

Active Polymers Tie Themselves in Knots

Simulations show that polymers that include inert and self-propelled components are more likely to form and retain knots, with possible applications in materials engineering.

By **Marric Stephens**

Long molecules can become spontaneously entangled with themselves. Sometimes—in strands of DNA, for example—those knots are a problem. But the ability to create knots in polymers on demand could lead to materials with bespoke properties. Simulations have now shown that a molecule comprising two different polymers joined end to end—one inert, the other self-propelling—can accumulate knots more readily than a single-component chain of the same length [1].

Marin Vatin at the University of Padua in Italy and his colleagues modeled diblock (two-component) polymers as strings of beads. Each 200–400-bead chain had an adjustable ratio of active to passive beads. Both types were affected by random thermal motion. However, each active bead also propelled itself along a tangent to the chain. The vigor of this self-propulsion varied from one modeling run to the next, in all cases being much greater than the vigor of the thermal motion.

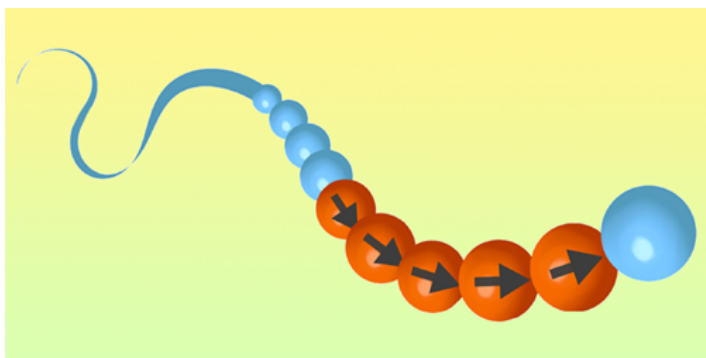
The likelihood of a diblock polymer hosting a knot at the end of a run turned out to be tiny when the polymer consisted solely of active or of passive beads. The likelihood peaked when the active length was around 40% of the total, and this peak was sharper when the self-propulsion was stronger. That behavior, the team found, arose from a competition between knot formation and dissolution. Knots tended to form in the active portion of a chain and migrated quickly along its length. Because migration slowed in the passive portion, any knot that reached this region was subsequently less likely to unravel.

So far, the researchers have studied simple knots in isolated strings. In the future, they hope to use these strings as building blocks for microknitted fabric with improved robustness and elastic properties.

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REFERENCES

1. M. Vatin *et al.*, “Upsurge of spontaneous knotting in polar diblock active polymers,” *Phys. Rev. Lett.* **134**, 168301 (2025).



Credit: M. Vatin *et al.* [1]