Complexity in surfaces of densest packings for families of polyhedra

DAPHNE KLOTSA, University of Michigan, ELIZABETH R. CHEN, Harvard University, MICHAEL ENGEL, PABLO F. DAMASCENO, SHARON C. GLOTZER, University of Michigan — Packings of hard polyhedra have been studied for centuries due to their mathematical aesthetic and more recently for their applications in fields such as nanoscience, colloidal matter, and biology. In all these fields, particle shape is important for structure and properties, especially upon crowding. In this talk, we explore packing as a function of shape. By combining simulations and analytic calculations, we study three 2-parameter families of hard polyhedra and report an extensive and systematic analysis of the densest known packings of more than 55,000 convex shapes. The three families have the symmetries of triangle groups (20-hedral, 8-hedral, 4-hedral) and interpolate between various symmetric solids (Platonic, Archimedean, Catalan). We find that maximum packing density surfaces reveal unexpected richness and complexity, containing as many as 130 different structures within a single family. Our results demonstrate the importance of thinking about shape not as a static property of an object, in the context of packings, but rather as but one point in a higher dimensional shape space whose neighbors in that space may have identical or markedly different packings. Finally, we propose a method to distinguish regions of packings and classify types of transitions between them.