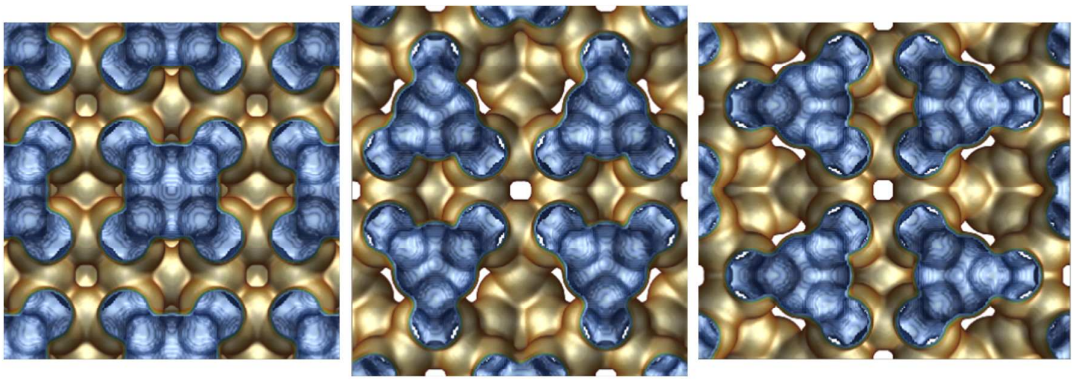


Figure S10: From left to right, *XY*, *YZ*, and *ZX* views of the energy grid profile of OBW. Brown and blue colors represent the accessible and inaccessible surface, respectively.

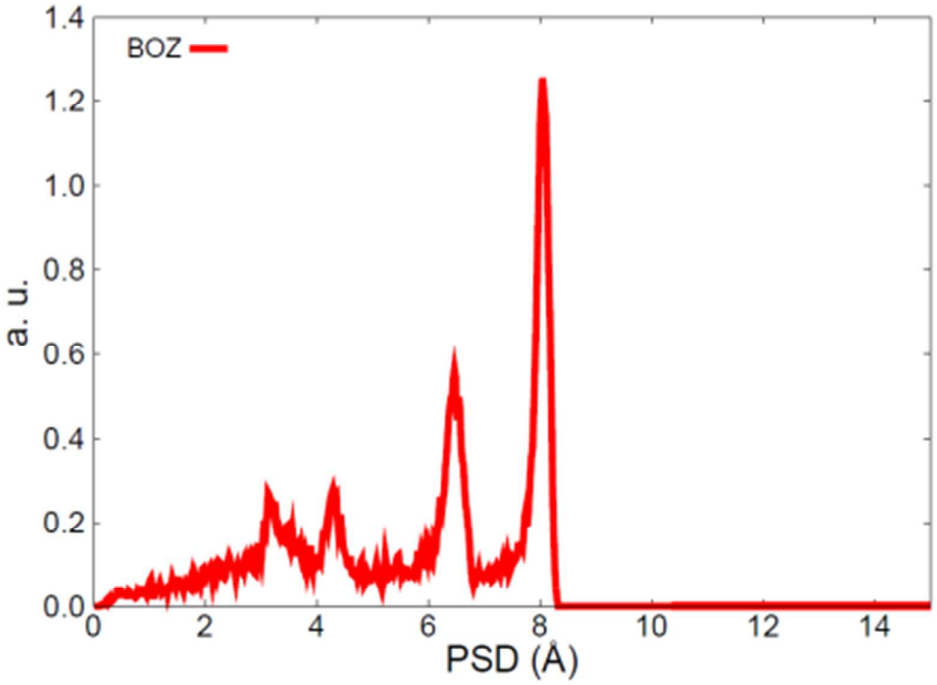


Figure S11: Computed pore size distribution of BOZ.

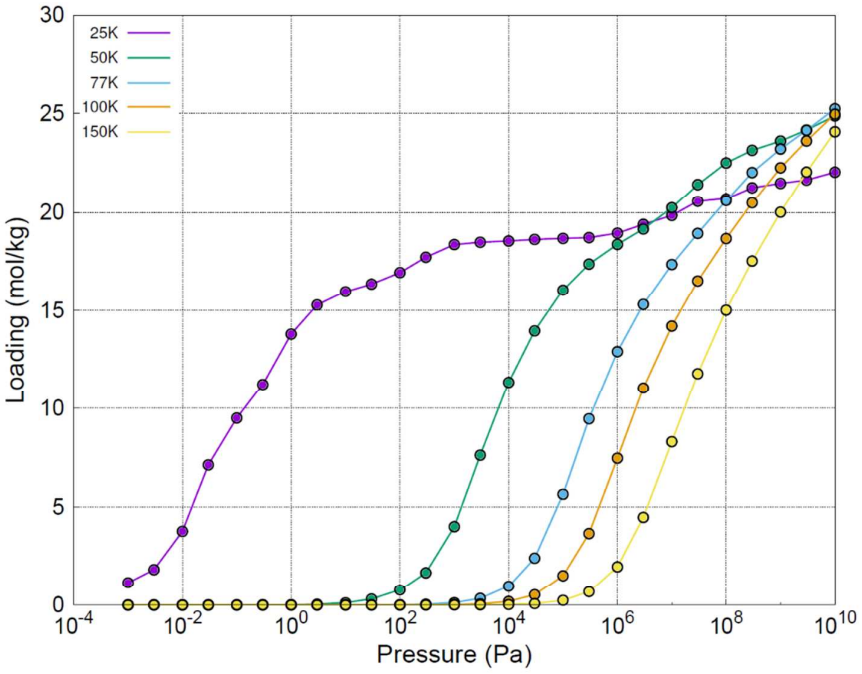


Figure S12: Adsorption isotherms of hydrogen in BOZ.

1. Duren, T.; Snurr, R. Q., Assessment of Isoreticular Metal-Organic Frameworks for Adsorption Separations: A Molecular Simulation Study of Methane/N-Butane Mixtures. *J. Phys. Chem. B* **2004**, *108*, 15703-15708.