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Multi-scale Modeling of the Nanomechanics of Microtubule Filaments

Microtubules are prime examples of large-size biomolecular systems that assemble, disassemble, and self-repair by controlled inputs. Despite the known role of mechanics in both the function of microtubules for example as motors driving the poleward chromosome motion during mitosis and in the remodeling of the microtubule lattice during depolymerization and severing by molecular motors, an understanding of the link between the structure of filaments and their dynamical properties is still in its infancy. Establishing such a link requires a combined experimental and computational approach. I will discuss the development of our approach to investigate the mechanics of filaments with relevance for chromosome motion and microtubule severing. Because of the modular architecture and strong inter- and intra-molecular coupling that influence the properties of microtubule filaments, we developed a multi-scale methodology, using coarse-graining and atomic details, to map out mechanical properties of microtubules on experimental timescales through large-scale molecular simulations. I will present our findings, combining results from simulations with results from in vitro experiments, of the microscopic origin of physico-chemical properties of microtubules and their protofilaments and the molecular mechanisms of their response to controlled mechanical inputs.