

[Talk 21] Effect of fluctuations on tracer diffusion in networks

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We present a recent study for the tracer diffusion in semi-flexible chain networks, using coarse-grained molecular dynamics simulations. Various equilibrium states of the network structure are nontrivially dependent on inter-(tracer-network) and intra-(network-network) interactions, where fluctuations arising in the structural transition largely affect the tracer diffusion and its partitioning inside and outside the network. The tracer diffusivities, throughout a wide range of the interaction strengths and the network bending rigidities, are found to abruptly decrease, signaling the network collapse transition. The network volume fluctuations associated with the network collapse transition become maximal around the transition point, notably enhanced by the network semi-flexibility. The tracer diffusivity is non-monotonic imparted by the tracer-network interactions in a collective manner. The tracer particle permeability finally shows a rich topology depending on the particles interactions, particularly for a semi-flexible network, which reveals a stark contrast between the diverse network structural states.