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Size-dependent mechanical properties of low-dimensional materials: coupling between deformation modes YITING DING, ZHIPING XU, Computational Energetics Laboratory, Department of Engineering Mechanics & Center for Nano and Micro Mechanics — Coupling between deformation modes, such as tension, bending, shear, and twisting, are widely observed in low-dimensional materials, especially biological materials. In this talk we will present our study on microtubules (MT) mechanics, where significance of mode coupling leads remarkable size-dependence in structural and mechanical properties. Using molecular dynamics (MD) simulations, we find a distinct dependence of bending rigidity on the contour length of a MT that agrees well with experimental data. We develop a simple model by including basic parameters to explain and predict this interesting phenomenon. An extended discussion will be made to general low-dimensional materials, with focuses not only on the mechanism, but also applications in optimal materials design.

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