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Molecular Adhesion of Curved Filaments: Self-Assembly of Bacterial Flagellar Bundles¹ LUIS CAJAMARCA, University of Massachusetts Amherst, Physics Department, GREGORY GRASON, University of Massachusetts Amherst, PSE Department — The self-assembly of chiral filaments, such as filamentous proteins, introduces an unavoidable frustration between inter-filament and intra-filament geometries. We study the self-assembly of bacterial flagella with a model that focuses on three geometric features: a preferred distance of closest approach; a preferred relatively-parallel orientation; and a mechanical cost for changes of helical shape. As a result, intrinsically curved filaments cannot simultaneously minimize all three driving forces, even in the limiting case of 2-filament contacts. Using a model of depletion-driven and electrostatically-stabilized interactions we present a phase diagram for two filament bundles depicting the complex thermodynamic behavior of adhesive contact using three ratios: one describes the shape of the filaments, and the other two capture the competition of the modulus associated with mechanical deformations and with the cost of having a non-zero twist vs the modulus associated to changes in inter-filament spacing. Finally, we describe the dependence of these ratios on experimentally-adjustable variables and predict critical concentrations of depletant molecules for known polymorphic configurations which may favor the filaments to undergo a transition from non-adhesive to adhesive state.

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