Design of colloidal particles to form 3-dimensional axial quasicrystals

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Aperiodic crystals (or quasicrystals, QCs) are materials that display long-range orientational order but lack periodicity. Initially discovered in metallic alloys [1], they have since been identified in a variety of soft matter systems [2]. QCs can be classified according to their symmetry, the main types being icosahedral and axial. While icosahedral QCs are aperiodic in all directions, axial QCs are aperiodic in two dimensions, but periodic in the third one.
We will show two examples of how we designed colloids with directional interactions to assemble into 3D quasicrystals with dodecagonal and octagonal symmetry. In the dodecagonal example, we generalize previous success in forming a 2D dodecagonal quasicrystal from 5-patch discs [3] and binary mixtures of 5- and 6-patch discs [4] by designing particles that forms stacks of such layers [5]. The nature of the interactions between such layers is simple with particles designed to sit directly above the particles in the previous layer.
For the octagonal quasicrystal the model design was obtained by looking at the local environments of a generalization to 3D of the 2D octagonal Ammann-Beenker tiling of squares and thin rhombs [6]. These environments have from 3 to 8 neighbours. An octagonal QCs can be obtained either from a binary system of 5-patch and 8-patch particles, or from a one-component system of 5-patch particles forms an octagonal quasicrystal. In both systems, edge dislocations are common. Additionally, a one-component system of the 8-patch particles assembled into an aggregate with multiple twinned crystalline domains whose diffraction pattern also exhibits 8-fold symmetry.
Finally, we will discuss the formation and stability of a decagonal QC from spherical particles with a soft corona [7]. Despite the fact that the decagonal QCs forms spontaneously upon quenching the fluid phase, our simulations indicate that this phase is less stable than a periodic approximant (i.e. a periodic crystal with local environments similar to those of the QCs).

Keywords:
colloids, self-assembly, quasicrystals, computer simulation, phase diagram, patchy particles

References:

[1] D. Shechtman, I. Blech, D. Gratias, J. W. Cahn, Phys. Rev. Lett. **53** (1984) 1951.
[2] X. Zeng, G. Ungar, Y. Liu, V. Percec, A.E. Dulcey, J.K. Hobbs, Nature 428, 157 (2004).
[3] M. N. van der Linden, J.P.K. Doye and A.A. Louis, J. Chem. Phys. 136, 054904 (2012)
[4] A. Reinhardt, J.S. Schreck, F. Romano and J.P.K. Doye, J. Phys: Condens. Matter, 29, 014006 (2017).
[5] D.F. Tracey, E.G. Noya and J.P.K. Doye, J. Chem. Phys. 154, 194505 (2021)
[6] A. Kowaguchi, S. Metha, J.P.K. Doye and Eva G. Noya, J. Chem. Phys. 163, 244904 (2025)
[7] S. Mosca, J.P.K. Doye, and Eva G. Noya, in preparation (2026).

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