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Force-Based Theory for the Center of Mass Dynamics of Dense Ring Polymer Liquids ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana Champaign — Recent simulations of concentrated ring polymer melts liquids have found they form collapsed globules on global scales but still significantly interpenetrate. In contrast to entangled chains, their internal modes relax relatively quickly compared to the center-of-mass (CM) motion time scale. Curiously, the ring diffusion constant scales roughly as the inverse square of the degree of polymerization (N), but with an onset well above that of the chain analog. The suggestion of a type of macromolecular glass transition at very large values of N has been made. We formulate a statistical mechanical theory to describe the CM dynamics of rings based on assuming the internal modes are relaxed, the effective time-dependent forces on the ring CM are related to the inter-ring packing structure, and the ring liquid equation-of-state is qualitatively the same as for chains. Solving the theory at the level of dynamic second order perturbation theory results in a near N^{-2} scaling of the long time diffusion constant, which is not predicted for non-interpenetrating strictly compact globules. A macromolecular glass-like localization transition is predicted as N becomes very large which signals a crossover to activated hopping transport controlled by an entropic barrier.

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