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A statistical model of protein binding in parallel actin bundles HOMIN SHIN, GREGORY GRASON, University of Massachusetts Amherst, KIRSTIN PURDY DREW, GERARD WONG, University of Illinois at Urbana-Champaign — We propose a coarse-grained lattice model of cross-linking proteins in parallel actin bundles. Based on this model that captures the interplay between geometrical frustration of binding and the intrinsic flexibility of filaments and linkers, we predict a unique regular ground-state structure of fully cross-linked bundles. We also discuss the linker-dependent thermodynamic transition of actin filaments from their native state to the overtwisted state and map out the "twist-state" phase diagram in terms of linker flexibility as well as the chemical potential. A flexible linker regime exhibits a continuous spectrum of intermediate twist states, while a stiff linker regime only allows for untwisted actin filaments and fully overtwisted bundles. Our predictions compare well with small-angle scattering studies of bundles formed in the presence of two types of reconstituted cross-linking proteins, fascin and espin. Additionally, this study reveals how subtle differences in crosslinking agents themselves may be used by cells to achieve self-organized bundles with dramatically different properties.

Homin Shin
University of Massachusetts Amherst

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