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Knotting and Unknotting Dynamics of DNA Strands in Nanochannels ANTONIO SUMA, SISSA, ENZO ORLANDINI, University of Padova, CRISTIAN MICHELETTI, SISSA — Confinement of dsDNA in nanochannels can enhance or suppress altogether the strands knotting probability, affecting their metric, mechanical properties and interfering with the elongation process in nanofuidics devices. We characterize, through Langevin dynamic simulations, how knottedness arise from the internal dynamics of the chain, recovering the well characterized equilibrium knotting probability. Different channel widths are considered, covering various metric scaling regimes from 50 to 300 nm [1], and different DNA lengths, from 1.2 to 4.8 nm [2]. We explain the interplay between knot and unknot lifetimes and the channel and DNA parameters, relating these quantities to the equilibrium knotting probability. We show the basic knotting mechanism, which involves deep looping and back-foldings of the chain ends. The results can aid the design of nanochannels capable of harnessing the self-knotting dynamics to quench or relax the DNA topological state as desired.

[1]C. Micheletti and E. Orlandini. **ACS Macro Lett** 3.9 (2014): 876-880.
[2]A. Suma, E. Orlandini and C. Micheletti. **J. Phys. Condens. Matter** 27.35 (2015): 354102.

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