

Abstract Submitted
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Mapping the energy landscape of tubulin under tension with molecular simulations HARSHAD JOSHI, RUXANDRA DIMA, University of Cincinnati — Microtubules (MTs) play major roles in the transport of organelles in the cell and in cell division. MTs are subject to permanent tension [1] and additional forces act on MTs when external mechanical perturbations are applied to cells. To elucidate the microscopic origins of the mechanical response in MTs, we have performed simulations of a self-organized polymer (SOP) model of tubulin, the building block of MTs. The SOP representation is an off-lattice minimalist description of a protein chain which allows us to perform force-induced unfolding simulations of large molecules at the loading rates and time scales of single-molecule experiments [2]. We show that the forced unfolding of tubulin involves a bifurcation in the unfolding pathways and map precise features of the complex energy landscape of tubulin by surveying the structures of the various metastable intermediates [3].

References:

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- [2] Hyeon C, Dima RI, Thirumalai D (2006) *Structure* 14:1633–1645.
- [3] Dima RI, Joshi H (2008) *Proc. Natl. Acad. Sci. USA* (accepted).

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