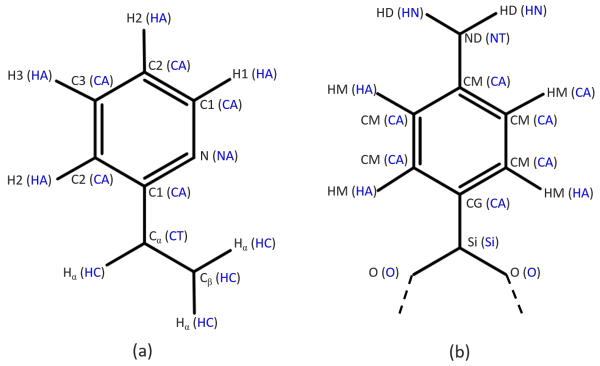

Figure 1 The structural formula of (a) 2-vinylpyridine unit and (b) octaaminophenyl polyhedraloligomeric silsesquioxane particle. Atomic types or labels given in black/blue are for nonboned/boned interaction parameters listed in the following tables. In OAPS particle, only one Si and two O atoms are shown for clarity.

Table 1 Nonbonded force-field parameters for poly(2-vinylpyridine) and octaaminophenyl polyhedraloligomeric silsesquioxane.

$V\left(r_{ij}\right) = 4\varepsilon\left[\left(\sigma/r_{ij}\right)^{12} - \left(\sigma/r_{ij}\right)^{6}\right] + \left(q_i q_j/4\pi\varepsilon_0 r_{ij}\right)\left[r_{ij}^{-1} + \left(\left(\varepsilon_{\mathrm{RF}^{-1}}\right)\left(2\varepsilon_{\mathrm{RF}}+1\right)\right)\left(\mathrm{r}_{ij}^{2}/r_{\mathrm{cuttoff}}\right)\right]$

atom type	bond type	$\varepsilon/kJmol^{-1}$	σ/nm	q/e
poly(2-vinylpyridine)				
NA	NC	0.7112	0.3250	-0.6560
C1	CA	0.2928	0.355	0.5145
H1	HA	0.1255	0.242	0.0120
C2	CA	0.2928	0.355	-0.422
H2	HA	0.1255	0.242	0.0835
C3	CA	0.2928	0.355	0.2270
H3	HA	0.1255	0.242	0.0650
C_α	CT	0.2761	0.350	-0.1080
H_α	HC	0.1255	0.250	0.1080
C_β	CT	0.2761	0.350	-0.1200
H_β	HC	0.1255	0.250	0.0600
octaaminophenyl polyhedral oligomeric silsesquioxane				
Si	Si	2.5104	0.3920	1.020
O	O	0.6368	0.3154	0.6368
CM	CA	0.2940	0.355	-0.115
CG	CA	0.2940	0.355	0.000
HM	HA	0.1260	0.242	0.115
CN	CA	0.2928	0.355	0.020
ND	NT	0.7112	0.330	-0.780
HD	HN	0.000	0.0000	0.380

Table 2 Bond stretching parameters.

harmonic bonds	r_0/nm	$V_{\mathrm{bond}} = (K_\mathrm{r}/2)(r-r_0)^2$ k_r/kJmol^{-1}nm^{-2}
poly(2-vinylpyridine)		
CA-NC	0.134	404174.4
CA-CA	0.140	392459.2
CA-CT	0.151	265265.6
CA-HA	0.108	307105.6
CT-HC	0.109	284512
CT-CT	0.153	224262.4
octaaminophenyl polyhedral oligomeric silsesquioxane		
Si-O	0.163	323984.0
CA-CA	0.139	393022.0
CA-Si	0.184	100000
CA-NT	0.134	402500.8
CA-HA	0.108	200000
NT-HN	0.101	363171.2

Table 3 Bond angle parameters.

harmoic bond angles	θ_0/	$V(\theta) = (k_\theta/2)(\theta-\theta_0)^2$ k_θ/kJ mol^{-1} rad^{-2}
poly(2-vinylpyridine)		
NC-CA-CA	124.0	585.760
NC-CA-CT	116.0	585.760
CA-CA-CT	120.0	585.760
CA-NC-CA	117.0	585.760
NC-CA-HA	116.0	292.880
CA-CA-HA	120.0	292.880
CA-CA-CA	120.0	527.184
CA-CT-HC	109.5	292.990
CA-CT-CT	114.0	527.184
CT-CT-HC	110.7	313.800
HC-CT-HC	107.8	276.144
octaaminophenyl polyhedral oligomeric silsesquioxane		
O-Si-O	109.5	469.72
Si-O-Si	144.0	209.60
CA-Si-O	114.9	469.72
CA-CA-Si	120.0	418.80
CA-CA-CA	120.0	376.60
CA-CA-HA	120.0	418.80
CA-CA-CT	120.0	585.76
CA-NT-HN	111.0	292.88
HN-NT-HN	106.4	364.85

Table 4 Dihedral parameters.

				$V_{rb}\left(\phi_{ijkl}\right) = \sum_{n=0}^{5} C_n(\cos(\psi))^n$		
Ryckaert-Bellemans dihedral angles	C0	C1	C2	C3	C4	C5
poly(2-vinylpyridine)						
A_{ring}-A_{ring}-A_{ring}-A_{ring}*	30.334	0.0	-30.334	0.0	0.0	0.0
A_{ring}-A_{ring}-A_{ring}-HA	30.334	0.0	-30.334	0.0	0.0	0.0
CA-CT-CT-HC	0.9665	2.8995	0.0	-3.8660	0.0	0.0
CA-CT-CT-CT	2.9288	-1.4644	0.2092	-1.6736	0.0	0.0
*A_{ring} includes CA NC bond type						
octaaminophenyl polyhedral oligomeric silsesquioxane						
CA-CA-NT-HN	16.987	0.0	-16.987	0.0	0.0	0.0

		$V(\varphi) = \left(k_\varphi/2\right)(\varphi - \varphi_0)^2$
harmonic dihedral angles	φ_0/ degrees	k_φ/kJmol^{-1}rad^{-2}
poly(2-vinylpyridine)		
HA-CA-CA-CA	180.0	10.460
HA-CA-CA-NC	180.0	10.460
NC-CA-CT-CA	180.0	10.460
octaaminophenyl polyhedral oligomeric silsesquioxane		
CA-CA-CA-HA	180.0	10.460
CA-CA-CA-CA	180.0	10.460
CA-CA-CA-Si	180.0	10.460
CA-CA-CA-NT	180.0	10.460