

Electronic Supplementary Information

Characterization of a Graphene Oxide/Poly(acrylic acid) Nanocomposite by means of Molecular Dynamics Simulations

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Shape parameters of polymer chains

Figure S1 compares the axes of the ellipsoid of inertia of the PAA chains molecules in bulk and in composite systems.

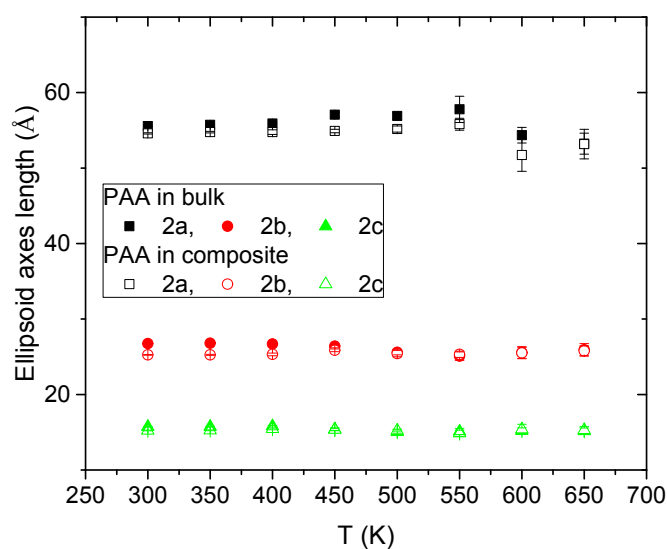


Figure S1. Axes of the ellipsoid of inertia of the polymer chains in the bulk (filled symbols) and in the nanocomposite (open symbols) at the examined temperatures

Orientalional parameter of the HO-OH bond of the PAA monomer with respect to the GO plane

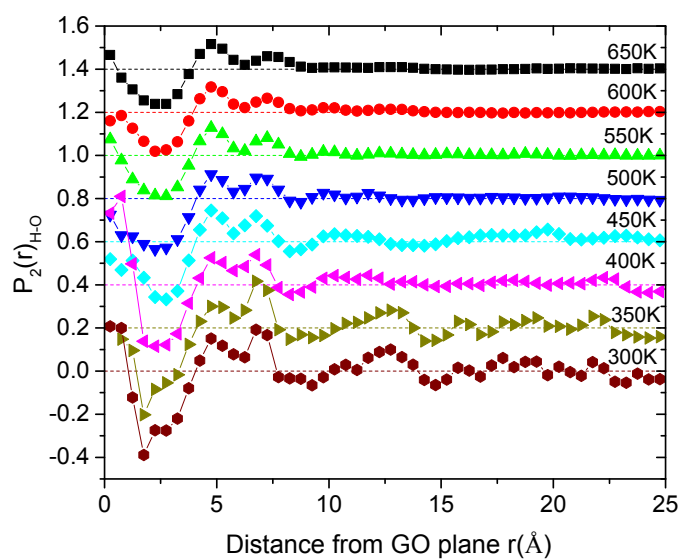


Figure S2: Polymer HO-OH orientational parameter as a function of the distance from a GO plane for all the examined temperatures. Each curve is shifted on the y-axis by 0.2 with respect to its previous temperature. Dashed lines denote the corresponding zero levels.

OH-OH pair correlation functions in the PAA pristine system

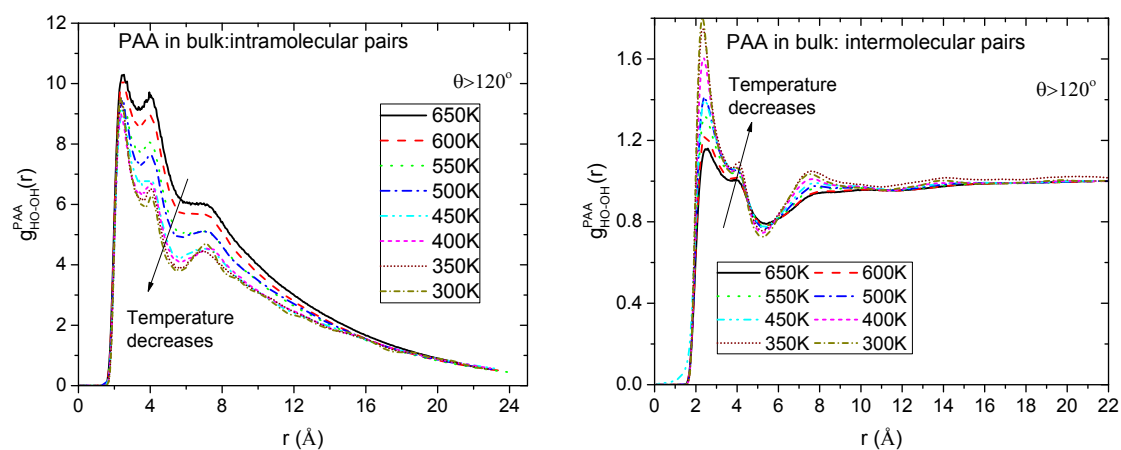


Figure S3. Pair correlation functions between hydroxyl hydrogen and hydroxyl oxygens for the intramolecular (left) and the intermolecular (right) pairs in the pristine PAA sample.

Hydrogen bond correlation functions for the PAA HO-OH pairs

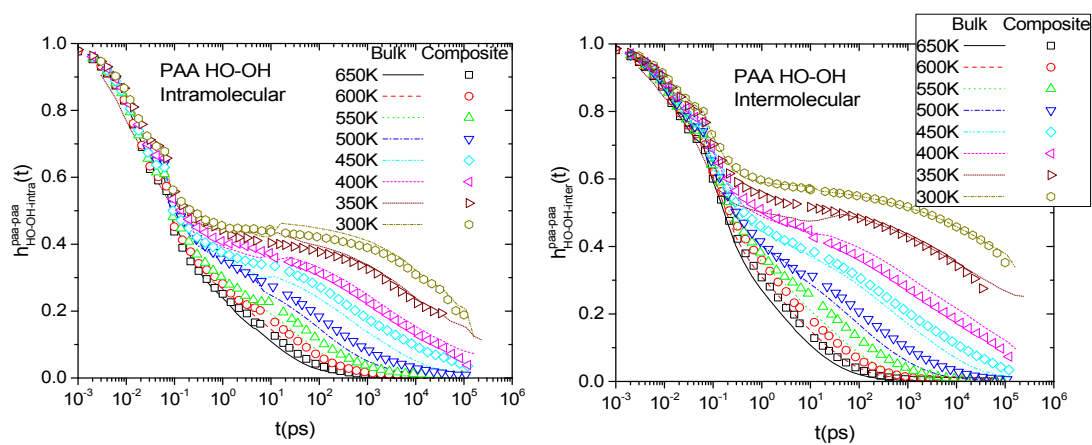


Figure S4. Hydrogen bond correlation functions describing intramolecular (left) and intermolecular (right) hydroxyl hydrogen and hydroxyl oxygens pairs of PAA. Symbols denote the behavior in the composite system and lines with the same color that in the pristine PAA model at the corresponding temperature.

Mastercurves and shift factors for the overall chain correlation functions

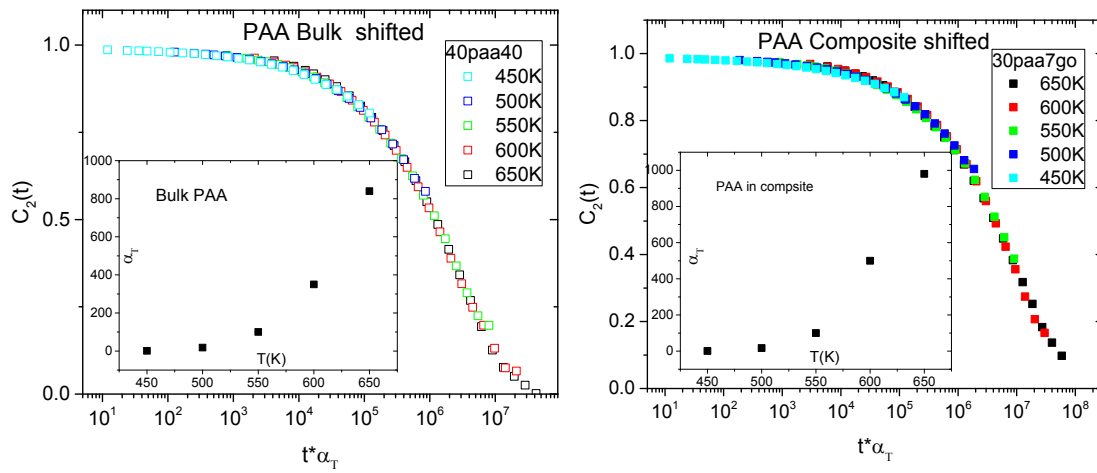


Figure S5: Resulted mastercurves (main panels) and shift factors (insets) for the overall rotational correlation function of PAA in the bulk (left) and in the composite (right)

Comparison between the spectra describing reorientational dynamics of bonds belonging to the 1st layer close to a GO plane and the corresponding overall average.

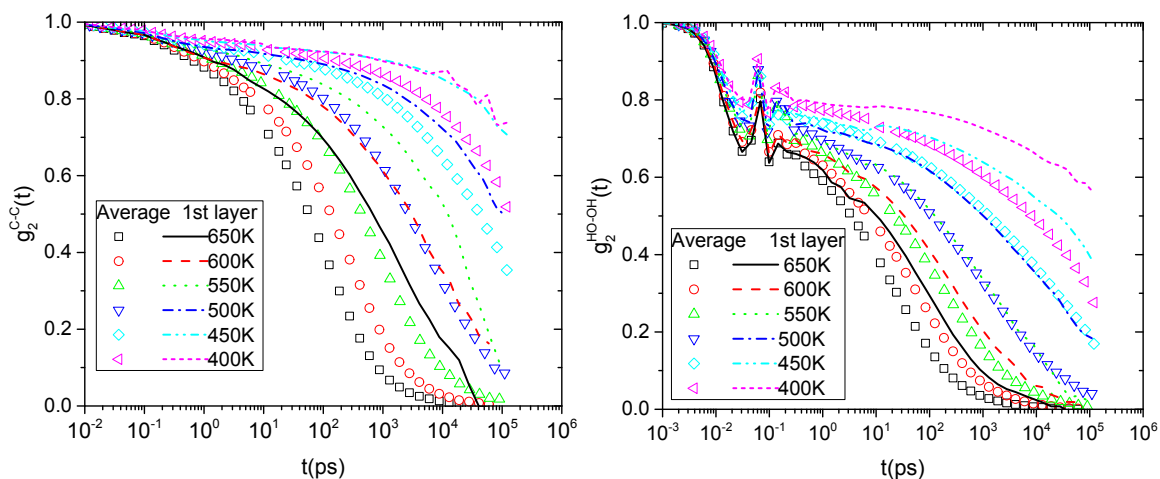


Figure S6: C-C (left) and HO-OH (right) bond reorientational spectra in the composite system. Symbols denote the correlation functions describing the overall average and lines those of the bonds belonging to the 1st layer adjacent to GO plane. Correlation functions with a very low degree of decorrelation in the examined temperature windows are omitted for clarity.

Comparison of torsional autocorrelation spectra at different distance ranges from a GO plane to those describing the average behavior of all the dihedrals

Figure S7 shows the torsional autocorrelation functions (ACFs) of the PAA backbone defined by the expression

$$P(\varphi(t)) = \frac{\langle \cos \varphi(t) \cos \varphi(0) \rangle - \langle \cos \varphi(0) \rangle^2}{\langle \cos \varphi(0) \cos \varphi(0) \rangle - \langle \cos \varphi(0) \rangle^2}$$

The distance of a dihedral angle from a GO plane is determined from the middle point of the first and the fourth atom participating in the dihedral.

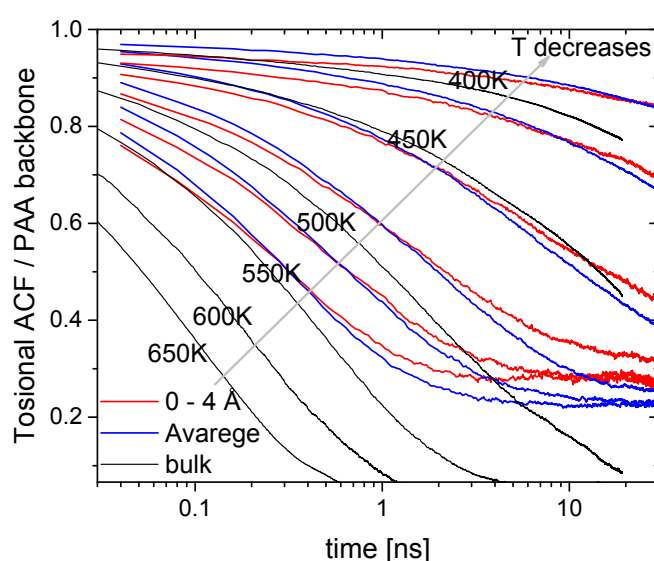


Figure S7: Torsional autocorrelation functions involving backbone carbon dihedrals for the nanocomposite, taking into account all (blue lines), and those torsional angles belonging to the 1st (red lines) layer adjacent to a GO plane. Also we compare with the respective autocorrelation functions for the bulk (black lines). Correlation functions for the sub-T_g region with a very low degree of decorrelation are not shown.