**Supplementary Material**

Molecular dynamics simulations of montmorillonite reinforcing amylose plasticized by Brazilian Cerrado oils: polymer-clay nanocomposite.

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In the following supplementary material, we present some snapshots of the studied systems helping to correlate the following data: energetic characteristics, number of components and control graphics of the dynamic trajectories.



**FIG. S1.** (Left) Snapshots of system fluctuations over MMT-O surface, at 0 ps, 20 ps and 200 ps of dynamic trajectory, at 363 K. The oligomer amylose (lilac) is shown in space-filling model of Corey, Pauling, Koltun (CPK model), as well the ions Na+ (violet) and N+ cetrimonium ions (cobalt blue), whose spheres have been reduced for clarity. The atoms of palmitic fatty acids are colored green, light blue for stearic and the ones of oleic acids, gray. The MMT is in white stick representation. (Right) Graphics of dynamic process control (Energy (kcal mol-1) vs. time (ps) and temperature (K) vs. time (ps)) to a 200 ps trajectory, at 363 K.

**TABLE SI.** Composition data of the molecular system and selected energetic values for three representative dynamic fluctuations for the first model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom numbers in the system: MMT = 5 458; Na+ = 128; cetrimonium ion = 682; amylose = 842; fatty acids: oleic = 702, palmitic = 400, stearic = 56; water = 2652. Total atoms number = 10 920 atoms.  Cell parameters: a = 103.84 Å; b = 54.09 Å; c = 50.05 Å;  = 90.00 0 | | | |
| Fluctuation time in the dynamic trajectory (ps) | **0** | **20** | **200** |
| Total energy (Etot) (kcal.mol-1) | -824 424.72 | -824 239.75 | -824 663.39  -5 496.441 |
| Most significant energetic contributions to Etot (kcal.mol-1) | | | |
| Valence energy  (diag. terms) | 18 871.86 | 18 928.07 | 18 823.09  -1 449.05 |
| Bond | 16 989.80 | 17 004.37 | 16 963.80  269.97 |
| Angle | 4 370.68 | 4 397.95 | 4 379.03  800.72 |
| Torsion | -2 488.88 | -2 474.53 | -2 520.03  -2 520.03 |
| Valence energy  (cross terms) | -367.59 | -373.72 | -369.22  -369.23 |
| Stretch-Bend-Stretch | -59.81 | -60.57 | -59.39  -59.39 |
| Torsion-Bend-Bend | -64.45 | -66.42 | -68.70  -68.70 |
| Bend-Torsion-Bend | -241.94 | -246.47 | -243.00  -243.00 |
| Non-bond energy | -842 928.98 | -842 794.11 | -843 117.26  -3 678.17 |
| van der Waals | -26.48 | -31.89 | -129.51  862.82 |
| Electrostatic | -842 902.49 | -842 762.22 | -842 987.75  -4 540.99 |
| rms force (kcal/mol/A) | 8.22 E-003 | 9.47 E-003 | 8.48 E-003 |
| max force (kcal/mol/A) | 7.33 E-002 | 1.78 E-001 | 1.65 E-001 |
| Radius of Gyration2 (Å) | 18.82 | 16.30 | 18.97 |

1Energetic values, highlighted in blue, exemplify the contributions to the system when MMT is excluded. Static values.

* Energy values were calculated by molecular mechanics from Forcite21 using PCFF-interface.15

2Radius of Gyration (Rg) were calculated only for the amylose chains by the Forcite Analysis tool in the Materials StudioTM suite.21



**FIG S2.** (Left) Snapshots of system fluctuations over MMT-O surface, at 0 ps, 20 ps and 200 ps of dynamic trajectory, at 363 K. (Center) top view of the previously described systems. The oligomer amylose (lilac) is shown in space-filling model of Corey, Pauling, Koltun (CPK model), as well the ions Na+ (violet) and N+ cetrimonium ions (cobalt blue), whose spheres have been reduced for clarity. The atoms of palmitic fatty acids are colored green, light blue for stearic and the ones of oleic acids, gray. The MMT is in white stick representation. (Right) Graphics of dynamic process control (Energy (kcal mol-1) vs. time (ps) and temperature (K) vs. time (ps)) to a 200 ps trajectory, at 363 K.

**TABLE SII.** Composition data for the second molecular system. Selected energetic values for three representative frames taken from a 200 ps dynamics trajectory, at 363 K, already optimized.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom numbers in the system: MMT = 5 458; Na+ = 128; cetrimonium ion = 682; amylose = 2 312; fatty acids: oleic = 756, palmitic = 500, stearic = 112; water = 2 604. Total atoms number = 12 555 atoms.  Cell parameters: a = 103.84 Å; b = 54.09 Å; c = 50.05 Å;  = 90.00 0 | | | |
| Fluctuation time in the dynamic trajectory (ps) | **0** | **60** | **200** |
| Total energy (Etot) (kcal.mol-1) | -823 212.18 | -824 176.15 | -825 096.37  -5 615.59 |
| Most significant energetic contributions to Etot (kcal.mol-1) | | | |
| Valence energy  (diag. terms) | 17 325.66 | 17 497.07 | 17 125.48  -2 838.8151 |
| Bond | 16 484.81 | 17 138.94 | 16 406.98  389.479 |
| Angle | 5 446.47 | 4 971.90 | 5 387.59  1 440.796 |
| Torsion | -4 605.91 | -4 614.13 | -4669.58  -4 669.58 |
| Valence energy  (cross terms) | -770.95 | -768.25 | -775.87  -775.87 |
| Stretch-Bend-Stretch | -91.65 | -90.05 | -89.15  -89.15 |
| Torsion-Bend-Bend | -208.00 | -201.80 | -199.58  -199.58 |
| Bend-Torsion-Bend | -499.02 | -498.25 | -515.48  -515.48 |
| Non-bond energy | -839 766.89 | -840 904.97 | -841 445.98  -2 000.90 |
| van der Waals | 51.98 | -431.05 | -488.53  405.37 |
| Electrostatic | -839 818.86 | -840 473.92 | -840 957.45  -2 406.27 |
| rms force (kcal/mol/A) | 6.16 E-002 | 7.94 E-003 | 7.47 E-003 |
| max force (kcal/mol/A) | 9.02 E-001 | 1.00 E-001 | 1.36 E-001 |
| Radius of Gyration2 (Å) | 22.1 | 19.57 | 18.97 |

1Energetic values, highlighted in blue, exemplify the contributions to the system when MMT is excluded. Static values.

* Energy values were calculated by molecular mechanics from Forcite21 using PCFF-interface.15

2Radius of Gyration (Rg) were calculated only for the amylose chains by the Forcite Analysis tool in the Materials StudioTM suite.21

**TABLE SIII.** Composition data for the third molecular system. Selected energetic values for five representative frames taken from the NPT dynamics trajectory, at 363 K, already optimized.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom numbers in the system: MMT =10 916; Na+ =243; cetrimonium ion =248; amylose =1054; fatty acids: oleic =540, palmitic =250, stearic = 56; water =. Total atoms number =14 771 atoms. | | | | | |
| Distance for reference: d O...O (A) | **43.48** | **42.20** | **30.24** | **23.54** | **15.92** |
| Total energy (Etot) | -1 629 722.01 | -1 629 679.26 | -1 629 546.53 | -1 629 330.32 | -1 629 692.67 |
| Most significant energetic contributions to Etot (kcal.mol-1) | | | | | |
| Valence energy (diag. terms) | 46 357.19 | 46 499.84 | 46 345.57 | 46 305.95 | 46 336.22 |
| Bond | 38 579.71 | 38 713.02 | 38 625.28 | 38 607.83 | 38 623.15 |
| Angle | 9 995.73 | 10 006.49 | 9 930.62 | 9 907.42 | 9 914.86 |
| Torsion | -2 218.42 | -2 219.84 | -2 210.60 | -2 209.50 | -2 202.01 |
| Valence energy (cross terms) | -371.97 | -371.03 | -363.65 | -359.03 | -358.25 |
| Stretch-Bend-Stretch | -47.23 | -47.20 | -47.55 | -46.18 | -46.01 |
| Torsion-Bend-Bend | -91.69 | -91.46 | -94.92 | -95.84 | -94.92 |
| Bend-Torsion-Bend | -243.88 | -243.20 | -233.08 | -226.45 | -227.89 |
| Non-bond energy | -1 675 707.23 | -1 675 808.07 | -1 675 528.45 | -1 675 277.24 | -1 675 670.65 |
| van der Waals | -870.68 | -832.92 | -665.06 | -664.68 | -919.58 |
| Electrostatic | -1 674 836.55 | -1 674 975.16 | -1 674 863.39 | -1 674 612.56 | -1 674 751.07 |
|  | | | | | |
| rms force (kcal/mol/A) | 8.315E-003 | 9.23 E-002 | 5.41 E-003 | 4.10 E-002 | 3.940E-004 |
| max force (kcal/mol/A) | 1.534E-001 | 9.083E-001 | 1.488E-001 | 5.667E-001 | 3.124E-003 |
| Cell parameters:  A (A);  B (A);  C (A);  alpha (0):  beta (0):  gamma (0): | 103.08;  53.70;  59.66;  90.00;  90.00;  90.00. | 103.16  53.65  58.33  90.06  89.72  89.91 | 103.17  53.66  46.30  91.55  89.08  89.91 | 103.17  53.66  39.56  91.35  87.87  89.90 | 103.17  53.66  31.81  93.13  87.53  89.91 |