Electronic Supplementary Information

Diffusion Mechanisms of Janus Nanoparticles in Cross-Linked Polymer Networks

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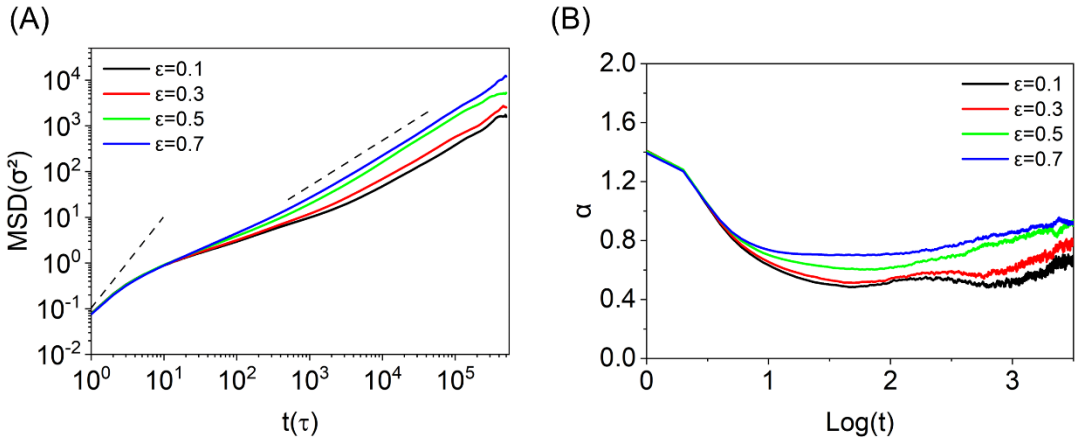

Fig. S1 Diffusion dynamics of JNPs with the adhesive component fixed at $\varepsilon=0.9k_BT$ and the non-adhesive side varied from 0.1 to $0.7k_BT$ in semi-flexible networks ($k_a = 25k_BT/\text{rad}^2$). (A) Mean square displacement (MSD); (B) anomalous diffusion exponent α corresponding to the MSD in (A).

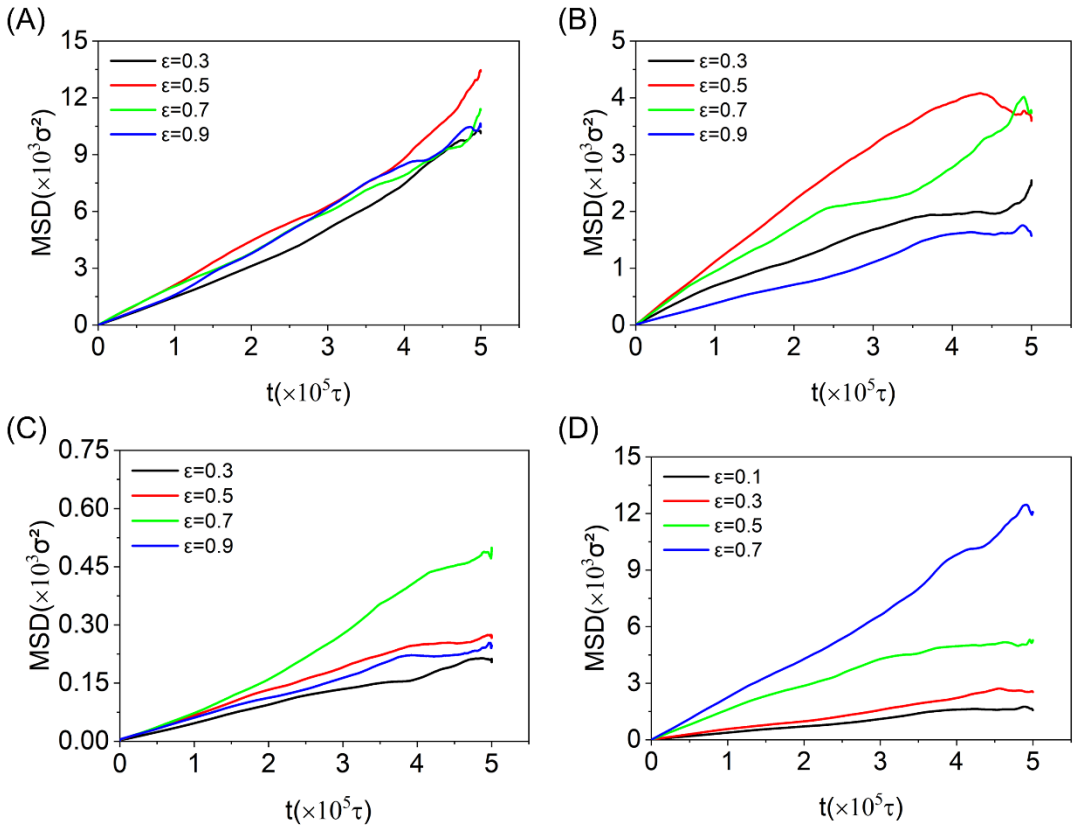

Fig. S2 Linear plots of the MSDs of the JNPs with varying interactions with cross-linked networks. (A-C) ε of non-adhesive component of JNP was fixed at $0.1k_BT$ in soft, semi-flexible and rigid networks (k_a = 2.5, 25 and $250k_BT$/rad^2), respectively; (D) ε of adhesive component of JNP was fixed at $0.9k_BT$ in semi-flexible network.

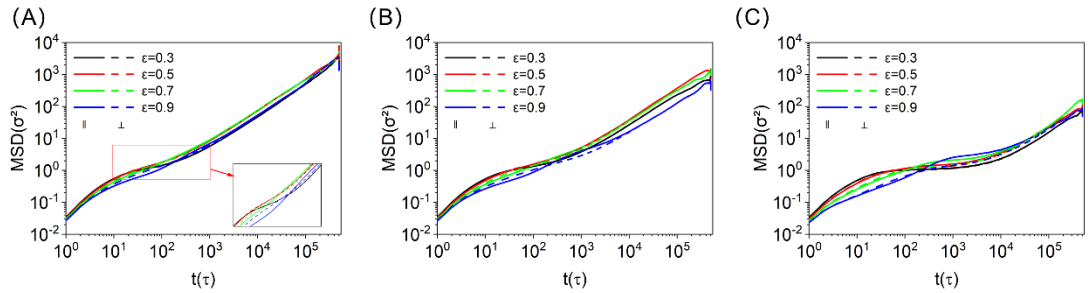

Fig. S3 MSD components of parallel and perpendicular to the major axes of JNPs with the non-adhesive component fixed at $\varepsilon = 0.1k_{\mathrm{B}}T$ in cross-linked networks of varying stiffness. (A) soft network (k_a = 2.5$k_{\mathrm{B}}T$/rad^2), (B) semi-flexible network (k_a = 25$k_{\mathrm{B}}T$/rad^2), (C) rigid network (k_a = 250$k_{\mathrm{B}}T$/rad^2). The adhesive-side ε is varied from 0.3 to $0.9k_{\mathrm{B}}T$.

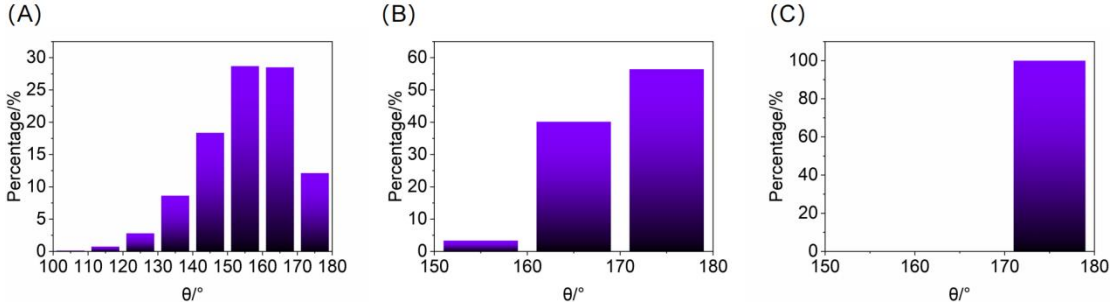

Fig. S4 Probability distribution of angles of every three consecutive CG beads in the network cell where the JNPs locate. (A) soft network (k_a = 2.5$k_{\mathrm{B}}T$/rad^2), (B) semi-flexible network (k_a = 25$k_{\mathrm{B}}T$/rad^2), (C) rigid network (k_a = 250$k_{\mathrm{B}}T$/rad^2).

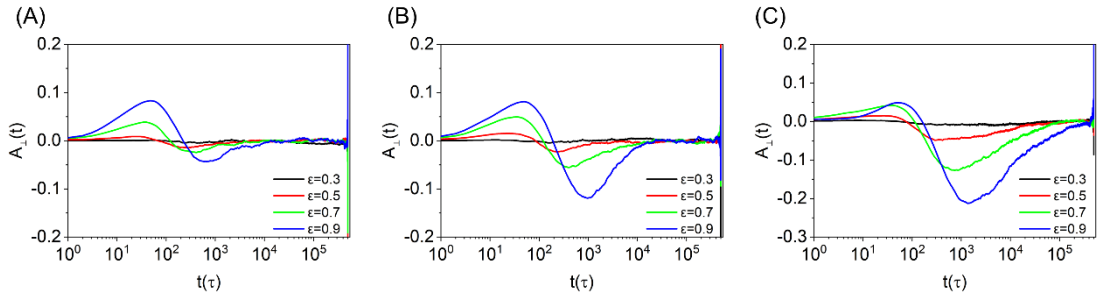

Fig. S5 Perpendicular anisotropic diffusion parameters $A_{\perp}(t)$ of JNPs with the non-adhesive component fixed at $\varepsilon = 0.1k_{\mathrm{B}}T$ in cross-linked networks of varying stiffness. (A) soft network (k_a = 2.5$k_{\mathrm{B}}T$/rad^2), (B) semi-flexible network (k_a = 25$k_{\mathrm{B}}T$/rad^2), (C) rigid network (k_a = 250$k_{\mathrm{B}}T$/rad^2). The adhesive-side ε is varied from 0.3 to $0.9k_{\mathrm{B}}T$.

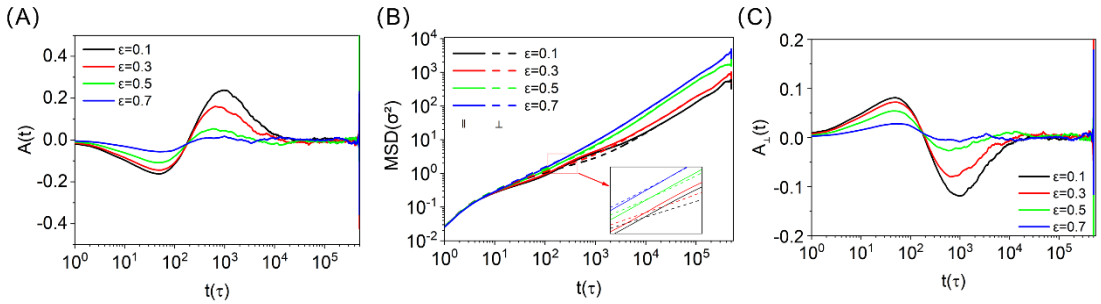

Fig. S6 Anisotropic dynamics of JNPs with the adhesive component fixed at ε=0.9$k_{\mathrm{B}}T$ and the non-adhesive side varied from 0.1 to $0.7k_{\mathrm{B}}T$ in semi-flexible networks (k_a = 25$k_{\mathrm{B}}T$/rad^2). (A) Anisotropic parameter; (B) parallel and perpendicular MSDs; (C) perpendicular anisotropic parameter.

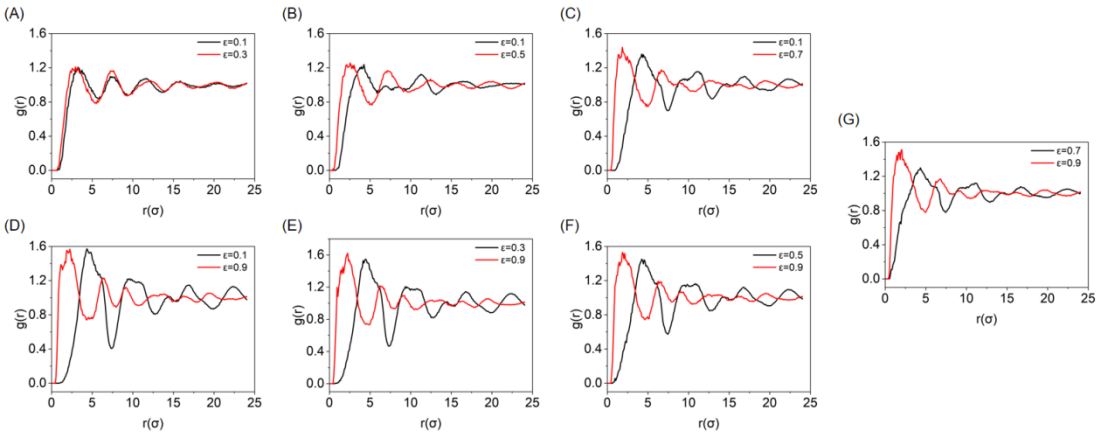

Fig. S7 Radial distribution function (RDF) plots of JNPs in cross-linked networks with $k_a = 25k_BT/\text{rad}^2$. (A) ε = 0.1 and $0.3k_BT$, (B) ε = 0.1 and $0.5k_BT$, (C) ε = 0.1 and $0.7k_BT$, (D) ε = 0.1 and $0.9k_BT$, (E) ε = 0.3 and $0.9k_BT$, (F) ε = 0.5 and $0.9k_BT$, (G) ε = 0.7 and $0.9k_BT$.

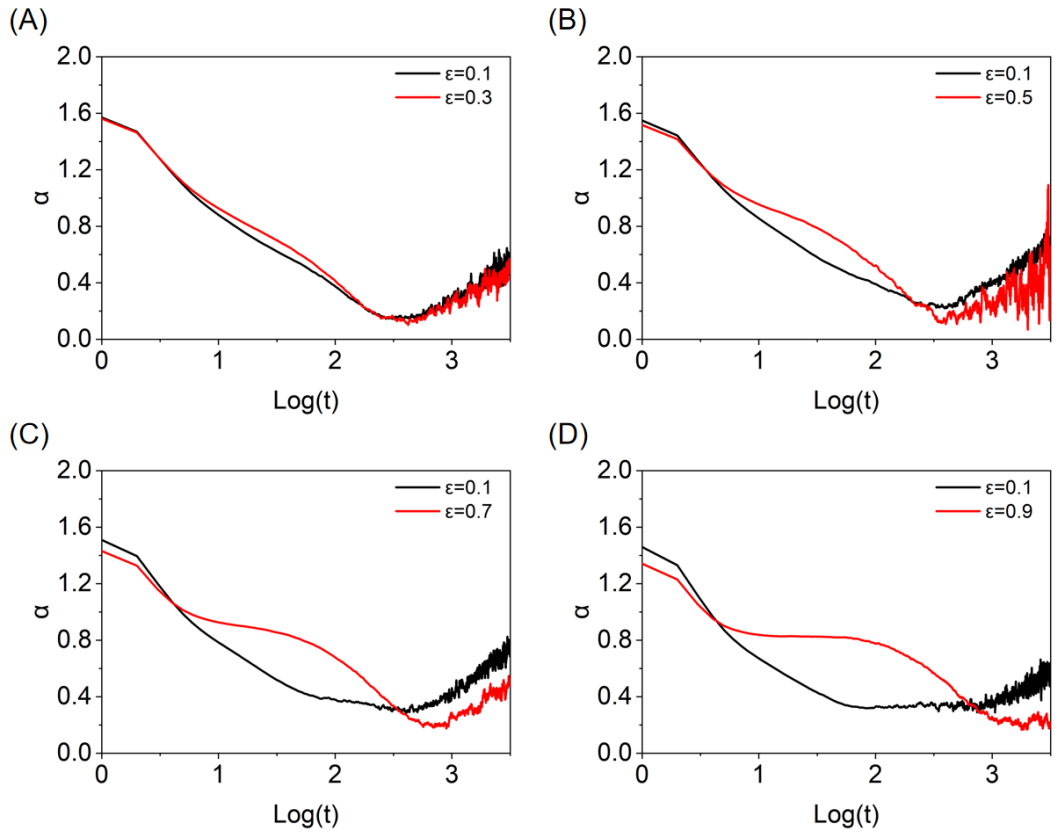

Fig. S8 Anomalous diffusion exponents α of the two vertices of JNPs in cross-linked networks with $k_a = 25k_BT/\text{rad}^2$. (A) ε = 0.1 and $0.3k_BT$, (B) ε = 0.1 and $0.5k_BT$, (C) ε = 0.1 and $0.7k_BT$, (D) ε = 0.1 and $0.9k_BT$.

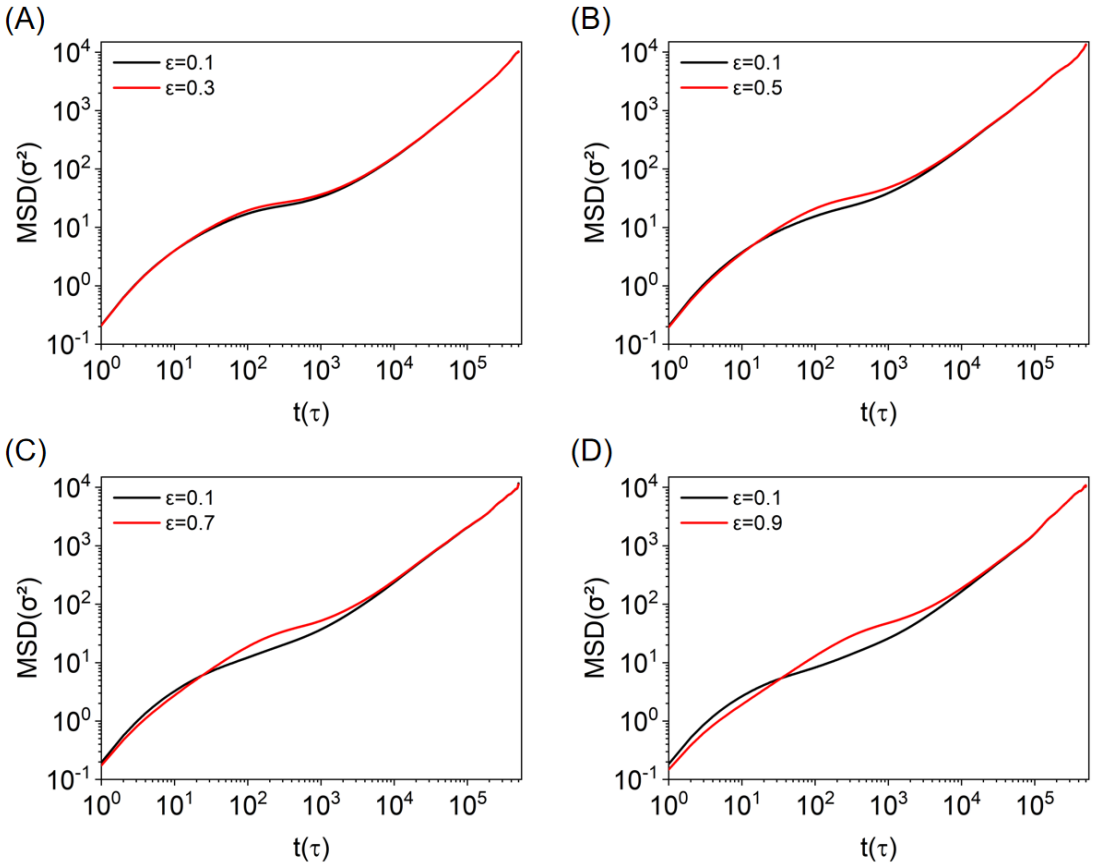

Fig. S9 MSDs of the two vertices of JNPs in cross-linked networks with k_a = 2.5 k_BT/rad^2. (A) ε = 0.1 and 0.3k_BT, (B) ε = 0.1 and 0.5k_BT, (C) ε = 0.1 and 0.7k_BT, (D) ε = 0.1 and 0.9k_BT.

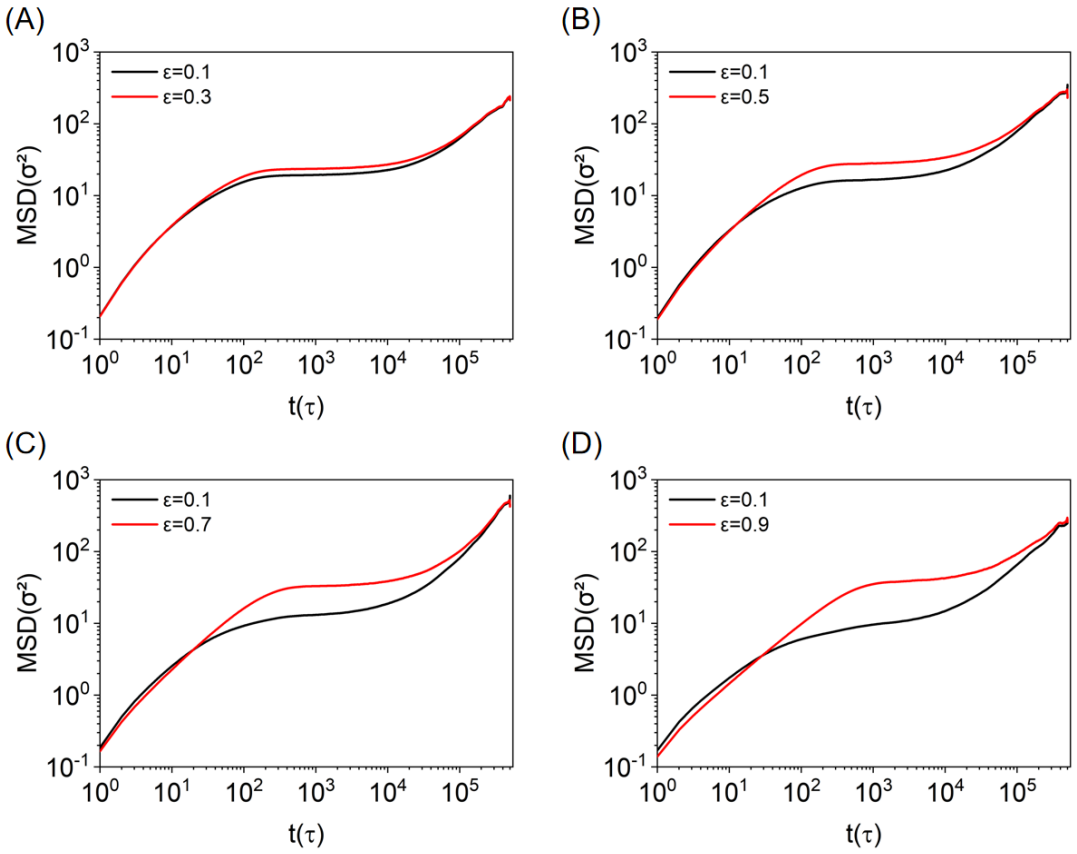

Fig. S10 MSDs of the two vertices of JNPs in cross-linked networks with k_a = 250 k_BT/rad^2. (A) ε = 0.1 and 0.3k_BT, (B) ε = 0.1 and 0.5k_BT, (C) ε = 0.1 and 0.7k_BT, (D) ε = 0.1 and 0.9k_BT.

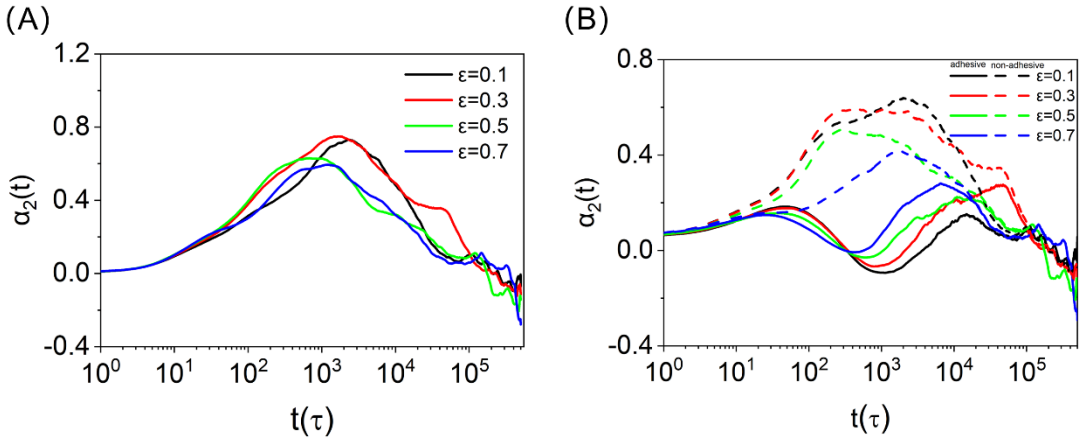

Fig. S11 Non-Gaussian parameters of JNPs with the adhesive component fixed at ε=0.9k_BT and the non-adhesive side varied from 0.1 to 0.7k_BT in semi-flexible networks (k_a = 25k_BT/rad^2). (A) Results of JNP centers; (B) results of two vertices of JNPs.

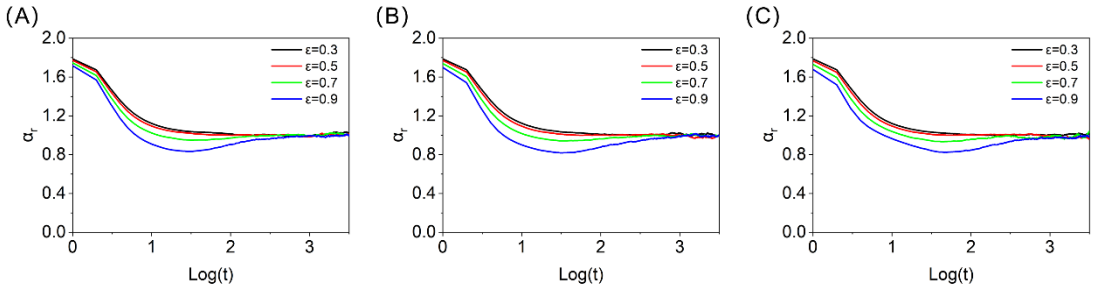

Fig. S12 Anomalous rotational diffusion exponents α_r of JNPs with the non-adhesive component fixed at $\varepsilon = 0.1k_BT$ in cross-linked networks of varying stiffness. (A) soft network (k_a = 2.5k_BT/rad^2), (B) semi-flexible network (k_a = 25k_BT/rad^2), (C) rigid network (k_a = 250k_BT/rad^2). The adhesive-side ε is varied from 0.3 to $0.9k_BT$.

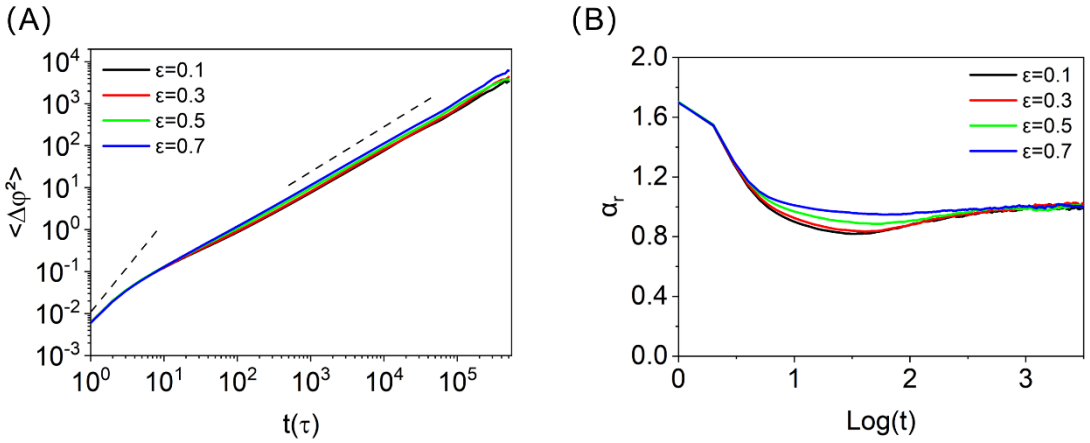

Fig. S13 Anomalous rotational diffusion exponents α_r of JNPs with the adhesive component fixed at ε=$0.9k_BT$ and the non-adhesive side varied from 0.1 to $0.7k_BT$ in semi-flexible networks (k_a = 25k_BT/rad^2). (A) Mean square angular displacement (MSAD); (B) anomalous rotational diffusion exponents α_r corresponding to the MSAD in (A).