

55b Self-Assembly of Patchy Particles into Diamond Structures through Molecular Mimicry

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Fabrication of the diamond structure by self-assembly is a fundamental challenge in making three-dimensional photonic crystals. In this study we perform molecular simulations of model hard particles with patches of attractive interactions and show that particles with these interactions can self-assemble into a diamond structure from an initially disordered state. We show that the formation of the diamond structure can be facilitated by “seeding” the system with small diamond crystallites or by introducing a rotation-inducing interaction to mimic a carbon-carbon bond rotation. Our results suggest the patchy particles may serve as colloidal “atoms” for the bottom-up self-assembly of three-dimensional photonic crystals.