Supplementary Information

Interactions of Long Chain Polyamines with Silica Studied by Molecular Dynamics Simulations and Solid-State NMR Spectroscopy

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Force Field Parameters

BONDS
$V(bond) = K_b(b - b0)^2$
K_b: kcal/mole/A^2

Silica surface (SiO)

atom type	Kb	b0
OC24 HOY	495.00	0.945
SC4 OC24	285.00	1.650
SC4 OC23	285.00	1.650

TIP3P water model (AmberFF10)

atom type	Kb	b0
HT HT	553.000	1.5136
OT HT	553.000	0.9572

Polyamine (LCPA)

atom type	Kb	b0
C3 C3	310.0	1.526
C3 H1	340.0	1.090
C3 HC	340.0	1.090
C3 HX	340.0	1.090
C3 N4	365.0	1.471

C3 N3	365.0	1.471
HN N3	435.0	1.010
HN N4	435.0	1.010

ANGLES

$V(angle) = K_\theta(\theta - \theta_0)^2$

Silica surface (SiO)

atom types	**K_ϑ**	**ϑ_0**
OC24 SC4 OC23	100.00	109.500
OC24 SC4 OC24	100.00	109.500
OC23 SC4 OC23	100.00	109.500
SC4 OC23 SC4	100.00	149.000
SC4 OC24 HOY	50.00	115.000

Polyamine (LCPA)

atom types	**K_ϑ**	**ϑ_0**
C3 C3 C3	40.0	109.50
C3 C3 H1	50.0	109.50
C3 C3 HC	50.0	109.50
C3 C3 HX	50.0	109.50
C3 C3 N4	80.0	111.20
C3 C3 N3	80.0	111.20
H1 C3 H1	35.0	109.50
H1 C3 N3	50.0	109.50
HC C3 HC	35.0	109.50
HX C3 HX	35.0	109.50
HX C3 N4	50.0	109.50
C3 N4 C3	50.0	109.50
C3 N4 HN	50.0	109.50
HN N4 HN	35.0	109.50
C3 N3 C3	50.0	109.50
C3 N3 HN	50.0	109.50
HN N3 HN	35.0	109.50

TIP3P water model (AmberFF10)

atom types	K_ϑ	ϑ_0
HT OT HT	100.000	104.520

DIHEDRALS

V(dihedral) = $K_\chi(1 + \cos(n(\chi) - \delta)$

K_χ: kcal/mole

n: multiplicity

δ: degrees

Polyamine (LCPA)

atom types	K_χ	n	δ
X C3 N4 X	0.156	3	0.0
X C3 C3 X	0.156	3	0.0
X C3 N3 X	0.300	3	0.0
C3 C3 N3 C3	0.300	3	0.0

NON BONDED

Van Der Waals

V(Lennard-Jones) = $\varepsilon_{,i,j}[(R_{min,i,j}/r_{i,j})^{12} - 2(R_{min,i,j}/r_{i,j})^{6}]$

Silica surface (SIO)

	ε	R_{min}
HOY	-0.015000	0.608936
OC23	-0.054000	1.947472
OC24	-0.122000	1.947472
SC4	-0.093000	2.329109
NA+	-0.094000	1.779102
CLA	-0.265000	1.948000

Polyamine (LCPA)

	ε	R_{min}
C3	-0.1094	1.9080
HX	-0.0157	1.1000
N4	-0.1700	1.8240
HC	-0.0157	1.4870
H1	-0.0157	1.3870
N3	-0.1700	1.8240
HN	-0.0157	0.6000

TIP3P water model (AmberFF10)

	ε	R_{min}
OT	-0.152000	1.768300
HT	-0.000000	0.000000

PARTIAL CHARGES

Silica surface (SIO)

	charge	mass
SC4	1.100000	28.0855
OC23	-0.550000	15.9994
OC24	-0.675000	15.9994
HOY	0.400000	1.0079
NA+	1.000000	22.9898
CLA	-1.000000	35.4500

Polyamine (LCPA)

	charge	mass
N4	-0.303900	14.0100
HN	0.352700	1.0080
HN	0.352700	1.0080
HN	0.352700	1.0080
C3	0.043300	12.0100
HX	0.128200	1.0080
HX	0.128200	1.0080
C3	-0.147100	12.0100
HX	0.155000	1.0080
HX	0.155000	1.0080
N4	-0.072900	14.0100
HN	0.286900	1.0080
HN	0.286900	1.0080
C3	-0.031100	12.0100
HX	0.125700	1.0080
HX	0.125700	1.0080
C3	-0.035400	12.0100
HC	0.064500	1.0080
HC	0.064500	1.0080
C3	-0.032600	12.0100
HX	0.103700	1.0080
HX	0.103700	1.0080
N4	-0.037600	14.0100
HN	0.254600	1.0080
HN	0.254600	1.0080
C3	0.026100	12.0100
HX	0.111100	1.0080
HX	0.111100	1.0080
C3	0.002300	12.0100
H1	0.082400	1.0080
H1	0.082400	1.0080
N3	-0.668300	14.0100
HN	0.368500	1.0080
C3	0.093700	12.0100
H1	0.088500	1.0080
H1	0.088500	1.0080
C3	-0.031500	12.0100
HC	0.063200	1.0080
HC	0.063200	1.0080

C3	-0.085000	12.0100
HX	0.100700	1.0080
HX	0.100700	1.0080
N4	-0.005500	14.0100
HN	0.255400	1.0080
HN	0.255400	1.0080
C3	-0.008300	12.0100
HX	0.108500	1.0080
HX	0.108500	1.0080
C3	-0.078200	12.0100
HC	0.069000	1.0080
HC	0.069000	1.0080
C3	-0.034500	12.0100
HX	0.114300	1.0080
HX	0.114300	1.0080
N4	-0.055000	14.0100
HN	0.276700	1.0080
HN	0.276700	1.0080
C3	-0.032900	12.0100
HX	0.114000	1.0080
HX	0.114000	1.0080
C3	-0.078800	12.0100
HC	0.068600	1.0080
HC	0.068600	1.0080
C3	-0.012500	12.0100
HX	0.109100	1.0080
HX	0.109100	1.0080
N4	0.000800	14.0100
HN	0.253800	1.0080
HN	0.253800	1.0080
C3	-0.116600	12.0100
HX	0.108200	1.0080
HX	0.108200	1.0080
C3	0.002700	12.0100
HC	0.056000	1.0080
HC	0.056000	1.0080
C3	0.079100	12.0100
H1	0.084400	1.0080
H1	0.084400	1.0080
N3	-0.666800	14.0100
HN	0.363800	1.0080
C3	-0.014000	12.0100
H1	0.086900	1.0080
H1	0.086900	1.0080
C3	0.004400	12.0100
HX	0.108700	1.0080
HX	0.108700	1.0080
N4	0.060300	14.0100
HN	0.221400	1.0080
HN	0.221400	1.0080
C3	-0.111100	12.0100
HX	0.089100	1.0080

HX	0.089100	1.0080
C3	0.025000	12.0100
HC	0.044400	1.0080
HC	0.044400	1.0080
C3	0.130900	12.0100
H1	0.070500	1.0080
H1	0.070500	1.0080
N3	-0.720300	14.0100
HN	0.368400	1.0080
C3	0.030100	12.0100
H1	0.088300	1.0080
H1	0.088300	1.0080
C3	0.027500	12.0100
HX	0.126700	1.0080
HX	0.126700	1.0080
N4	-0.346800	14.0100
HN	0.334900	1.0080
HN	0.334900	1.0080
HN	0.334900	1.0080

TIP3P water model (AmberFF10)

	charge	**mass**
OT	-0.834000	15.9994
HT	0.417000	1.0080
HT	0.417000	1.0080