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Modeling of long DNA electrophoresis in inverse opals NABIL LAACHI, KEVIN DORFMAN, University of Minnesota — We investigate the electrophoretic motion of long DNA molecules in periodic geometries with a spherical confinement. The confining spheres, also called lakes, are spatially organized in a cubic, crystal-like lattice whereby DNA can only travel between spheres through narrow holes connecting them, also called straits. When the radius of the spheres exceeds the radius of gyration of the molecules, an entropic trapping-like mechanism is well suited to describe the dynamics of the chain. In the context of this study, however, we consider confining spheres with a radius on the order of a few Kuhn segments, so that chains can simultaneously span a fluctuating number of lakes. Adjacent spheres can then exchange segments through the straits, resulting in a net motion of the center of mass of the chain when an electric field is applied. In this study, we model the sequential exchange of segments -or translocation events- between neighboring lakes as a discrete stochastic chemical reaction. We employ kinetic Monte Carlo methods combined with free energy calculations to monitor the lake occupancies. Results on the chain mobility as a function of various parameters at play will be presented.

Nabil Laachi
University of Minnesota

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