WINTER SEMESTER 2025 / 2026

RTG 2756 CYTAC SEMINAR SERIES

TUESDAY, JANUARY 6
17:00 IN HS5

CYTAC
RTG 2756

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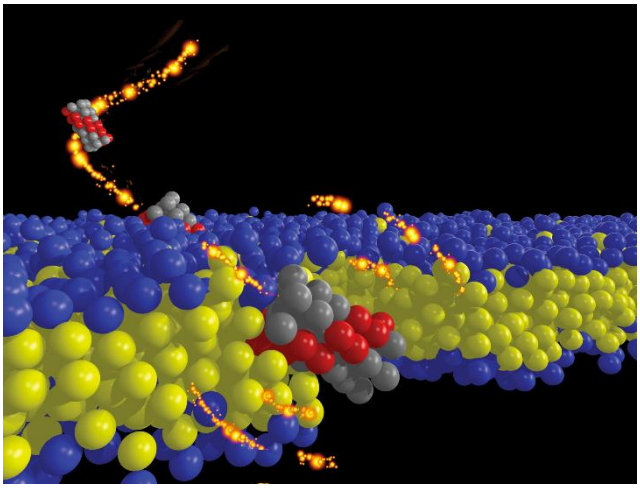
TWISTERS IN ACTION: HOW PROTEINS DEFORM MEMBRANES

An individual torque-applying filament can induce membrane deformations via two mechanisms: the Twister and the Darboux torque mechanism [1]. Whereas the latter has been shown to explain membrane deformations by a polymer in several important biological systems, the former has been studied only recently in more detail.

In my talk I will discuss how the Twister mechanism together with numerical simulations can explain the membrane translocation of botulinium toxins, which are among the most powerful toxins in nature [2]. The initial deformation of the membrane by the toxin is caused by the presence of local torques arising from asymmetric positions of hydrophobic residues. Different torque distributions are observed in the simulations and permit an origin for the mechanism opening the membrane to be proposed.



Further coarse-grained molecular dynamics simulations of a simplified model protein allow for a systematic study [3]. The protein is modeled as a cylinder stabilized by a tensegrity scheme, leading to an elasticity similar to that observed in real proteins. The Twister mechanism is induced by a hydrophobic helical strip displayed by the protein. The entire configuration space is explored by systematically varying the hydrophobic strip width, the twisting of the strip as well as the range of hydrophobic interactions between the cylinder and the membrane. The results are explained using a qualitative model based on the total hydrophobic moment of the protein.

[1] J. Fierling et al., Soft Matter 12, 5747 (2016). [2] A. Delort et al., IJMS 25, 2481 (2024). [3] J. Klein et al., Soft Matter 21, 4336 (2025).