Abstract Submitted
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Hopping Diffusion of Nanoparticles Subjected to Topological Constraints[1] LI-HENG CAI, Department of Chemistry, University of North Carolina at Chapel Hill, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, Russian Academy of Sciences, MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina at Chapel Hill — We describe a novel hopping mechanism for diffusion of large non-sticky nanoparticles subjected to topological constraints in polymer solids (networks and gels) and entangled polymer liquids (melts and solutions). Probe particles with size larger than the mesh size of unentangled polymer networks (tube diameter of entangled polymer liquids) are trapped by the network (entanglement) cages at time scales longer than the relaxation time of the network (entanglement) strand. At long time scales, however, these particles can move further by hopping between neighboring confinement cages. This hopping is controlled by fluctuations of surrounding confinement cages, which could be large enough to allow particles to slip through. The terminal particle diffusion coefficient dominated by this hopping diffusion is appreciable for particles with size slightly larger than the network mesh size (tube diameter). Very large particles in polymer solids will be permanently trapped by local network cages, whereas they can still move in polymer liquids by waiting for entanglement cages to rearrange on the relaxation time scale of the liquids.

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