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Densest packings of hard spheres in a cylinder LIN FU, WILLIAM STEINHARDT, HAO ZHAO, JOSHUA SOCOLAR, PATRICK CHARBONNEAU, Duke University — Densely packing hard spheres (HS) within a cylinder is remarkably complex. Little is known about the densest achievable packings when the cylinder diameter, D, is larger than 2.85 times the sphere diameter, s. Here, we extend the identification of the densest packings up to D = 4.00s by adapting Torquato-Jiaos adaptive-shrinking-cell formulation and sequential-linear-programming technique to this geometry. We identify 17 new structures, almost all of them chiral. Beyond D, approx2.85s , most of the structures consist of an outer shell and of an inner core that compete for being close packed. In some cases the shell adopts a periodic configuration that is optimal and the stacking of core spheres within it is quasiperiodic, while in other cases a direct interplay between the two layers is observed. For some packings the very distinction between the core and shell vanishes, which results in exotic geometries, including some that are a three-dimensional extension of packing hard disks in a circle. In order to connect our results with experiments on comparable systems, we also consider the ease with which these structures assemble. Using kinetic Monte Carlo simulations, we find that some of the structures promtply assemble while others simply do not.

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