Optimal arrangement of lamellar and triangular lattices confined to cylindrical fibers

KEVIN KOHLSTEDT, University of Michigan, GRAZIANO VERNIZZI, Northwestern University, FRANCISCO SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University — The optimal packing of ionic lamellar and triangular lattices on the surface of a nanofiber is computed to determine the effects of the surface curvature. In ionic triangular lattices, electrostatic interactions prefer chiral arrangements only for special families of lattices that depend on the fiber diameter. However, there are families of triangular lattices that energetically promote achiral configurations. We also consider the behavior of short-range elastic forces, represented by interconnected springs between neighboring components. In this case a different family of achiral lattices is preferred. We also determine the optimal packing of lamellar lattices of cationic-anionic components. In lamellar packing of cylinders a chiral angle emerges that depends on the cylinder radius and the different dielectric constants of the interior and exterior of the cylinder. We discuss the effect of salt concentration inside and outside the cylinders on the chiral angle, and the implication of our results in ion channels structures.

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