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Analysis of the morphology, stability, and folding pathways of ring polymers with supramolecular topological constraints using molecular simulation and nonlinear manifold learning JIANG WANG, ANDREW FERGUSON, Univ of Illinois - Urbana — Ring polymers offer a wide range of natural and engineered functions and applications, including as circular bacterial DNA, crown ethers for cation chelation, and "molecular machines" such as mechanical nanoswitches. The morphology and dynamics of ring polymers are governed by the chemistry and degree of polymerization of the ring, and intramolecular and supramolecular topological constraints such as knots or mechanically-interlocked rings. We perform molecular dynamics simulations of polyethylene ring polymers as a function of degree of polymerization and in different topological states, including a knotted state, catenane state (two interlocked rings), and borromean state (three interlocked rings). Applying nonlinear manifold learning to our all-atom simulation trajectories, we extract low-dimensional free energy surfaces governing the accessible conformational states and their relative thermodynamic stability. The free energy surfaces reveal how degree of polymerization and topological constraints affect the thermally accessible conformations, chiral symmetry breaking, and folding and collapse pathways of the rings, and present a means to rationally engineer ring size and topology to preferentially stabilize particular conformational states.

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