TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

Institut für Physik
Physikalisches Kolloquium

Donnerstag, 01.02.2024, 15:30 Uhr

Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude, Raum C10.013

Prof. Dr. Peter Virnau

Institut für Physik,
Johannes Gutenberg-Universität Mainz

Knots in polymers, DNA and proteins

Ever since Kelvin has conjectured that atoms are composed of knots in the ether, these peculiar objects have stimulated the imagination of mathematicians and natural scientists alike. In recent years the field went through a renaissance and progressed considerably, spurred by the discovery of knotted DNA and proteins. Interestingly, our intuitive understanding of knots at the macroscopic level often applies to objects at the nanometer scale as well.

After providing a general introduction to the topological classification of knots, I will discuss their occurrence in computer simulations of coarse-grained polymers. Amongst others this allows us to test from a topological point of view a long-standing paradigm of polymer physics, namely that chains in a polymer melt are well-represented by random walks [1]. Coarse-grained polymer models can also be parametrized to capture topology in dsDNA [2] and serve as a basis for modelling biological processes such as loop extrusion at experimentally relevant time and length scales.

From an evolutionary point of view protein knots occur in all kingdoms of life and topology is typically preserved amongst homologs. Nowadays, knotted protein structures can even be created artificially in the context protein engineering. I will demonstrate why the folding of knotted proteins may not be so difficult after all by explaining coarse-grained folding simulations of a topologically complex protein [3]. While knots in globular homopolymers are abundant, protein knots are rare and occur in less than one percent of all known structures. To address this conundrum, I will argue on the basis of a coarse-grained heteropolymer model that the introduction of sequence may enable evolution towards mostly unknotted proteins [4]. Finally, I will report on very recent developments facilitated by the artificial intelligence system AlphaFold, which has predicted millions of previously unknown three-dimensional protein structures. We have discovered in this data several novel knotted folds [5] including a composite knot consisting of two methyltransferases. In the meantime, this fold has been confirmed experimentally, serving as an impressive validation of the prowess of AlphaFold.

[1] H. Meyer, E. Horwath, P. Virnau, ACS Macro Lett. 7, 757 (2018).
[2] S. Wettermann, R. Datta, P. Virnau, Front. Chem. 10, 1096014 (2023).
[3] D. Bölinger, J. Sulkowska et al, PLoS Comp. Biol. 6, e1000731 (2010).
[4] T. Wüst, D. Reith, P. Virnau, Phys. Rev. Lett. 114, 028102 (2015).
[5] M. Brems, R. Runkel, T. Yeates, P. Virnau, Prot. Sci. 31, 4380 (2022).

Alle Zuhörer sind ab 15:15 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt:
Prof. Dr. Martin Weigel, Tel. 0371 531 34570

www.tu-chemnitz.de/physik