Abstract Submitted
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**Multipolar interaction model for microtubule self-assembly**[1] KYLE GUSTAFSON, Univ. of MD, Dept. of Physics, IREAP, JUSTIN STAMBAUGH, MIT Lincoln Lab., WOLFGANG LOSERT, Univ. of MD, Dept. of Physics, IPST and IREAP — Tubulin protein monomers (m = 50 kDa, d = 4-5 nm) are known to self-assemble into biologically significant structures called microtubules. Calculations for microtubule models using the full crystallographic structure of tubulin are prohibitive. As a substitute, we investigate a simpler multipolar interaction model of tubulin which can capture important features of microtubules. We present energy-minimization calculations showing that a four point-charge rectangular model reproduces the 0.93 nm staggering of observed microtubules. We then attempt to validate these static Coulomb calculations with molecular dynamics (MD) using NAMD (from the Theoretical and Computational Biophysics group at the University of Illinois). These simulations include electrostatic interactions, stiff bonded interactions, a Lennard-Jones potential and Langevin damping. The results of the MD simulations are strongly dependent on each of these influences. We find stable filaments of tubulin using the multipole model in MD simulations. When these filaments are combined into a realistic microtubule in MD, an energy minimum is found which supports a stable tube. The study encompasses fraying of tube ends, staggering angle, and ring stability for tubulin and microtubules based on our simple, four charge multipolar model.

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