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Monte Carlo simulation studies of diffusion in crowded environments PRITHVIRAJ NANDIGRAMI, Kent State University, BRANDY GROVE, Case Western Reserve University, ANDREW KONYA, ROBIN SELINGER, Kent State University — Anomalous diffusion has been observed in protein solutions and other multi-component systems due to macromolecular crowding. Using Monte Carlo simulations, we investigate mechanisms that govern anomalous diffusive transport and pattern formation in a crowded mixture. We consider a multi-component lattice gas model with "tracer" molecules diffusing across a density gradient in a solution containing sticky "crowder" molecules that cluster to form dynamically evolving obstacles. The dependence of tracer flux on crowder density shows an intriguing re-entrant behavior as a function of temperature with three distinct temperature regimes. At high temperature, crowders segregate near the tracer sink but, for low enough overall crowder density, remain sufficiently disordered to allow continuous tracer flux. At intermediate temperature, crowders segregate and block tracer flux entirely, giving rise to complex pattern formation. At low temperature, crowders aggregate to form small, slowly diffusing obstacles. The resulting tracer flux shows scaling behavior near the percolation threshold, analogous to the scenario when the obstacles are fixed and randomly distributed. Our simulations predict distinct quantitative dependence of tracer flux on crowder density in these temperature limits.

Prithviraj Nandigrami
Kent State University

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