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Molecular Dynamics Simulation of semi-flexible filament assembly LAM T. NGUYEN, Florida State Univ., QI WANG, ZIYAD MUSLIMANI, LINDA S. HIRST — An MD simulation has been developed to study semi-flexible filament bundling and network formation by cross-linkers in solution. We aim to model and understand the ordered mesoscale structures observed experimentally by F-actin, in which different network configurations occur for different concentrations of cross-linking protein. [1]. We use a bead-rod model for the semi-flexible filament and linkers, which can be easily adapted to different cross-linking proteins. Electrostatic interactions were shown to be the main mechanism for the aggregation process, Coulombic forces between excess charges on the proteins dominate at the long range inducing the assembly, while at short range the Van der Waals interaction and specific binding potentials of the proteins have been taken into account. We discuss the effects of screening the Coulomb interaction not only for the linker conc. at which a phase transition occurs but also on bundling and network configuration above the transition point. These results are in good agreement with experimental observations of actin filament bundling and assembly. [1] **L.S. Hirst** et al J. CHEM. PHYS. 123, 104902 (2005)

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