

Supporting Information

Simulation study on the subdiffusion of polymer chains in crowded environments containing nanoparticles

Rong-Xing Lu¹, Jian-Hua Huang^{1*}, Meng-Bo Luo²

¹ *Department of Chemistry, Key Laboratory of Surface & Interface Science of Polymer Materials of Zhejiang Province, Zhejiang Sci-Tech University, Hangzhou 310018, China.*

² *Department of Physics, Zhejiang University, Hangzhou 310027, China.*

*Corresponding author. Email: jhhuang@zstu.edu.cn

1. The diffusion exponent α is roughly independent of the damping constant Γ , though the mean square displacement $\langle \Delta r^2(t) \rangle$ of polymer chain is larger for smaller Γ since the viscosity is proportional to Γ .

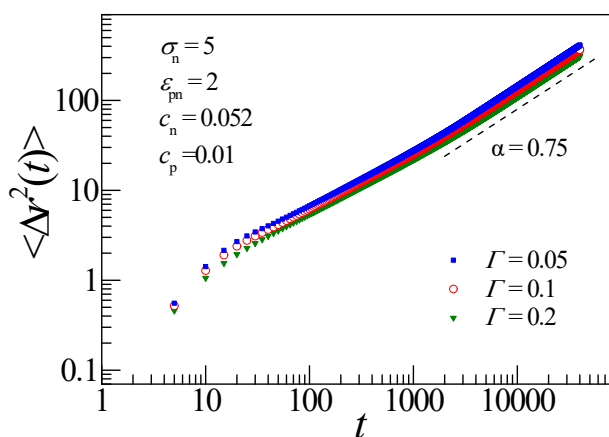


Fig. S1 Log-log plot of $\langle \Delta r^2(t) \rangle$ versus simulation time t for the system with $c_p = 0.01$ and $c_n = 0.052$ under three Γ values. The dashed straight line shows the diffusion exponent $\alpha = 0.75$.

2. Time averaged number of contacted NPs for every polymer chain in one simulation sample at different polymer concentrations.

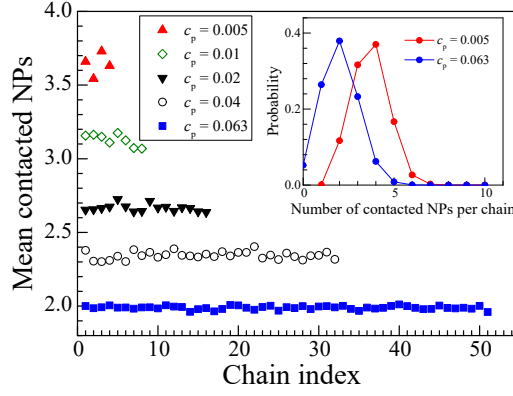


Fig. S2 Time averaged number of contacted NPs of each polymer chain in one simulation sample at five polymer concentrations with $c_n = 0.052$ and $\sigma_n = 5$. Inset: Probability distribution of the number of contacted NPs per chain.

3. The variation of diffusive exponent α with c_n is similar for different polymer concentrations. With an increase in c_n , α drops and gradually approaches a convergent value. The convergent value α_{conv} increases with c_p and finally tends to 1.

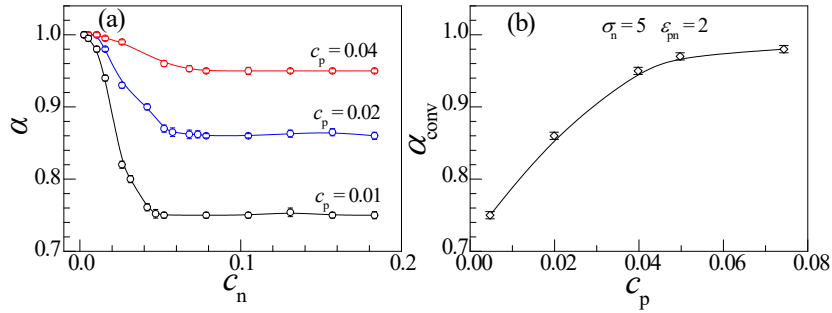


Fig. S3 (a) The diffusive exponent α as a function of NP concentration c_n for three polymer concentrations $c_p = 0.01, 0.02,$ and 0.04 . (b) Variation of the convergent value α_{conv} with c_p .