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Linking the dynamics of molecular prime knots to topological and local structural properties HYO JUNG PARK[1], Dickinson College, LAKSHMINARAYANAN MAHADEVAN, ANNA LAPPALA, Harvard University — Molecular knots (MKs) are structures entangled into the form of knots at a molecular level. Since the synthesis of the first artificial knot in 1989, various topologies of synthetic MKs have been realized, revealing their potential applications in biomedicine and nanotechnology. MKs have shown to perform specific functions based on their dynamic behaviors. Some protein-based knots, for example, can alternate between entangled and loose states and thus act as molecular machines that trap and release other molecules as desired. In defining their dynamics, the topology of MKs is known to play an important role, as knotting reduces degrees of freedom of molecular strands. However, understanding of what specific structural factors give rise to or allow certain types of dynamics is lacking. To understand these relationships, we build a methodology for studying knot dynamics in terms of topological and local structural properties. Specifically, we explore the dynamics of prime knots—knots that cannot be decomposed into two non-trivial knots—using Molecular Dynamics simulations and relate their principal motions to knot complexity, linking numbers, curvature, and torsion. We also investigate and compare the dynamics of symmetric and asymmetric prime knots.

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