

SUPPLEMENTARY MATERIAL

Parameters used in the united-atom (UA) model for alkane chains.

Intramolecular Potential Functions

Bond Potential: Constrained

Valence Angle Potential:

$$U(\theta_{jik}) = \frac{k}{2} (\theta_{jik} - \theta_0)^2$$

Dihedral Angle Potential:

$$U(\theta_{jikn}) = A_i [1 + \cos(m_i \theta_{jikn})]$$

$i=1,6$

Intermolecular Potential Functions

Short Ranged Potential:

$$U(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right]$$

Long Ranged Electrostatic Potential:

$$U(r_{ij}) = \frac{q_i q_j e^2}{r_{ij}} + \frac{e^2}{n(\sigma_i + \sigma_j)} \left(\frac{\sigma_i + \sigma_j}{r_{ij}} \right)^9$$

Bond Parameters

Bond	Length (Å)
C-C	1.53

Valence Angle Parameters

Bond	k (kJ mol ⁻¹ rad ⁻²)	θ (deg)
C-C-C	520.0	112.5

Dihedral Angle Parameters

C-C-C-C torsion, <i>i</i>	<i>M_I</i>	<i>A_I</i>
1	0	-9.840
2	1	9.823
3	2	6.560
4	3	10.607
5	4	3.280
6	5	1.968

Short Ranged Parameters

Pair	ϵ (kJ mol⁻¹)	σ (Å)
CH ₃ - CH ₃	0.64230	3.7400
CH ₃ -CH ₂	0.62009	3.8230
CH ₂ -CH ₂	0.59864	3.9230
Fe- CH ₃	0.38450	3.8920
O-CH ₂	0.37120	3.9835
O- CH ₃	0.50710	3.3870
O-CH ₂	0.48960	3.4785

Long Ranged Parameters

Atom	<i>q</i> (e)	σ (Å)
Fe	2.6175	0.785
O	-1.7450	1.240
CH ₂	0.0	-
CH ₃	0.0	-