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Knots along DNA Confined in Nanochannels[1] C. BENJAMIN RENNER, MIT, LIANG DAI, SMART, PATRICK DOYLE, MIT — We study the size distribution of spontaneous knots on semiflexible chains confined in square channels using Monte Carlo simulations. The most probable knot size is shown to vary non-monotonically with the channel size. For knotted polymers confined in channels larger than the size of a knot in bulk, our analysis reveals that the metastable knot size in weak confinement is larger than the knot size in absence of confinement because the confinement free energy gained by shrinking the knot is lessened when the chain experiences the confinement of a channel. In the case of strong confinement, the metastable knot size is smaller than the knot size in the absence of confinement because the segments in the core of the knot experience more confinement free energy, and the channels pushes the segments out of the core of the knot. We demonstrate that a simple theory can capture this non-monotonic behavior and quantitatively explain the metastable knot size as a function of the channel size. These results may have implications for tuning the channel size to either generate or screen knots.

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Christopher Renner
MIT

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