Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**A coarse-grained model of microtubule self-assembly** CHOLA REGMI, SHENGFENG CHENG, Virginia Polytechnic Institute and State University — Microtubules play critical roles in cell structures and functions. They also serve as a model system to stimulate the next-generation smart, dynamic materials. A deep understanding of their self-assembly process and biomechanical properties will not only help elucidate how microtubules perform biological functions, but also lead to exciting insight on how microtubule dynamics can be altered or even controlled for specific purposes such as suppressing the division of cancer cells. Combining all-atom molecular dynamics (MD) simulations and the essential dynamics coarse-graining method, we construct a coarse-grained (CG) model of the tubulin protein, which is the building block of microtubules. In the CG model a tubulin dimer is represented as an elastic network of CG sites, the locations of which are determined by examining the protein dynamics of the tubulin and identifying the essential dynamic domains. Atomistic MD modeling is employed to directly compute the tubulin bond energies in the surface lattice of a microtubule, which are used to parameterize the interactions between CG building blocks. The CG model is then used to study the self-assembly pathways, kinetics, dynamics, and nanomechanics of microtubules.

Chola Regmi
Virginia Polytechnic Institute and State University

Date submitted: 04 Nov 2015 Electronic form version 1.4