

Packing and Assembling Spheres in Cylindrical Confinement

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Hard spheres confined to cylinders model systems as varied as fullerenes in nanotubes and fruit displays. Although identifying the densest packing of spheres of diameter s within a cylinder of diameter D is a purely geometric problem, solving it grows increasingly difficult with D/s . In fact, little is known for $D/s > 2.87$. Here, we present our work extending the identification of close packings up to $D/s = 4.00$. By adapting Torquato–Jiao’s adaptive-shrinking-cell formulation and sequential-linear-programming (SLP) technique we identify 17 new structures, almost all of them chiral. Beyond $D/s = 2.85$, most structures consist of an outer shell and an inner core that compete for being close packed. Remarkably, in some cases the shell density is maximized and the core spheres are stacked quasi-periodically, but other order types are also observed. In order to assess what structures are dynamically accessible, we also examine the self-assembly pathway in systems with $D/s < 2.82$.