On the performance of FAU and MFI zeolites for the adsorptive removal of a series of Volatile Organic Compounds from air using molecular simulation

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Table S1 Force field parameters used in this work.

- ▪ **VOCs: propane, propene, butane, 1-butene**

  - ✓ Intermolecular interactions: Lennard-Jones parameters[1] (σ_{ij} in Å and ε_{ij}/K_B in K)

	O		$CH_3(sp^3)$		$CH_2(sp^3)$		$CH_2(sp^2)$		$CH(sp^2)$	
	σ_{ij}	ϵ_{ij}/k_B	σ_{ij}	ϵ_{ij}/k_B	σ_{ij}	ϵ_{ij}/k_B	σ_{ij}	ϵ_{ij}/k_B	σ_{ij}	ϵ_{ij}/k_B
$CH_3(sp^3)$	3.48	93	3.76	108	3.86	77.77	3.72	100.22	3.75	75.66
$CH_2(sp^3)$	3.58	60.5	3.86	77.77	3.96	56	3.82	72.17	3.85	54.48
$CH_2(sp^2)$	*3.53*	*82.05*	3.72	100.22	3.82	72.17	*3.685*	*93*	3.71	70.21
$CH(sp^2)$	*3.502*	*55.215*	3.75	75.66	3.85	54.48	3.71	70.21	*3.74*	*53*

  - ✓ Intramolecular interactions[1,2]

$$U^{intra} = U^{bond} + U^{bend} + U^{torsion}$$
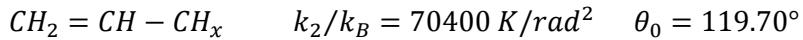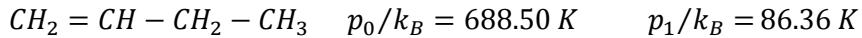
$$U^{bond} = \frac{1}{2}k_1(r - r_0)^2$$

$CH_x - CH_x$ $k_1/k_B = 96500\ K/Å^2$ $r_0 = 1.54\ Å$ $\boxed{\text{Subscript } x = 2 \text{ or } 3}$

$CH_2 = CH$ $k_1/k_B = 96500\ K/Å^2$ $r_0 = 1.33\ Å$

$$U^{bend} = \frac{1}{2}k_2(\theta - \theta_0)^2$$

$CH_x - CH_2 - CH_x$ $k_2/k_B = 62500\ K/rad^2$ $\theta_0 = 114°$ $\boxed{\text{Subscript } x = 2 \text{ or } 3}$

$CH_2 = CH - CH_x$ $k_2/k_B = 70400\ K/rad^2$ $\theta_0 = 119.70°$

$$U^{torsion} = p_0 + p_1[1 + cos\emptyset_{ijkl}] + p_2[1 - cos2\emptyset_{ijkl}] + p_3[1 + cos3\emptyset_{ijkl}]$$

$CH_3 - CH_2 - CH_2 - CH_3$ $p_0/k_B = 0.0\ K$ $p_1/k_B = 335.03\ K$

$p_2/k_B = -68.19\ K$ $p_3/k_B = 791.32\ K$

$CH_2 = CH - CH_2 - CH_3$ $p_0/k_B = 688.50\ K$ $p_1/k_B = 86.36\ K$

$p_2/k_B = -109.77\ K$ $p_3/k_B = -282.24\ K$
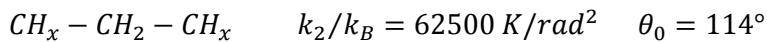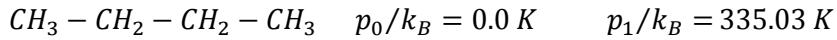
[1] B. Liu, B. Smit, F. Rey, S. Valencia, and S. Calero, *J. Phys. Chem. C*, 2008, **112**, 2492-2498 (ref. 20 of the manuscript). It includes parameters for alkanes of the earlier work of Dubbeldam *et al.* [2].

[2] D. Dubbeldam, S. Calero, T. J. H. Vlugt, R. Krishna, T. L. M. Maesen, and B. Smit, *J. Phys. Chem. B.*, 2004, **108**, 12301-12313 (ref. 19 of the manuscript).

- **Nitrogen N$_2$, Oxygen O$_2$, and Argon Ar**

  ✓ Point charges and Lennard-Jones (L-J) parameters

Atom	Charge / e⁻	L-J parameters[3]		Cross L-J parameters with O$_{zeo}$[4]	
		$\varepsilon/\kappa_B/K$	$\sigma/\text{Å}$	$\varepsilon/\kappa_B/K$	$\sigma/\text{Å}$
N (N$_2$)	-0.405	38.298	3.306	60.58	3.261
Dummy (N$_2$)	0.810	-	-	-	-
O (O$_2$)	-0.112	53.023	3.045	65.189	3.129
Dummy (O$_2$)	0.224	-	-	-	-
Ar	-	124.070	3.380	107.69	3.15

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