*Supplementary Material for*

# Grafting-Induced Structural Ordering of Lactide Chains

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**1. Mean square end-to-end distance of grafted lactide chains**

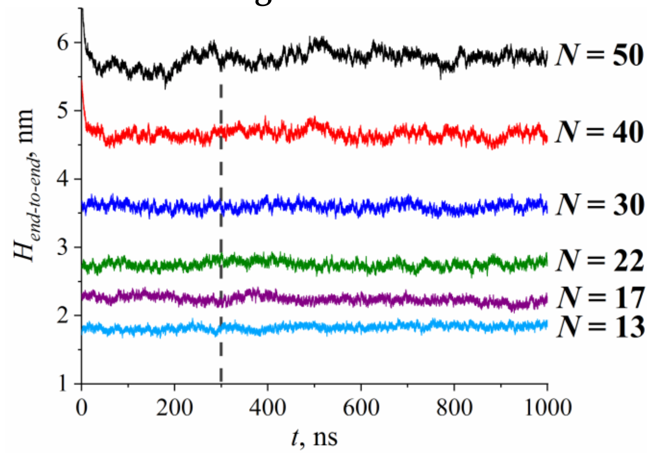


**Figure S1.** Time dependence of the mean square end-to-end distance $H_{end\text{-}to\text{-}end}$ for the grafted lactide chains with different lengths $N$. The vertical dash line shows the preliminary simulations time of 300 ns. Note that the decrease of $H_{end\text{-}to\text{-}end}$ for the grafts with $N = 40$ and 50 can be ascribed with the fact that the grafted chains were vertically oriented at the very beginning of the simulations (before compression); it takes some time for the grafts to stretch, since their length is higher than the one of the other grafts.

## 2. Distribution of center-of-mass position of grafted chains

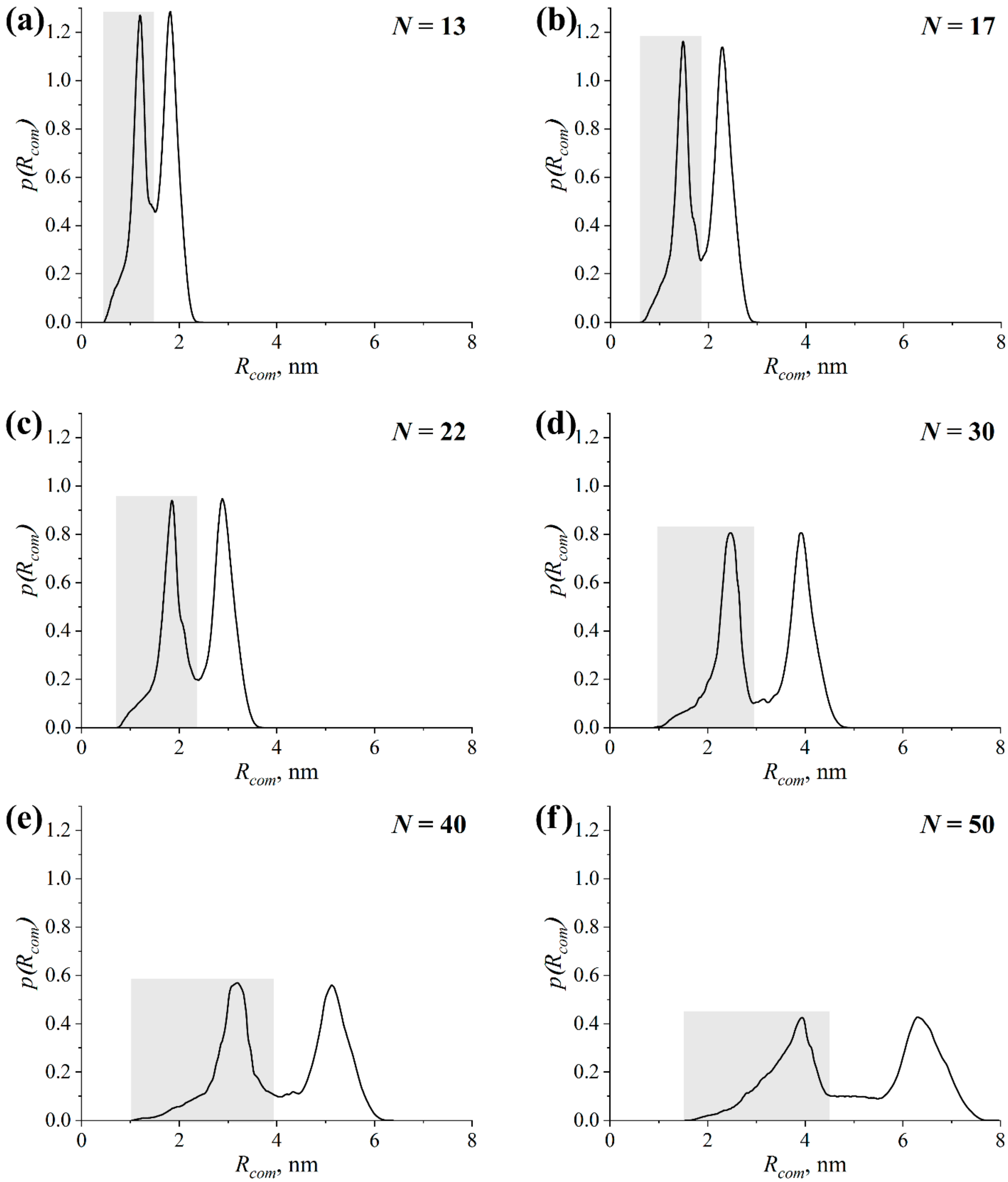


**Figure S2.** Probability density $p(R_{com})$ to find the center-of-mass of the graft at the distance $R_{com}$ relative to the filler surface in the systems with different graft's length $N$. Area colored in gray indicates the maximum corresponding to the fraction of the backfolded chains.

## 3. Normal density profiles of the grafted chains

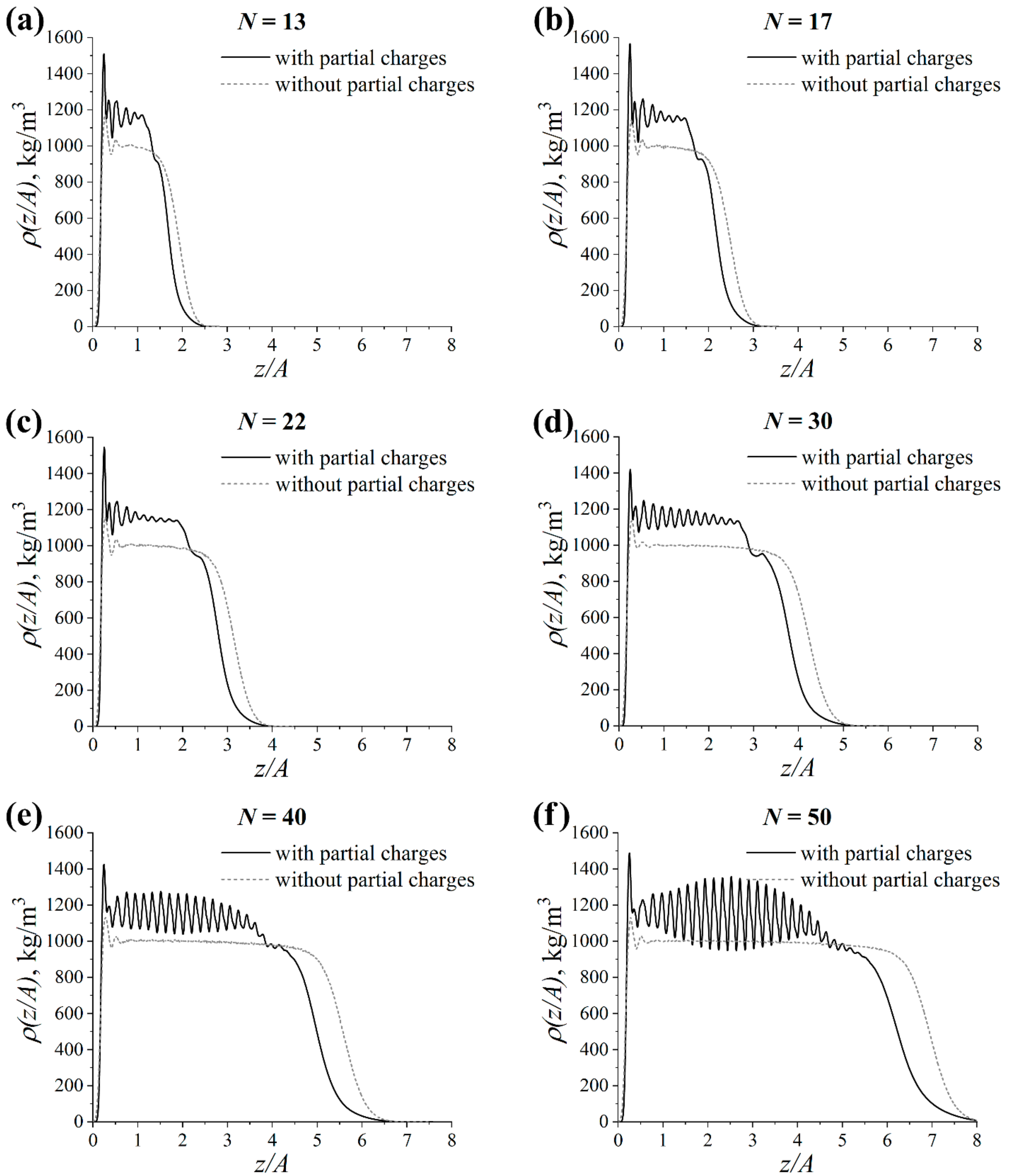


**Figure S3.** Normal density profiles of the grafted chains $\rho(z/A)$ related to the CNC surface at different graft's length $N$ in the systems with and without partial charges. $A$ is the Kuhn segment length for the lactide chains.

## 4. Order parameter for the grafts' monomers

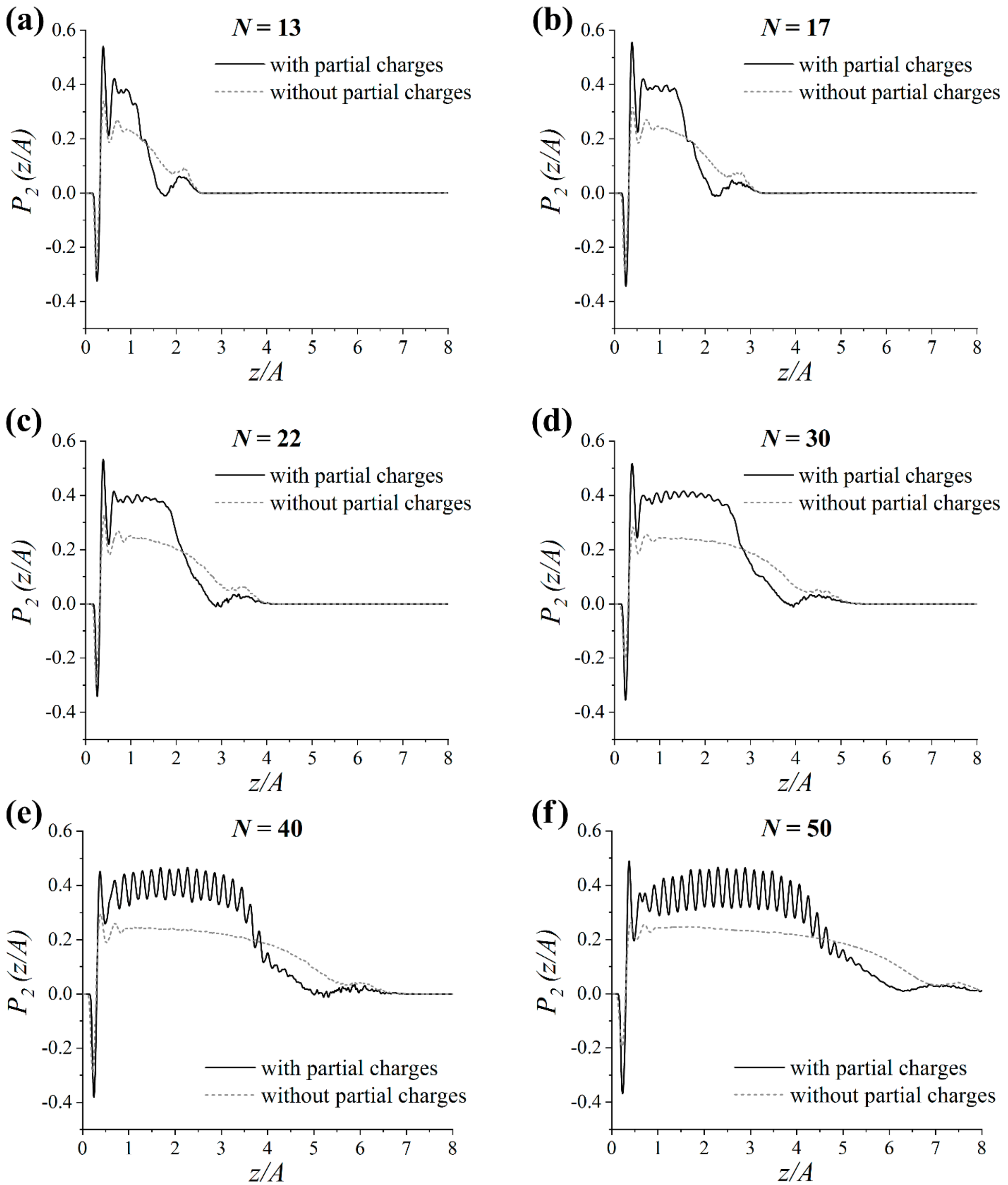


**Figure S4.** Order parameter $P_2(z/A)$ for the grafts' monomers as a function of their normalized distance from the filler surface $z/A$ at different chain length $N$ for the systems with and without partial charges. $A$ is the Kuhn segment length for the lactide chains.

## 5. Lateral density profiles for the grafted chains stretched from the surface

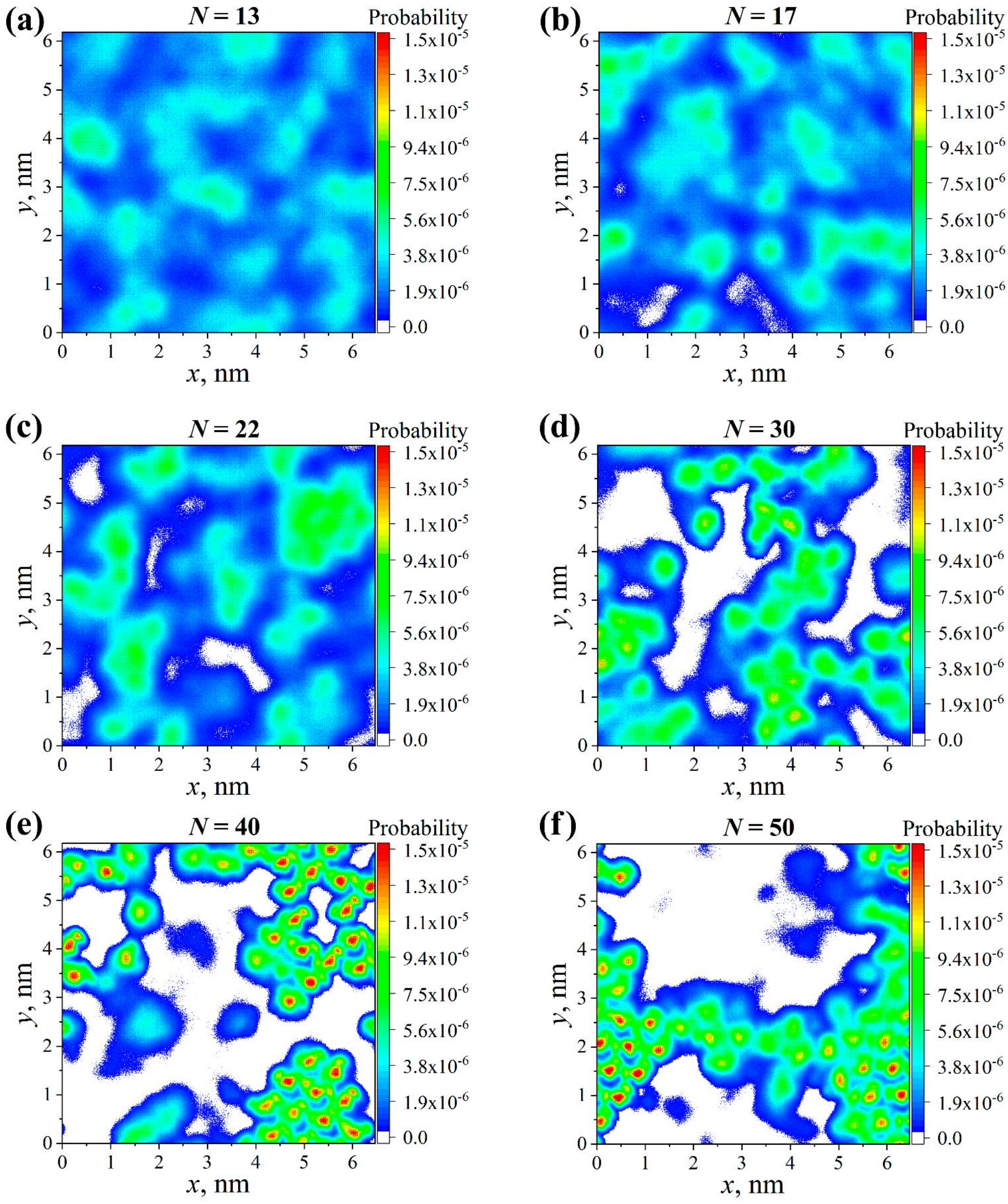


**Figure S5.** Lateral density profiles of the grafted chains stretched from the filler surface at different chain length *N* for the systems with partial charges.

**6. Comparison of the systems with different sizes simulated in the GAFF and PLAFF force fields**

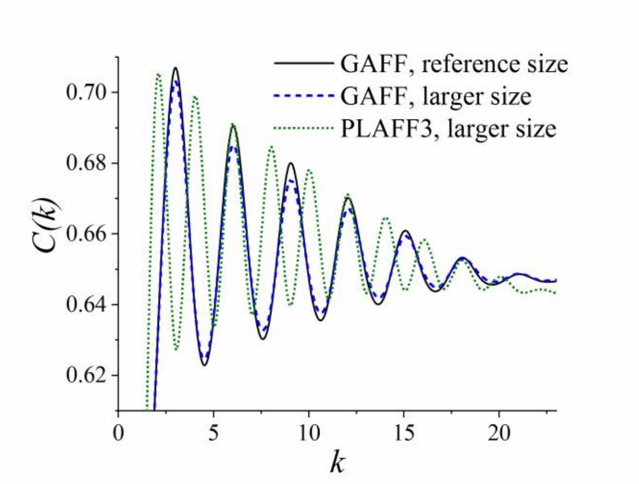


**Figure S6.** Autocorrelation function $C(k)$ for the grafts with the chain length $N = 50$ in the systems with reference sizes (used in the present paper) and larger sizes simulated in the GAFF and PLAFF force fields.