

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Molecular Simulations of Actomyosin Network Self-Assembly and Remodeling**<sup>1</sup> JAMES KOMIANOS, Univ of Maryland-College Park, KONSTANTIN POPOV, Univ of North Carolina-Chapel Hill, GAREGIN PAPOIAN, Univ of Maryland-College Park, PAPOIAN LAB TEAM — Actomyosin networks are an integral part of the cytoskeleton of eukaryotic cells and play an essential role in determining cellular shape and movement. Actomyosin network growth and remodeling in vivo is based on a large number of chemical and mechanical processes, which are mutually coupled and spatially and temporally resolved. To investigate the fundamental principles behind the self-organization of these networks, we have developed a detailed mechanochemical, stochastic model of actin filament growth dynamics, at a single-molecule resolution, where the nonlinear mechanical rigidity of filaments and their corresponding deformations under internally and externally generated forces are taken into account. Our work sheds light on the interplay between the chemical and mechanical processes governing the cytoskeletal dynamics, and also highlights the importance of diffusional and active transport phenomena. Our simulations reveal how different actomyosin micro-architectures emerge in response to varying the network composition.

<sup>1</sup>Support from NSF Grant CHE-1363081.

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Date submitted: 03 Nov 2015

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