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Computational prediction of an icosahedral quasicrystal

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From the first quasicrystal discovered in the laboratory 30 years ago to the only known specimen of naturally occurring quasicrystals, quasicrystals with icosahedral symmetry have received great attention. There are more than one hundred stable icosahedral quasicrystals in metallic alloys; all are identified by their diffraction spectra. Despite this abundance, resolving the positions of the atoms within the solid has been possible only indirectly. Moreover, unlike dodecagonal and other axial quasicrystals, icosahedral quasicrystals have been observed neither in simulations nor in non-atomic (e.g. micellar or colloidal) systems, where real-space information would be available. Here we present an icosahedral quasicrystal discovered in computer simulation via self-assembly from the liquid phase. We provide a structure model by analyzing atomic surfaces and report the presence of phason flips. Our results constitute a direct microscopic confirmation of the higher-dimensional crystallographic description of icosahedral quasicrystals.

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