Supporting Information

Percolation analysis of the electrical conductive network in a polymer nanocomposites by nanorod functionalization

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Fig. S1 The distribution of A and B beads in each nanorod (NR) at different NR functionalization degree $\lambda_A$. The red spheres denote the A beads and the blue spheres denote the B beads.

Fig. S2(a) The coordination number and (b) snapshots for different nanorods (NR) functionalization degree $\lambda_A$, where the polymer chains are neglected for clarity and the red spheres denote the NRs. ($T^* = 1.0, \varphi = 4.0\%$)
Fig. S3(a) The local order structure $\langle P_z(r) \rangle$ of the nanorod (NR) aggregation and (b) the probability distribution $P_n$ of the nearest neighbor NRs surrounding one NR at a separation closer than $1.5\sigma$ (Nnum) for different NR functionalization degree $\lambda_A$. $(T^*=1.0$, $\varphi=4.0\%$, $\tilde{Y}=0.0)$
Fig. S4 RDF of nanorods for different interaction $\varepsilon_{PA}$ between polymer and A beads. ($\bar{T}=1.0$, $\varphi=4.0\%$)
Fig. S5(a) The local order structure \(< P_z(r) >\) of the nanorod (NR) aggregation and (b) the probability distribution \(P_N\) of the nearest neighbor NRs surrounding one NR at a separation closer than \(1.5\sigma\) (Nnum) for different interaction \(\varepsilon_{pd}\) between polymer and A beads. \((T^* = 1.0, \varphi = 0.0, \gamma = 0.0)\)

Fig. S6 Change of the main cluster size \(C_n\) as a function of the nanorod (NR) volume fraction \(\varphi\) for different interaction \(\varepsilon_{pd}\) between polymer and A beads. \((T^* = 1.0, \gamma = 0.0)\)
Fig. S7 RDF of nanorods (NR) for different NR functionalization degree $\lambda_{\Lambda}$. ($T^*=1.0$, $\varphi=4.0\%$, $\dot{\gamma}=0.1$)
Fig. S8(a) The local order structure $< P_2(r) >$ of the nanorod (NR) aggregation and (b) the probability distribution ($P_N$) of the nearest neighbor NRs surrounding one NR at a separation closer than $1.5\sigma$ (Nnum) for different NR functionalization degree ($\lambda_A$). ($T^*=1.0$, $\varphi=4.0\%$, $\dot{\gamma}=0.1$)

Fig. S9 The orientation degree $< P_2 >$ of the nanorods (NR) with respect to the NR functionalization degree ($\lambda_A$). ($T^*=1.0$, $\varphi=4.0\%$, $\dot{\gamma}=0.1$)
Fig. S10 Change of the main cluster size $C_n$ as a function of the nanorod (NR) volume fraction $\varphi$ for different NR functionalization degree ($\lambda_A$). ($T^* = 1.0$, $\dot{\gamma} = 0.1$)

Fig. 11 The percolation threshold $\varphi_c$ with respect to the shear rate $\dot{\gamma}$. ($T^* = 1.0$, $\lambda_A = 0.1$)
Fig. S12 Change of the main cluster size $C_n$ as a function of the nanorod volume fraction $\varphi$ for different shear rate $\dot{\gamma}$. ($T^*=1.0, \lambda_d=0.1$)

Fig. S13 the NR orientation $\langle P_z \rangle$ with respect to the shear rate $\dot{\gamma}$. ($T^*=1.0, \varphi=4.0\%, \lambda_d=0.1$)
Fig. S14 RDF of nanorods with respect to the shear rate $\dot{\gamma}$. ($T^*=1.0$, $\varphi=4.0\%$, $\lambda_u=0.1$)

Table S1 Nonbonded interaction parameters used in this work.

<table>
<thead>
<tr>
<th>Interaction types</th>
<th>$\varepsilon_{ij}^a$ ($\varepsilon$)</th>
<th>$r_{cutoff}^b$ ($\sigma$)</th>
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<tr>
<td>PB*-PB*</td>
<td>1.0</td>
<td>$2 \times 2^{1/6}$</td>
</tr>
<tr>
<td>PB*-NRu</td>
<td>1.0</td>
<td>2.5</td>
</tr>
<tr>
<td>PB*-NRf</td>
<td>1.0-5.0</td>
<td>2.5</td>
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<tr>
<td>NRu-NRu</td>
<td>1.0</td>
<td>2.5</td>
</tr>
<tr>
<td>NRu-NRf</td>
<td>1.0</td>
<td>2.5</td>
</tr>
<tr>
<td>NRf-NRf</td>
<td>1.0</td>
<td>2.5</td>
</tr>
</tbody>
</table>

$a$ $\varepsilon_{ij}$ the energy parameters between interacting sites $i$ and $j$.

$b$ $r_{cutoff}$ is the cut-off distance.

$c$ PB is the bead on polymer chain.

$d$ NR is the unfunctionalized bead on nanorod.

$e$ NR is the functionalized bead on nanorod.