Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Branched versus Linear Lactide Chains for Cellulose Nanoparticle Modification: An Atomistic Molecular Dynamics Study

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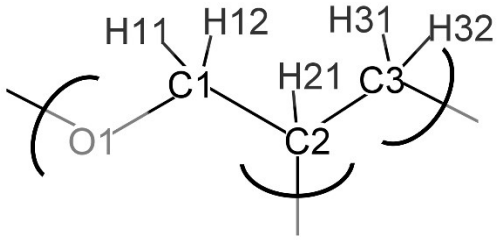
Values of atomic partial charges of branching points



Atom name	Partial charge, e
O1	-0.45
C1	-0.05
H11	0.10
H12	0.10
C2	0.05
H21	0.10
C3	-0.05
H31	0.10
H32	0.10

Order parameter of the grafted linear chains, as well as the root and free branches of the grafted branched chains

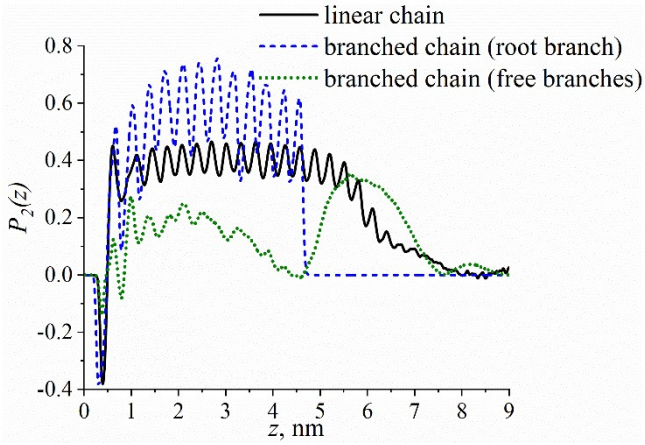


Fig. S1 Order parameter $P_2(z)$ of the grafted linear chains, as well as the root and free branches of the grafted branched chains relative to the CNC surface (z = 0 nm) at the grafting density σ = 1.76 nm^{-2}. The data for the linear chains were taken from ref. [Glova et al., Polymers 2019, 11, 2056]

Density profile of the free PLA chains in the composites

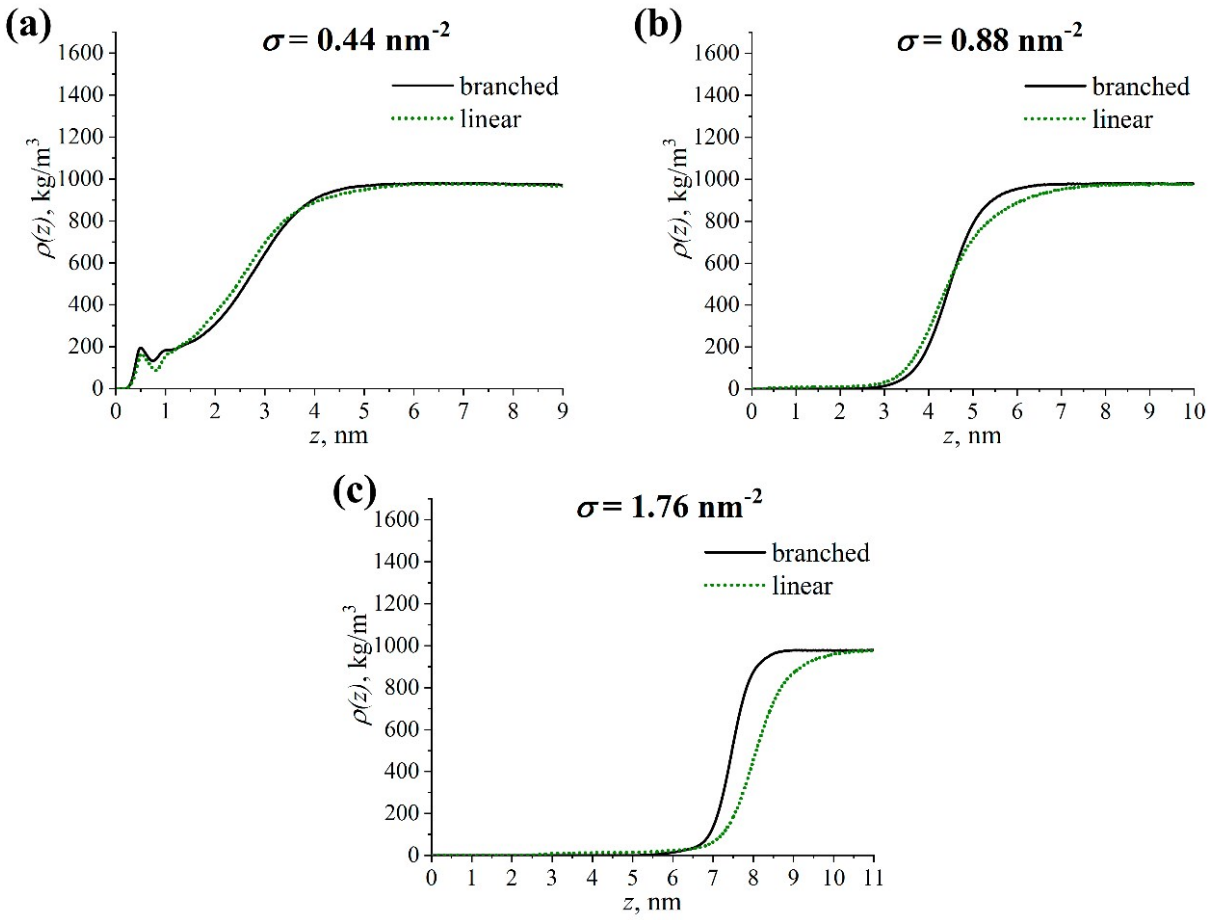
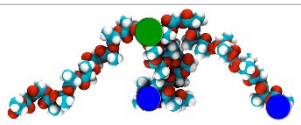
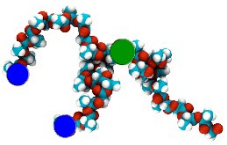
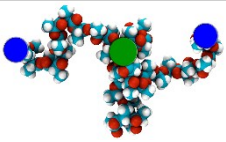
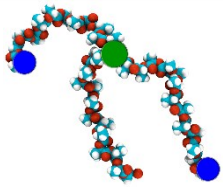
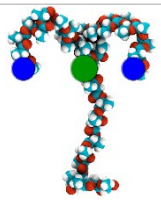
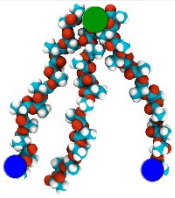
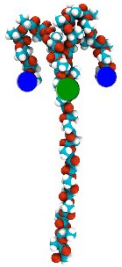


Fig. S2 Density profile *ρ(z)* of the free PLA chains in the composites filled with CNPs surface-modified by grafting branched and linear OLA chains with respect to the filler surface (z = 0 nm) at grafting densities σ of (a) 0.44 nm^{-2}, (b) 0.88 nm^{-2}, and (c) 1.76 nm^{-2}. Note that (1) the bulk density is the same for all model systems, and (2) an increase in the grafting density results in a greater expelling of the free PLA chains from the filler surface and in a greater difference in the density data for the cases of branched and linear grafted chains.

Regions on the bivariate joint probability distribution

Table S1. The boarders of the regions on the bivariate joint probability distribution $P(z_{e1}, z_{e2})$ used to calculate the fractions of the grafted chains in the observed preferable conformations.

Grafting density σ, nm^{-2}	Conformation snapshot	Boarders of the region in $P(z_{e1}, z_{e2})$
0.44		$z_{e1} \in \{0, 1\}$ nm $z_{e2} \in \{0, 1\}$ nm
		$z_{e1} \in \{0, 1\}$ nm $z_{e2} \in (1, 3\}$ nm and $z_{e1} \in (1, 3\}$ nm $z_{e2} \in \{0, 1\}$ nm
		$z_{e1} \in \{1, 3\}$ nm $z_{e2} \in \{1, 3\}$ nm
0.88		$z_{e1} \in \{0, 1\}$ nm $z_{e2} \in \{0, 1\}$ nm
		$z_{e1} \in \{0, 1\}$ nm $z_{e2} \in \{2, 5\}$ nm and $z_{e1} \in \{2, 5\}$ nm $z_{e2} \in \{0, 1\}$ nm
		$z_{e1} \in \{2, 5\}$ nm $z_{e2} \in \{2, 5\}$ nm
1.76		$z_{e1} \in \{0, 2\}$ nm $z_{e2} \in \{0, 2\}$ nm
		$z_{e1} \in \{4, 7\}$ nm $z_{e2} \in \{4, 7\}$ nm