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Structure and stability of self-assembled actin-lysozyme complexes studied via computer simulation CAMILO GUAQUETA, ERIK LUIJTEN, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801 — Using both molecular dynamics and grand-canonical Monte Carlo simulations, we have studied the structure and stability of complexes of filamentous actin (an anionic polyampholyte) and lysozyme (a cationic globular protein) in aqueous solution. We find that lysozyme initially bridges pairs of filaments, which then relax into hexagonally-coordinated bundles comprised of actin rods held together by one-dimensional arrays of lysozyme macroions. In order to connect to small-angle x-ray scattering results, we have examined the role of the concentration of monovalent salt. We find that exclusion of salt from the bundled phase is essential for bundle stability, and we address with our simulation results the different competing effects which could be responsible for this salt repartitioning.

Camilo Guaqueta
University of Illinois at Urbana-Champaign

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