Electronic Supporting Information

Study of Short-Chain Alcohol and Alcohol-Water Adsorption in MEL and MFI Zeolites

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Table S1 Non-bonded force field parameters used in the molecular simulations.

	Atom/Site	ε/k_B [K]	σ [Å]	q [e]
Water [1]	**O**	93.2	3.1589	-
	H	-	-	0.5564
	M	-	-	-1.1128
Alcohols [2]	**[CH_3]-OH**	98.0	3.750	0.265
	[CH_3]-CH_2	98.0	3.750	-
	[CH_2]-OH	46.0	3.950	0.265
	[CH_2]-CH_2	46.0	3.950	-
	O	93.0	3.020	-0.700
	H	-	-	0.435
Zeolite [3]	**O**	53	3.3	-0.75
	Si	22	2.3	1.5

Lorentz-Berthelot mixing rules[4] were used to account for the LJ parameters of the crossed interactions.

Figure S1. Simulated single-component adsorption isotherms in pure silica MEL zeolite at 298 K (closed symbols) and 323 K (open symbols) for **a)** alcohols (methanol in red, ethanol in green, 1-butanol in blue) and **b)** water.

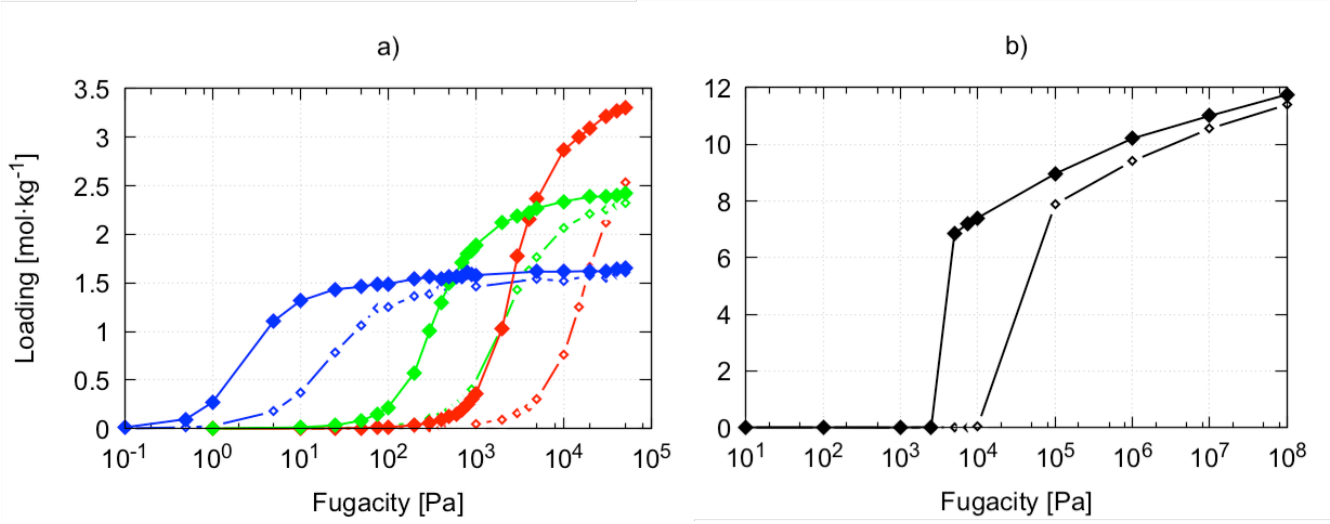
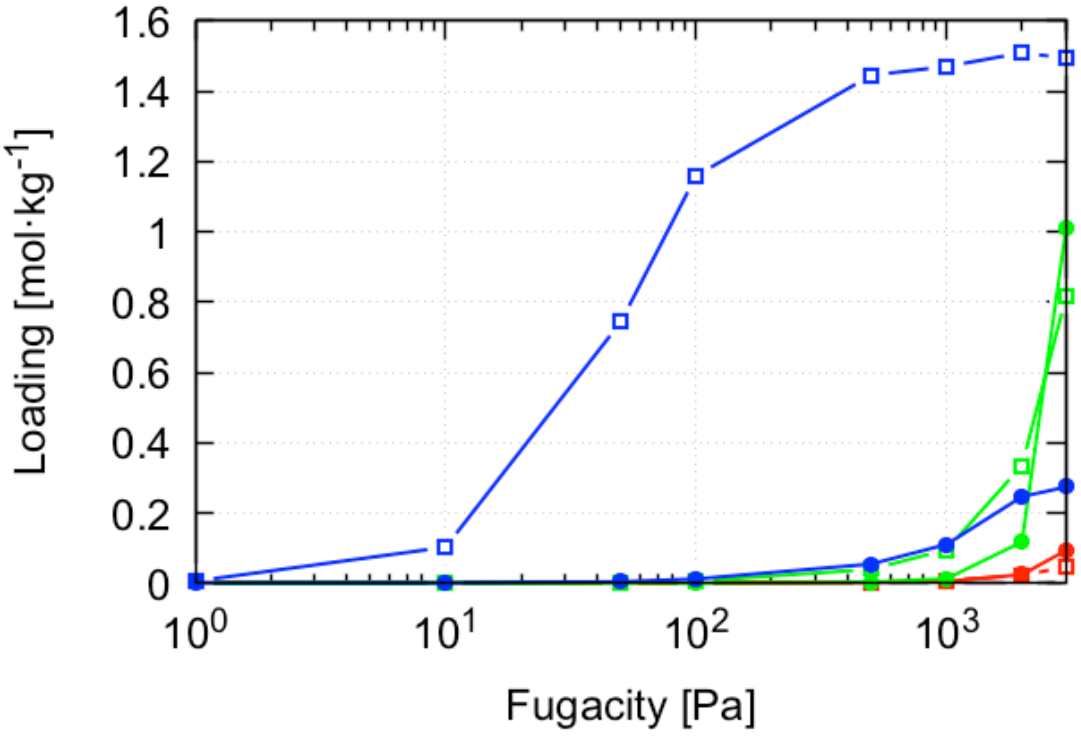


Figure S2. Simulated vapor adsorption isotherms at 298 K of 5/95 methanol/water (red), ethanol/water (green) and 1-butanol/water (blue) binary mixtures in pure silica MEL zeolite. Open square and closed circle symbols correspond to alcohol and water adsorption, respectively.



References

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