Microsymposium

Simple particles, complex structures

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Quasicrystalline structures, and complex compounds in general, have been found in a wide range of intermetallic systems over the last half-century. Their occurrence and stability is most commonly attributed to chemical and electronic factors and the systems that compose them are viewed with a focus on composition and stoichiometry. Recent studies, however, have shown that the same complex structures are found in soft-matter systems, either on vastly different length scales - in experimental investigations of colloids or nanoparticles - or in computational work that can agnostically explore phase space with almost unlimited flexibility.

We simulated one-component systems of attractive particles that interact via isotropic pair potentials. These have shown to produce crystalline structures of high complexity, when the first simulated icosahedral quasicrystal was reported [1]. Inspecting large areas of these parameter spaces, we find a variety of crystal structures - some known and some novel, some simple and others of varying complexity.

We observe the emergence of long-range periodicity from short-range potentials and the emergence of complex structures from simple interactions. In addition, the continuous variability of the applied interaction potentials results in a range of structures that spans nearest-neighbor coordination numbers from 4 through 14. We thus observe arrangements that occur in structures from a wide scope of chemical systems, mimicking interactions that range from directed, covalent bonds, leading to low-coordination geometries, to metallic ones, such as in the dense sphere packings. [1] Engel, M., Damasceno, P. F., Phillips, C. L., Glotzer, S. C. (2015), Nature Materials, 14, 109-116.

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