Supporting information

Lennard-Jones potential

The general form of the Lennard-Jones potential between atom i and atom j is given by:

$$V_{ij} = \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}}$$

In which A_{ij} and B_{ij} are calculated by the following expressions:

$$A_{ij} = \sqrt{A_i A_j}$$
$$B_{ij} = \sqrt{B_i B_j}$$

All Lennard-Jones potentials have been applied with a cut-off from 0 to 40 Å, except for the C_{sp3} – O Lennard-Jones potentials which is applied between 2 and 40 Å to avoid interference with the bond describing Morse potential.

The following parameters A and B have been used:

atom	A (eV Å^{12})	B (eV Å^{6})
C_{sp3}	77636.68281260	22.91719173
C_{sp2}	128737.36099524	57.48815803
C_{arom}	128737.36099524	57.48815803
H	308.25289998	1.42541402
Si	136561.43622211	30.78857787
Al	136561.43622211	30.78857787
O	11833.86243143	21.63347716

Overview of the potentials added to the zeolite force field and the applied cut-off distances

1. Morse potential

$$E_{Morse} = D_e\left[\left(1 - exp\left(-a\left(r - r_0\right)\right)\right)^2 - 1\right]$$

Bonds (Morse)*	D_e **(eV)**	a **(Å^{-1})**	r_0 **(Å)**	**cut-off (Å)**
H–C	1.4284	2.2707	1.1172	0.0 – 1.5
C_{sp2}–C_{sp2}	1.9947	2.5977	1.3271	0.0 – 2.0
C_{sp3}–C	1.4262	2.2722	1.4814	0.0 – 2.0
C_{arom}–C_{arom}	1.5206	2.3718	1.4009	0.0 – 2.0
C_{sp3}–O	0.9526	1.3651	1.8288	0.0 – 2.0

* If the carbon atom type is not specified (“C”), the respective potential function applies for any combination of the three types of carbon atoms (C_{sp2}, C_{sp3} and C_{arom})

2. Three-Body potential

$$E_{Three-Body} = \frac{1}{2}k\left(\theta - \theta_0\right)^2$$

Angle (Three-Body)*	k **(eV rad^{-2})**	θ_0 **(degrees)**	**cut-off (Å)****		
at2 – at1 – at3 **			$\mathbf{r_{12}}$	$\mathbf{r_{13}}$	$\mathbf{r_{23}}$
H–C_{sp2}–H	1.0074	120.00	0.0 – 1.5	0.0 – 1.5	0.0 – 4.0
H–C_{sp2}–C	1.6048	120.00	0.0 – 1.5	0.0 – 2.0	0.0 – 4.0
C–C_{sp2}–C	1.7965	120.00	0.0 – 2.0	0.0 – 2.0	0.0 – 4.0
H–C_{sp3}–H	1.1704	109.47	0.0 – 1.5	0.0 – 1.5	0.0 – 4.0
H–C_{sp3}–C	1.5839	109.47	0.0 – 1.5	0.0 – 2.0	0.0 – 4.0
C–C_{sp3}–C	2.2766	109.47	0.0 – 2.0	0.0 – 2.0	0.0 – 4.0
H–C_{arom}–C_{arom}	1.4335	120.00	0.0 – 1.5	0.0 – 2.0	0.0 – 4.0
C– C_{arom}–C_{arom}	1.7782	120.00	0.0 – 2.0	0.0 – 2.0	0.0 – 4.0
C–C_{sp3}–O	1.9585	109.47	0.0 – 2.0	0.0 – 2.0	0.0 – 4.0

* If the carbon atom type is not specified (“C”), the respective potential function applies for any combination of the three types of carbon atoms (C_{sp2}, C_{sp3} and C_{arom})

** See Figure below for a clarification of the atom numbers and the cut-off distances