Supporting Information

Molecular dynamics simulation of the conductivity mechanism of nanorod filled polymer nanocomposites

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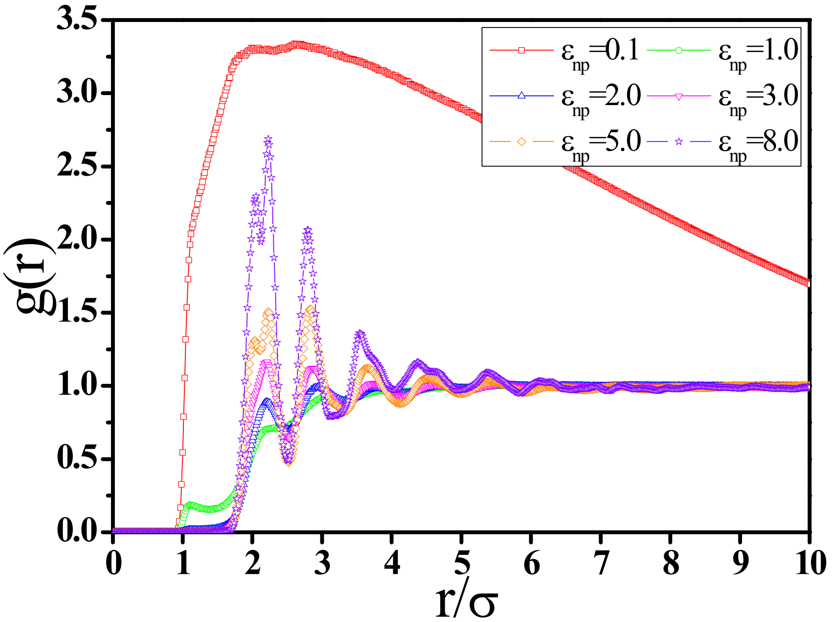
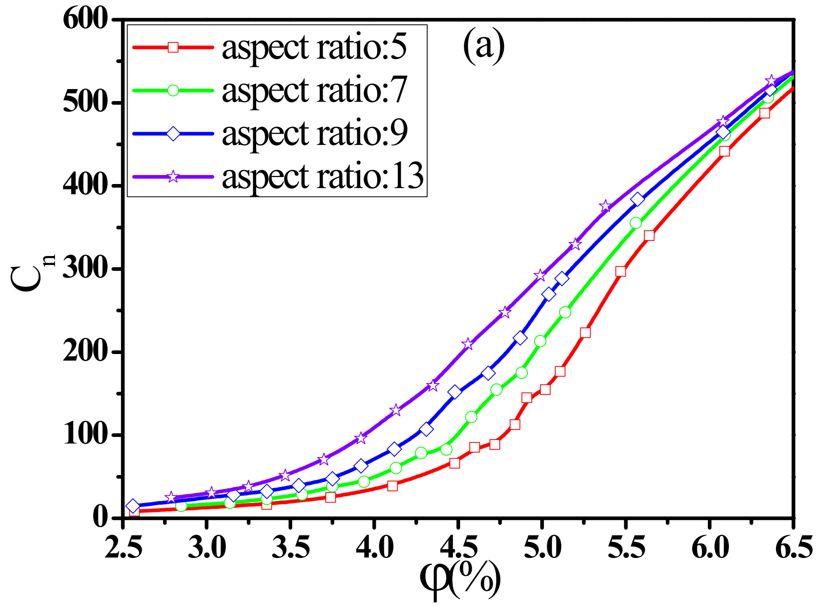


Fig. S1 RDF of nanorods for different polymer-nanorod interactions ε_{np}. (T=1.0, $\varphi = 4.49\%$)



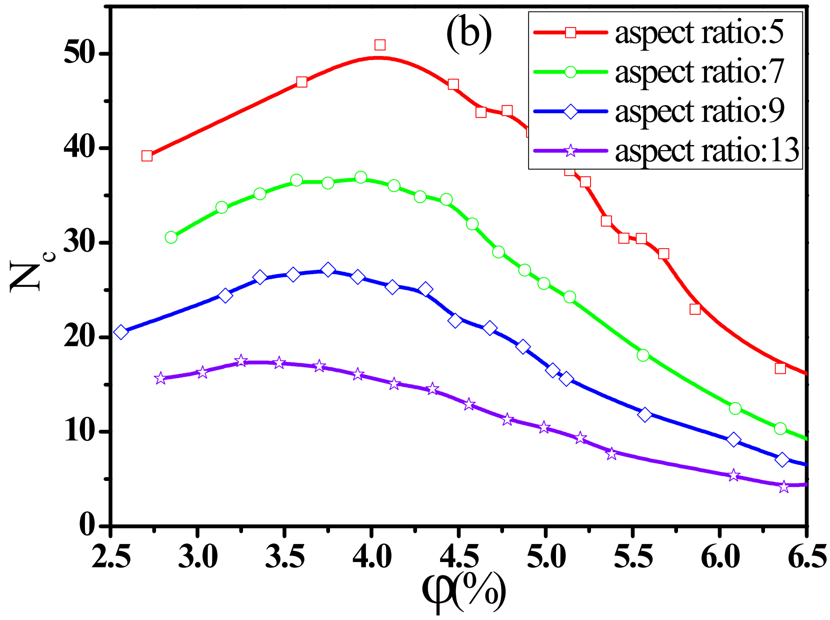
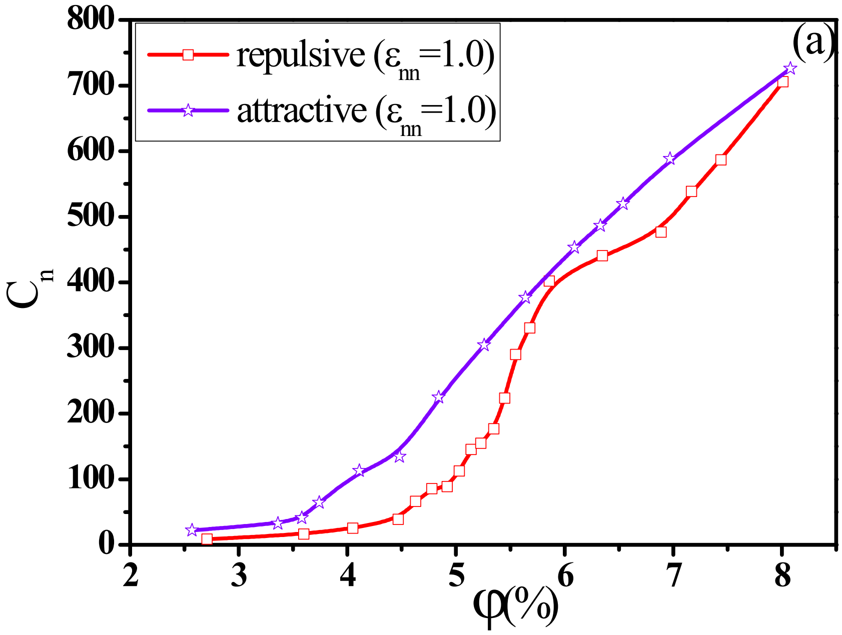


Fig. S2(a) The maximum cluster size C_n, (b) The total number of clusters N_c as a function of the volume fraction φ of nanorods for different aspect ratios. (T=1.0, $\varepsilon_{np}=1.0$)



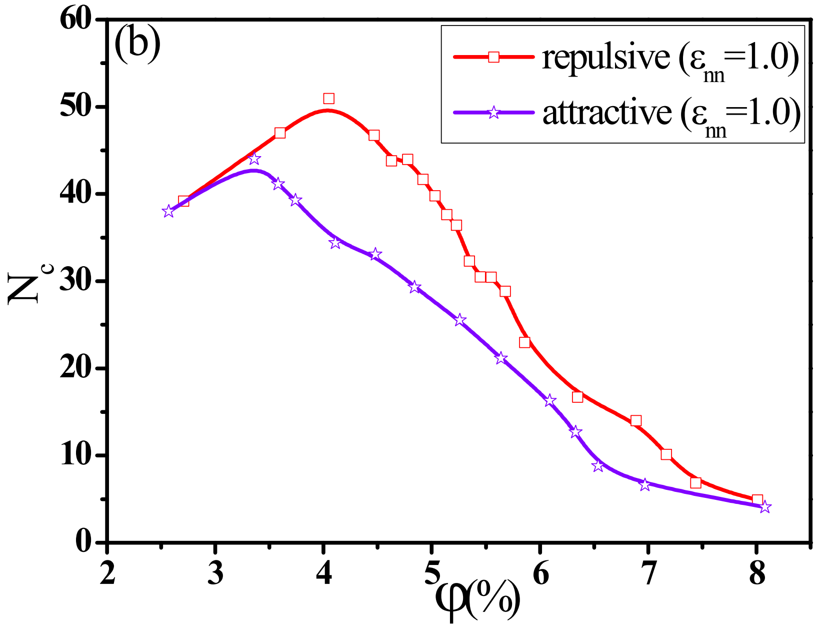


Fig. S3(a) The maximum cluster size C_n, (b) The total number of clusters N_c as a function of the volume fraction φ of nanorods for repulsive and attractive filler-filler interaction ε_{nn}. (T=1.0, $\varepsilon_{np}=1.0$)

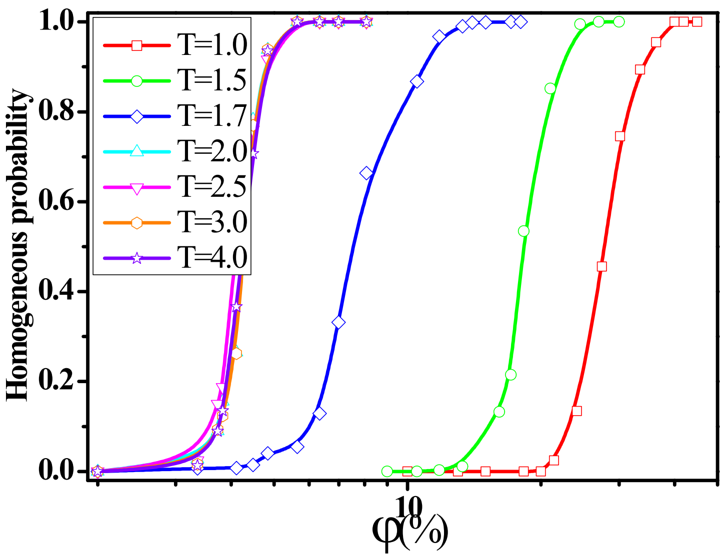


Fig. S4 Homogeneous probability as a function of the volume fraction φ of nanorods for different temperatures T. ($\varepsilon_{np}=0.1$)

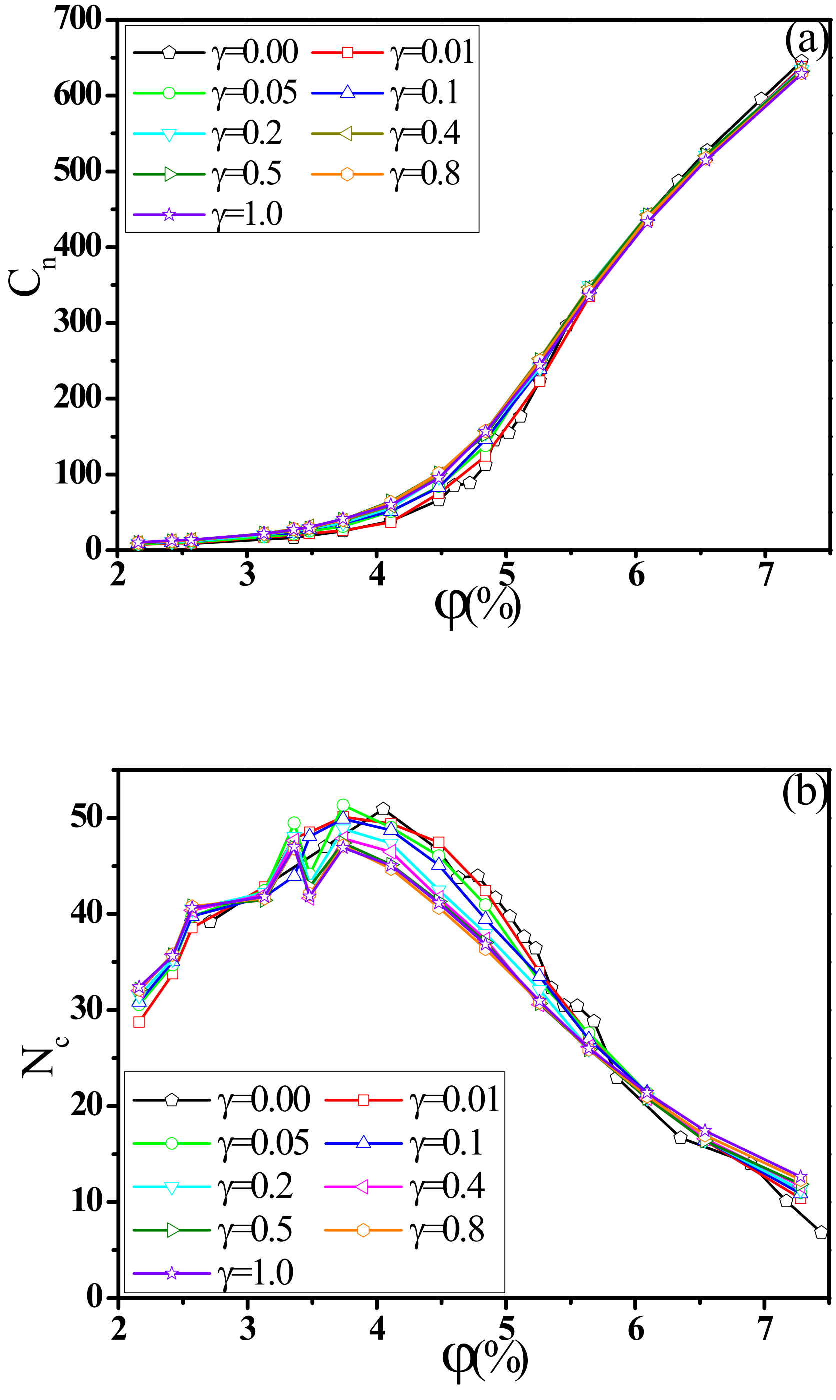
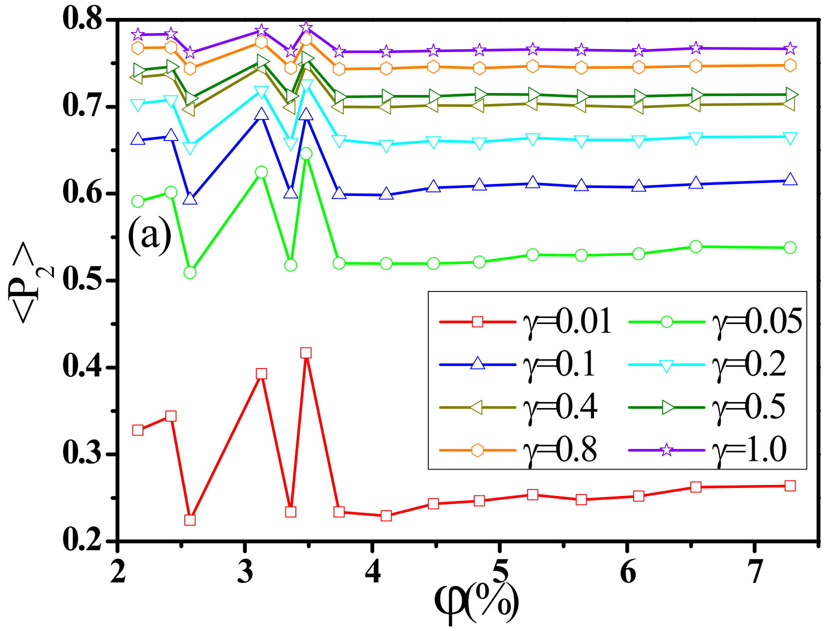


Fig. S5(a) The maximum cluster size C_n, (b) The total number of clusters N_c as a function of the volume fraction φ of nanorods for different shear rates γ. (T=1.0, $\varepsilon_{np}=1.0$)



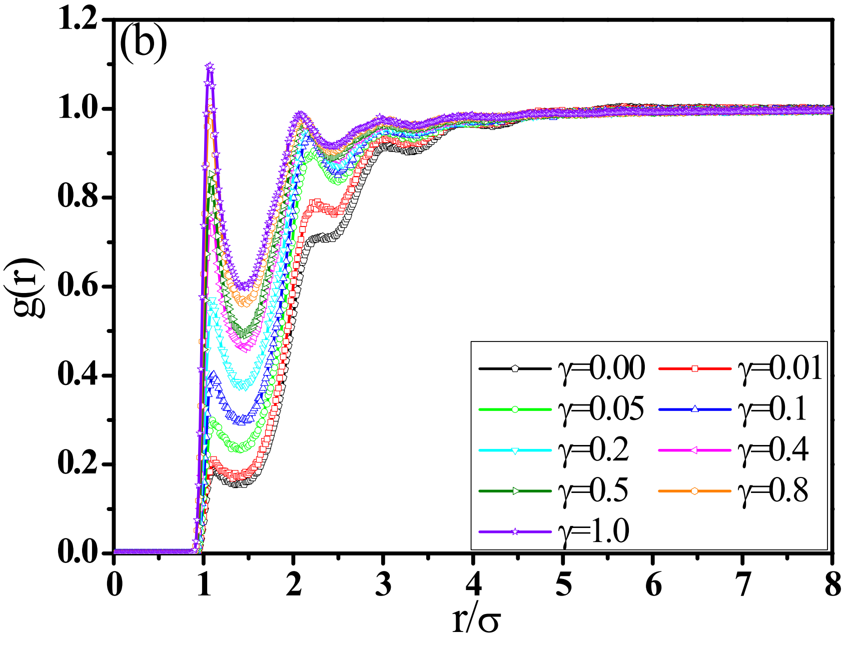


Fig. S6(a) The second-order Legendre polynomials $< P_2(\cos\theta(t)) >$ **as a function of the volume fraction** φ **of nanorod. (b) RDF of nanorods for different shear rates** γ **. (T=1.0,** $\varepsilon_{np} = 1.0$ **)**

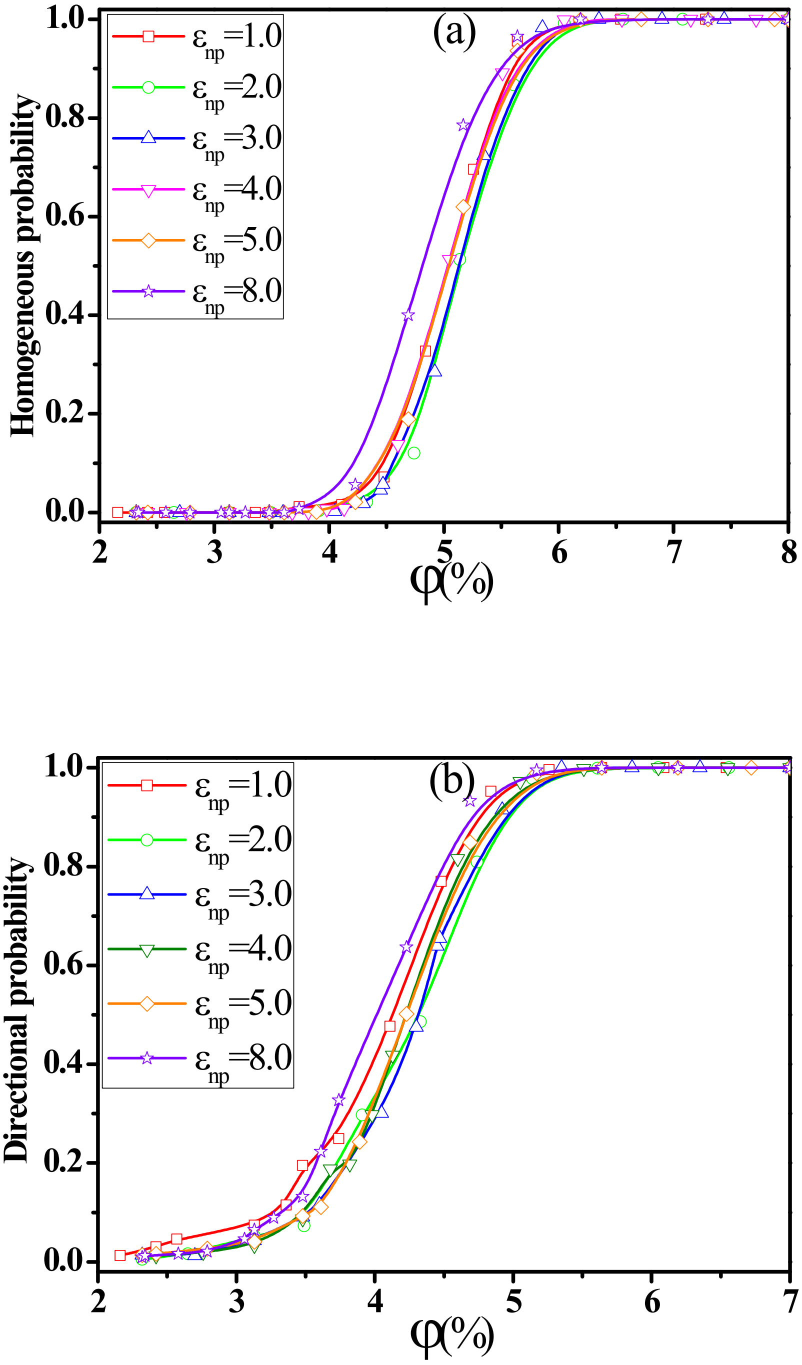


Fig. S7(a) Homogeneous probability and (b) directional probability of PNC as a function of the volume fraction φ of nanorods for different interfacial strengths ε_{np}. (T=1.0, $\gamma = 0.1$)

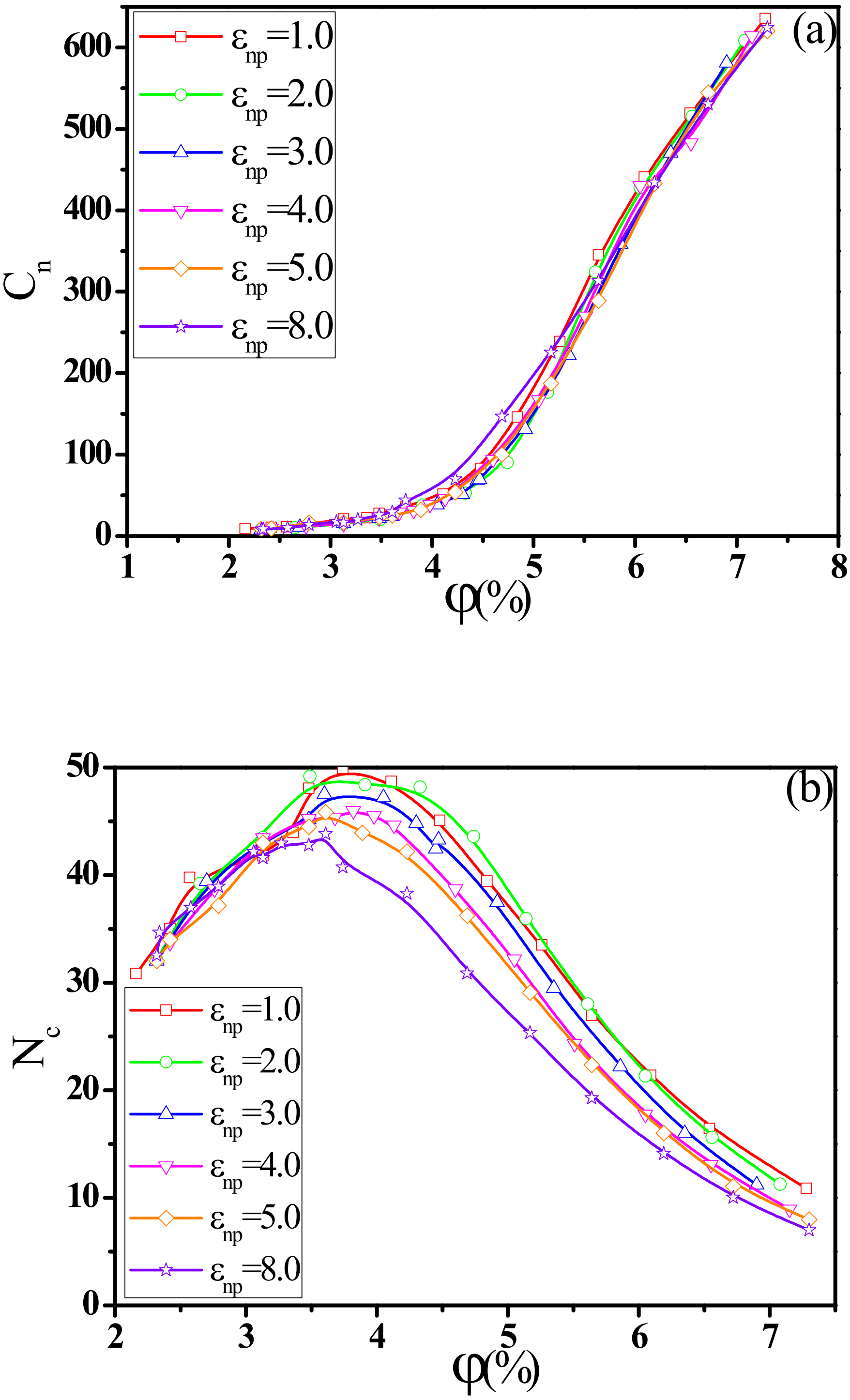


Fig. S8(a) The maximum cluster size C_n, (b) The total number of clusters N_c as a function of the volume fraction φ of nanorods for different interfacial strengths ε_{np}. (T=1.0, $\gamma = 0.1$)

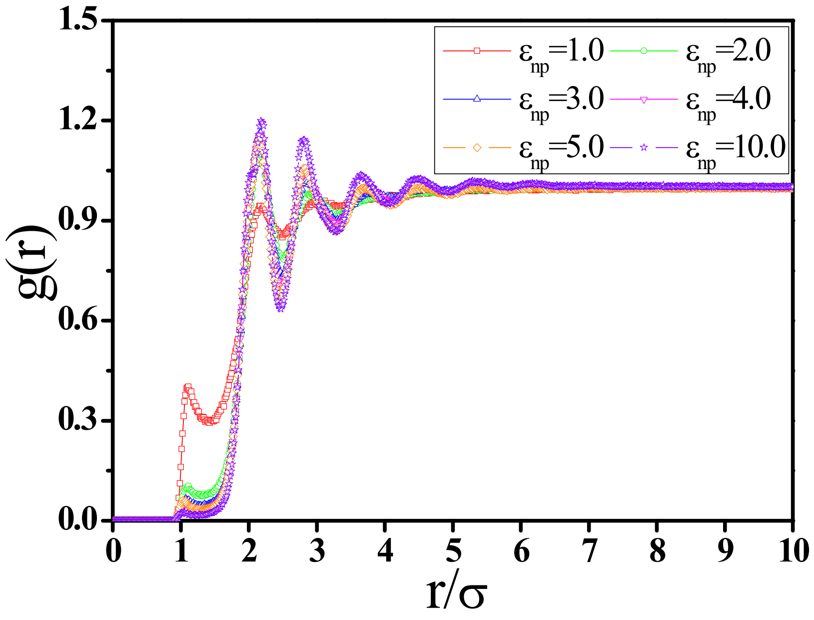
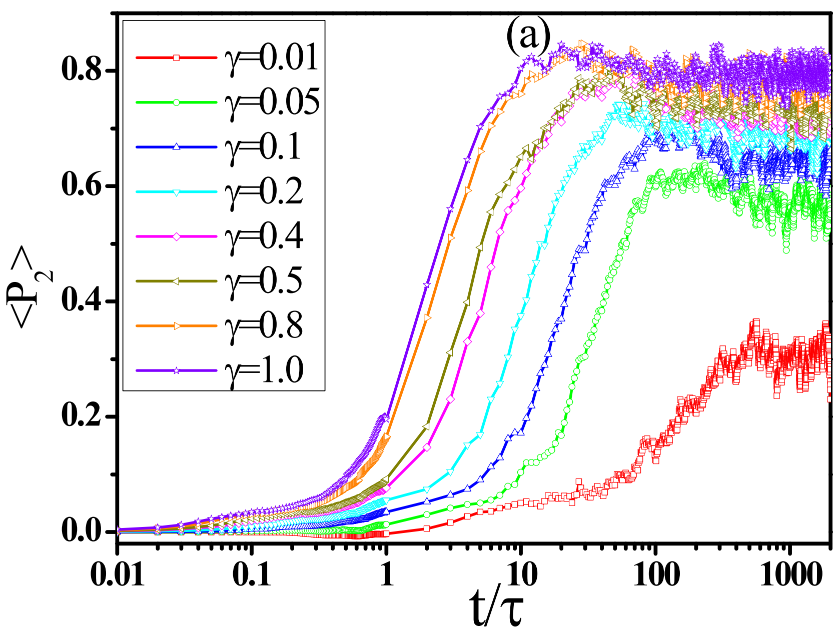


Fig. S9 RDF of nanorods for different interfacial interactions ε_{np}. (T=1.0, $\gamma = 0.1$)



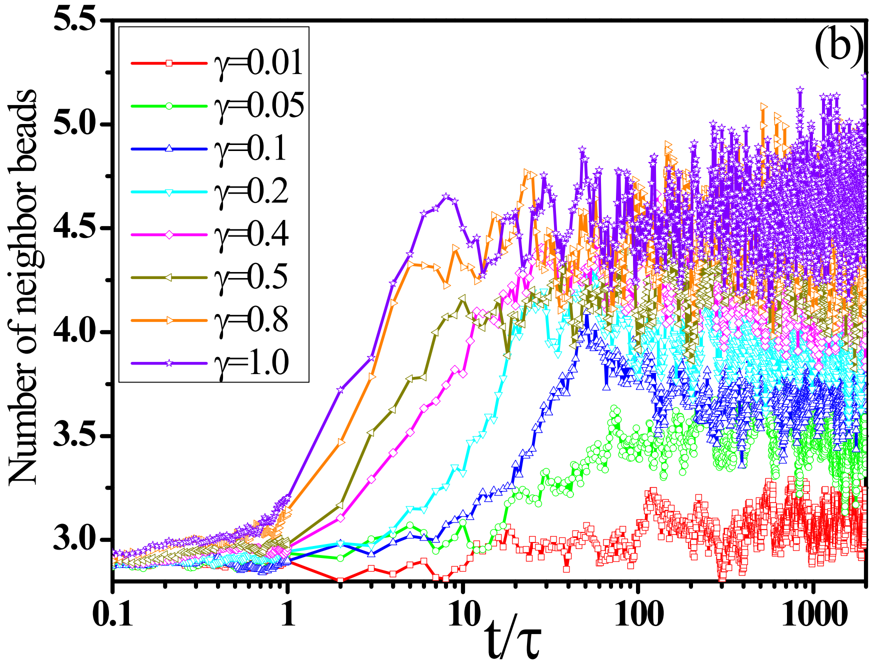


Fig. S10 The change of (a) the coordination number and (b) the second-order Legendre polynomials $< P_2 >$ as a function of the shear time t for different shear rates γ. (T=1.0, $\varepsilon_{np} = 1.0$, $\varphi = 4.49\%$)

Here we calculated the rotational diffusivity D_{rot} and the rotational Peclet number Pe_{rot} ($Pe_{rot} = \frac{\gamma}{D_{rot}}$). As shown in Fig. S11(a), for the case of $\varepsilon_{np} = 1.0$, the rotational diffusivity D_{rot} increases with the shear rate, while the effect of the volume fraction is little because of low interfacial interaction. And D_{rot} decreases significantly with the increase of the interfacial interaction shown in Fig. S11(b) because stronger interaction can inhibit the mobility of nanorods. From Fig. S12(a), the values of Pe_{rot} for different volume fractions are nearly the same, while they increase with the shear rate. Meanwhile, the percolation threshold of the directional conductivity also increases with the shear rate, which is similar to the trend of Pe_{rot}. From Fig. S12(b), the effect of the interfacial interaction on Pe_{rot} is small except the case $\varepsilon_{np} = 1.0$. This is consistent with the percolation threshold of conductivity for different interactions. The reason why Pe_{rot} is low at the case $\varepsilon_{np} = 1.0$ results from the fact that some nanorods aggregate directly (the peak at r =2σ in Fig. S9), which leads to the low rotational diffusivity D_{rot}. And for other interfacial interactions, nanorods do not aggregate directly.

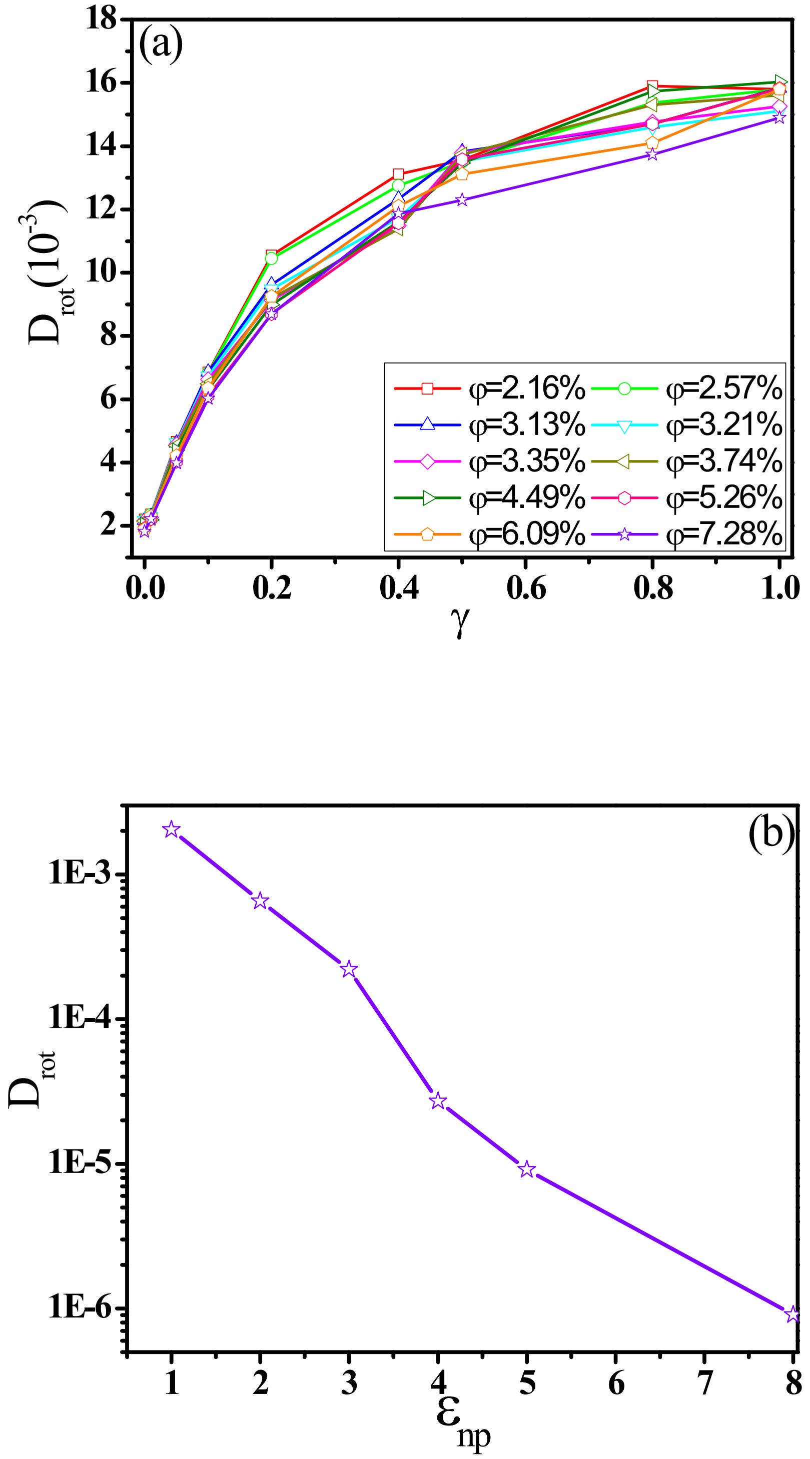


Fig. S11 The rotational diffusivity D_{rot} as a function of (a) shear rate γ for different volume fractions φ ($\varepsilon_{np} = 1.0$) and (b) the interfacial interaction ε_{np} ($\gamma = 0.0$, $\varphi = 4.49\%$). (T=1.0)

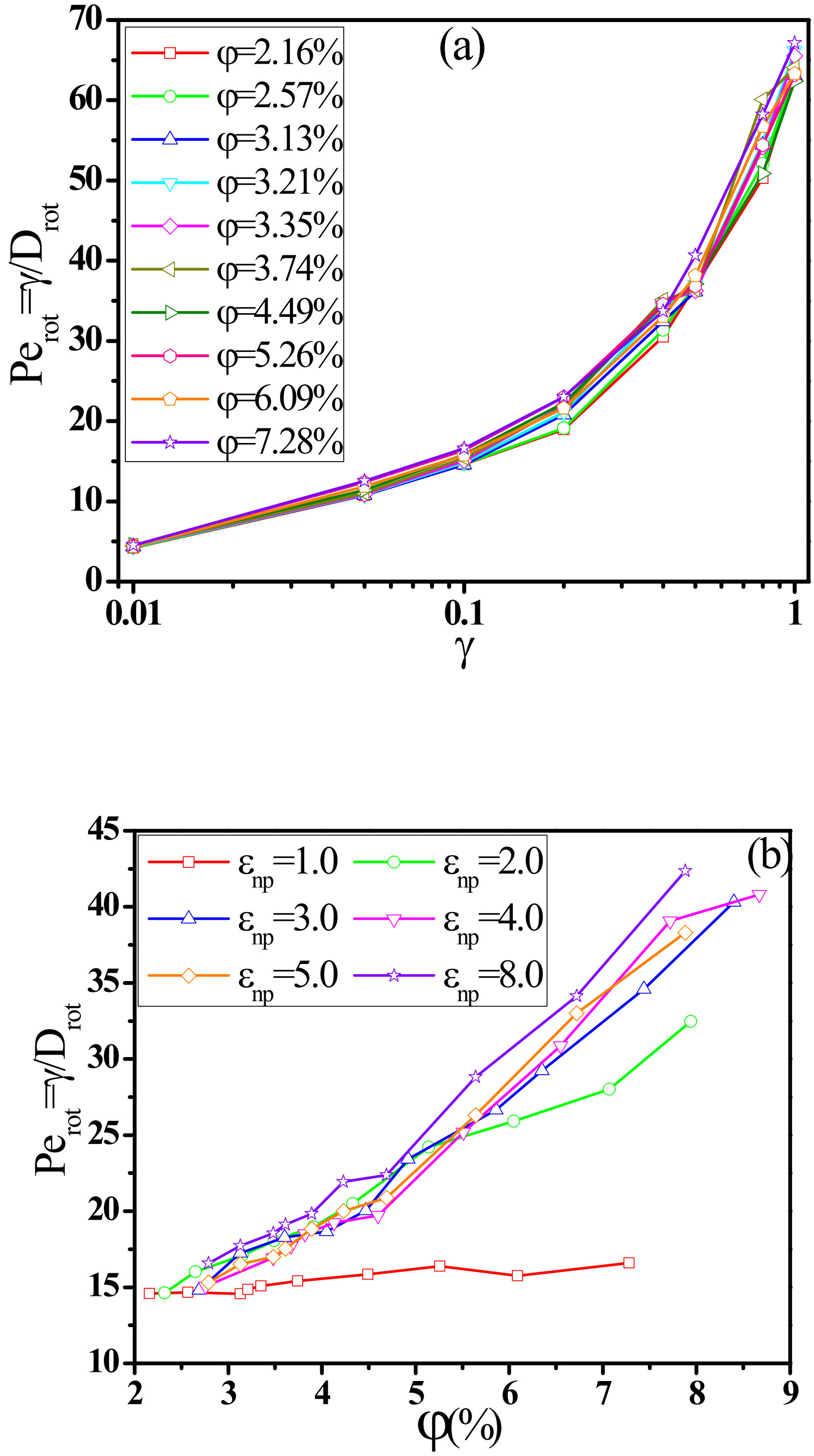
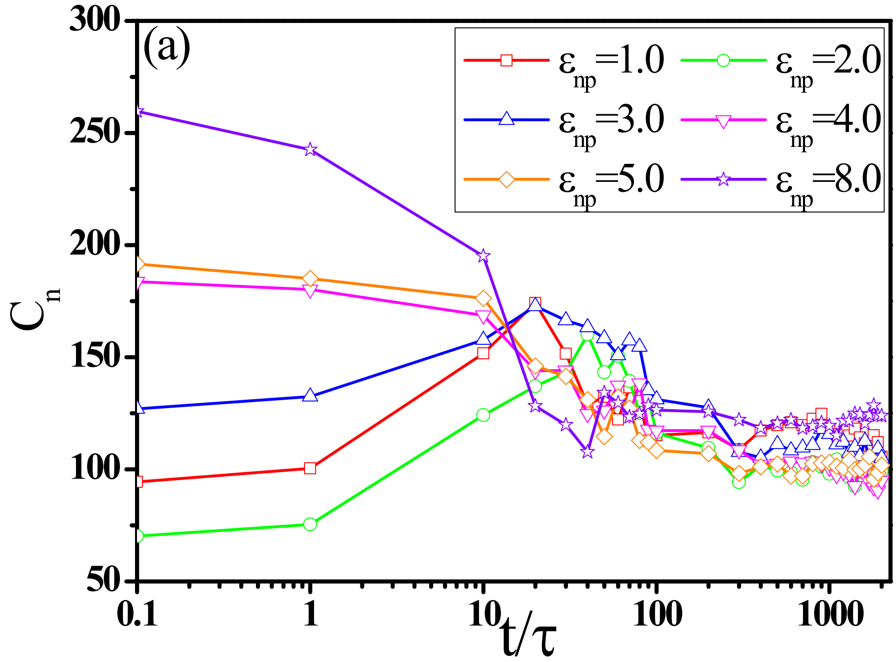


Fig. S12 The rotational Peclet number (a) as a function of shear rate γ for different volume fractions φ ($\varepsilon_{np} = 1.0$). (b) as a function of the volume fraction φ for different interfacial interaction ε_{np} with $\gamma = 0.1$. (T=1.0)



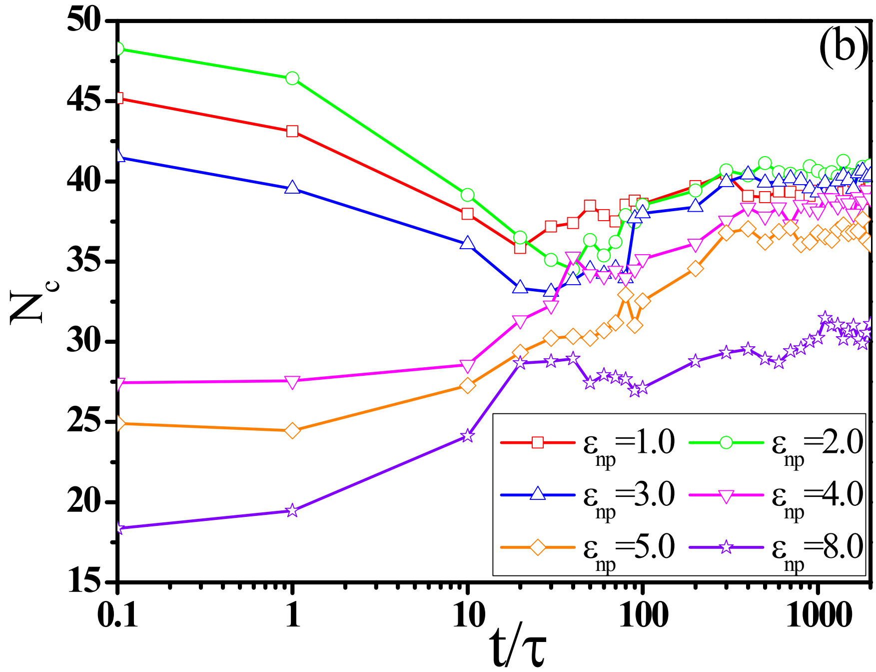


Fig. S13(a) The maximum cluster size C_n**, (b) The total number of clusters** N_c **as a function of the shear time** t **for different interfacial strengths** ε_{np}**. (T=1.0,** $\gamma = 0.1$**,** $\varphi = 4.49\%$**)**