Edge-Functionalized Graphene as a Nanofiller:

Molecular Dynamics Simulation Study

SUPPORTING INFORMATION

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In the present Supporting Information we show additional figures to the article entitled Edge-Functionalized Graphene as a Nanofiller: Molecular Dynamics Simulation Study. We refer to the graphs in the main text, therefore we provide only basic description of the figures.
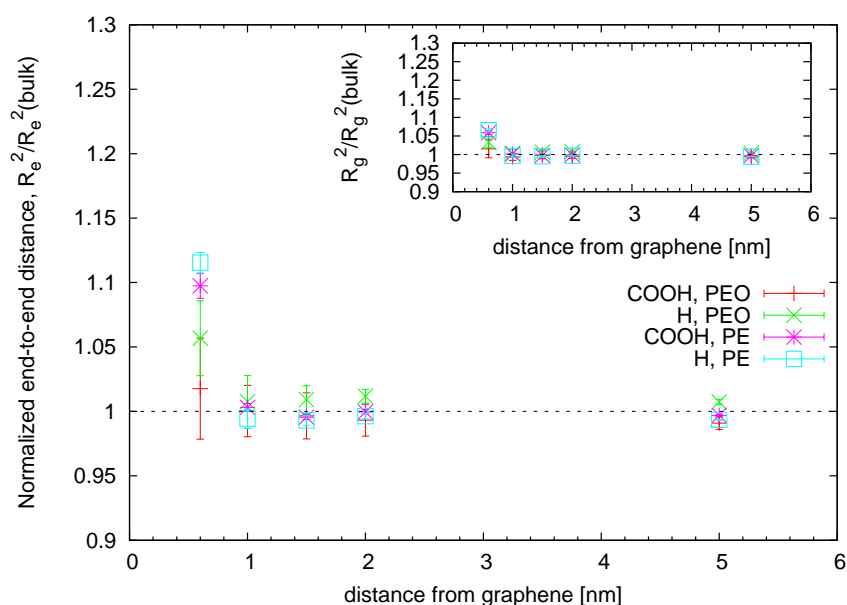
1   Static properties

Figure S1: Polymer end-to-end distance as a function of the distance from the edge of the graphene sheet normalized by the same quantity measured in the bulk. Inset: Square radius of gyration divided by the corresponding bulk values for the same set of data.
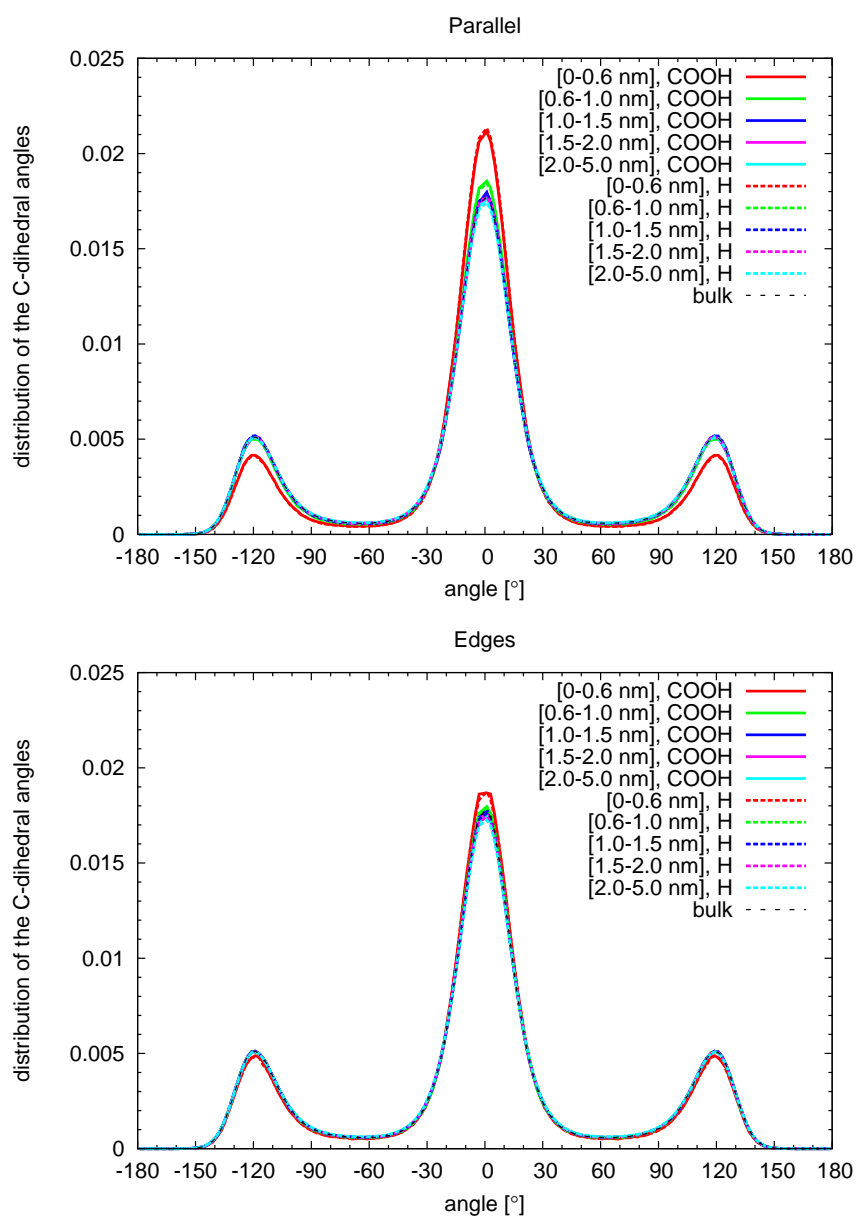
Figure S2: Distributions of the dihedral angles in the graphene/PE nanocomposites. Top: data for the region parallel to the graphene surface. Bottom: data obtained for the edge region. The binning of the layers is specified in the legend.
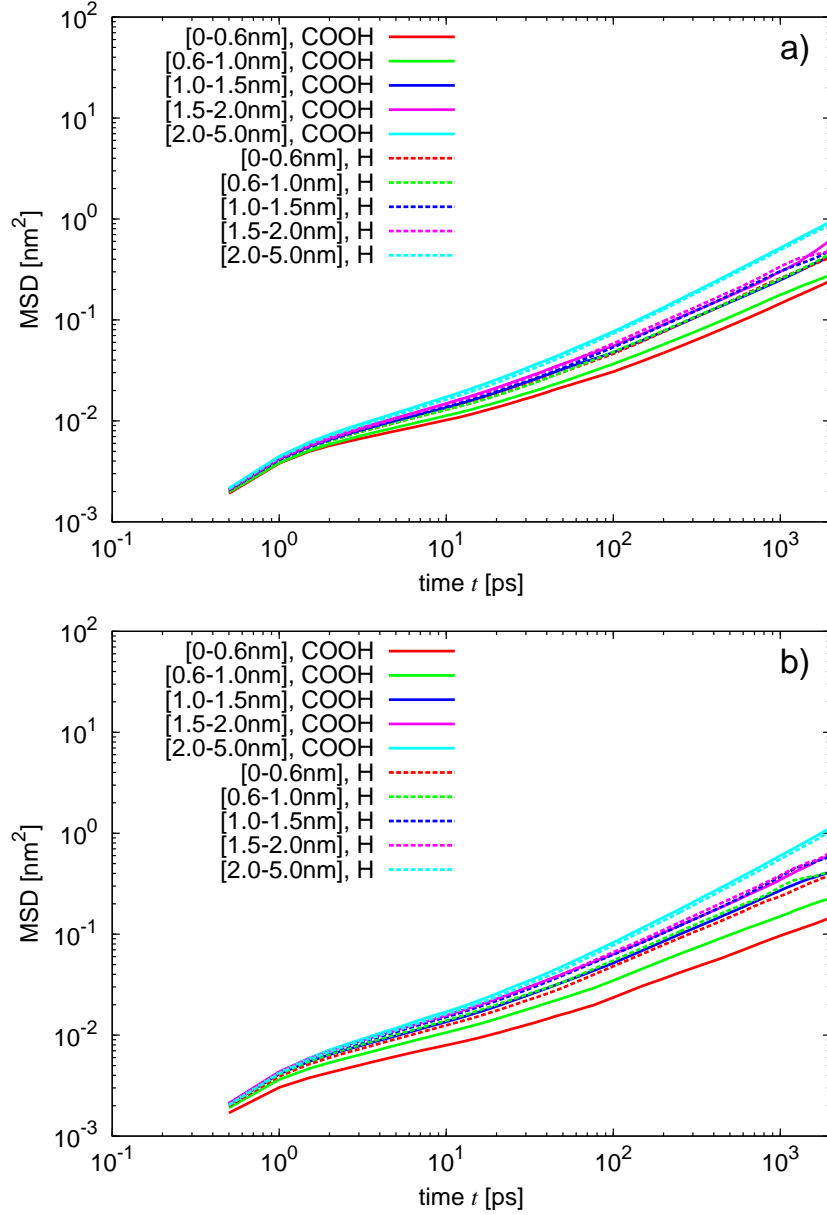
2 Dynamic properties

Figure S3: Mean square displacement of the centre of mass of the polymer situated a) in the parallel and b) in the edge region in the graphene/PEO nanocomposites. Only chains whose centres of masses belong to the same layer during the whole time t are taking into account.

Table S1: Stretching exponent β_s estimated from the correlation function of 1-3 vectors by fitting to KWW function.

	β_s(KWW) [ps]							
system	COOH PE		H PE		COOH PEO		H PEO	
layer	parallel	edges	parallel	edges	parallel	edges	parallel	edges
0-1.5 nm	0.35±0.01	0.4±0.04	0.35±0.03	0.44±0.02	0.37±0.02	0.327±0.006	0.44±0.06	0.40±0.03
1.5-3.0 nm	0.55±0.03	0.49±0.01	0.46±0.02	0.50±0.03	0.44±0.01	0.428±0.007	0.41±0.03	0.424±0.008
3.0-5.0 nm	0.48±0.07	0.56±0.05	0.48±0.02	0.6±0.1	0.43±0.01	0.46±0.01	0.43±0.03	0.451±0.004

*bulk values: β_s(KWW) $= 0.51 \pm 0.02$ ps for PE and β_s(KWW) $= 0.47 \pm 0.03$ ps for PEO

Table S2: Stretching exponent β_r estimated from the correlation function of end-to-end vectors.

	β_r(KWW) [ps]							
system	COOH PE		H PE		COOH PEO		H PEO	
layer	parallel	edges	parallel	edges	parallel	edges	parallel	edges
0-1.5 nm	0.8±0.1	0.9±0.2	0.64±0.08	0.9±0.1	0.7±0.2	0.54±0.03	0.7±0.1	0.8±0.2
1.5-3.0 nm	0.9±0.1	0.88±0.03	1.0±0.2	0.89±0.08	0.9±0.2	0.88±0.07	0.88±0.08	0.93±0.07
3.0-5.0 nm	0.9±0.1	0.99±0.04	0.9±0.1	1.0±0.03	0.99±0.06	0.95±0.02	1.0±0.2	0.94±0.02

*bulk values: β_r(KWW) $= 0.99 \pm 0.09$ ps for PE and β_r(KWW) $= 0.9 \pm 0.1$ ps for PEO
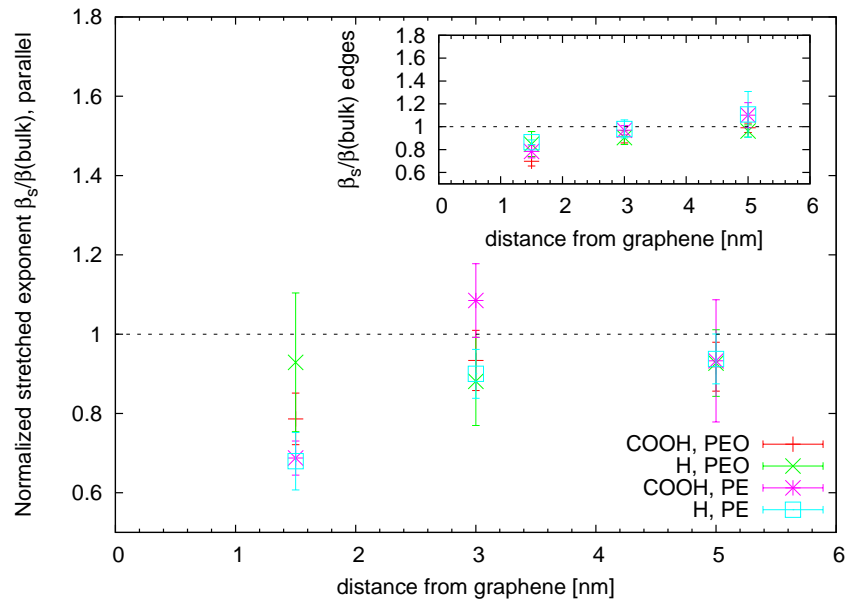

Figure S4: Stretching exponent β_s characteristic for the segmental relaxation in nanocomposites divided by the same observable measured in bulk polymer and plotted as a function of distance from the graphene sheet.
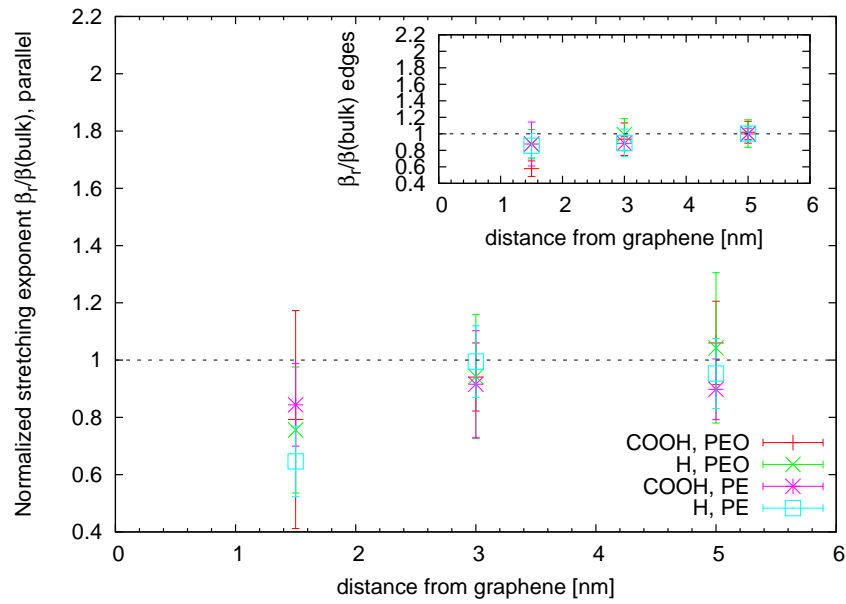
Figure S5: Stretching exponent β_r obtained from the end-to-end relaxation functions of the polymer matrices in nanocomposites normalized by the bulk value.