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Untying molecular friction knots SERDAL KIRMIZIALTIN, DMITRII MAKAROV, The University of Texas at Austin — Molecular knots tied in individual polymer strands have fascinated researchers from many fields. Recently, laser tweezers have been used to tie knots in individual DNA and protein molecules and to observe their dynamics. Unlike their macroscopic counterparts, knots in tensioned polymer strands undergo rapid diffusion caused by thermal fluctuations. Here, we use computer simulations to study the dynamics of a "friction knot" joining a pair of polymer strands. While a friction knot splicing two ropes is jammed when the ropes are pulled apart, molecular friction knots eventually become undone by thermal motion. We show that depending on the knot type and on the polymer structure, a friction knot between polymer strands can be strong (the time τ the knot stays tied increases with the force F applied to separate the strands) or weak (τ decreases with increasing F). We further propose a simple model explaining these behaviors.

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