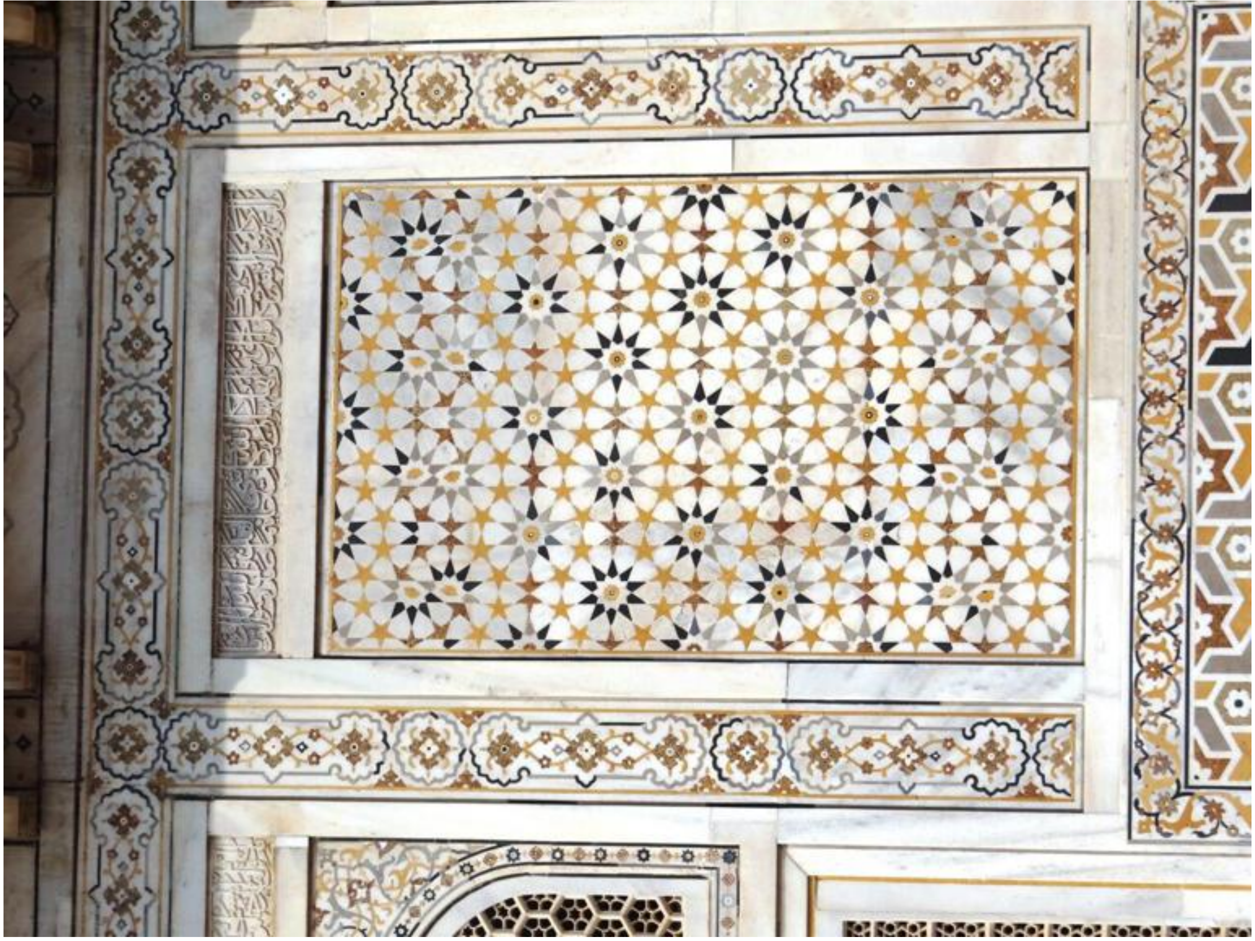
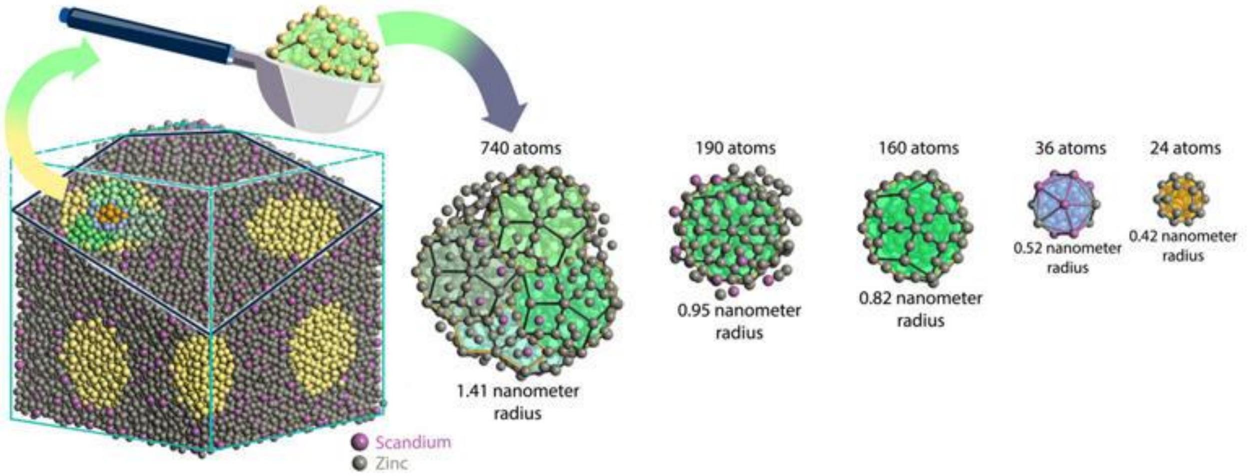
First quantum-mechanical model of quasicrystals reveals why they exist



While the symmetry of quasicrystals preclude sequential patterns, their atoms still form repeating motifs similar to the patterns in traditional islamic tile art. This panel on the Tomb of I'timād-ud-Daulah in Agra, India is one example—each individual building block doesn't repeat in a regular sequence from left to right, nor up and down, but the ten-pointed star repeats across the panel. Photo credit: Wikimedia commons.

A rare and bewildering intermediate between crystal and glass can be the most stable arrangement for some combinations of atoms, according to a study from the University of Michigan.

The findings come from the first quantum-mechanical simulations of quasicrystals—a type of solid that scientists once thought couldn't exist. While the atoms in quasicrystals are arranged in a lattice, as in a crystal, the pattern of atoms doesn't repeat like it does in conventional crystals. The new simulation method suggests quasicrystals—like crystals—are fundamentally stable materials, despite their similarity to disordered solids like glass that form as a consequence of rapid heating and cooling.



To calculate the stability of a solid whose atoms don't repeat in a sequence, the researchers simulated scoops of quasicrystal that were randomly sampled out of a larger block. The energy within each nanoparticle can be calculated using quantum mechanics because the particle has defined boundaries. Repeating the calculations over a range of scoop sizes allows the researchers to extrapolate their energy calculations to the bulk quasicrystal. Credit: Woohyeon Baek, Sun Research Group, University of Michigan.

"We need to know how to arrange atoms into specific structures if we want to design materials with desired properties," said Wenhao Sun, the Dow Early Career Assistant Professor of Materials Science and Engineering, and the corresponding author of the paper published today in *Nature Physics*. "Quasicrystals have forced us to rethink how and why certain materials can form. Until our study, it was unclear to scientists why they existed."

Quasicrystals seemed to defy physics when they were first described by Israeli scientist Daniel Shechtman in 1984. While experimenting with alloys of aluminum and manganese, Shechtman realized that some of the metals' atoms were arranged in an icosahedral structure resembling many 20-sided dice joined at their faces. This shape gave the material five-fold symmetry—identical from five different vantage points.

Scientists at the time thought that the atoms inside crystals could only be arranged in sequences repeating in each direction, but five-fold symmetry precluded such patterns. Shechtman initially faced intense scrutiny for suggesting the impossible, but other labs later produced their own quasicrystals and found them in billion-year-old meteorites.

Shechtman eventually earned the Nobel Prize in Chemistry in 2011 for his discovery, but scientists still couldn't answer fundamental questions on how quasicrystals formed. The roadblock was that density-functional theory—the quantum-mechanical method for calculating a crystal's stability—relies on patterns that infinitely repeat in a sequence, which quasicrystals lack.

"The first step to understanding a material is knowing what makes it stable, but it has been hard to tell how quasicrystals were stabilized," said Woohyeon Baek, a U-M doctoral student in materials science and engineering and the study's first author.

The atoms in any given material usually arrange into crystals so that the chemical bonds achieve the lowest possible energy. Scientists call such structures enthalpy-stabilized crystals. But other materials form because they have high entropy, meaning there are a lot of different ways for its atoms to be arranged or vibrate.

Glass is one example of an entropy-stabilized solid. It forms when melted silica quickly cools, flash-freezing the atoms into a patternless form. But if the cooling rates slow, or a base is added to heated silica, the atoms can arrange into quartz crystals—the preferred, lowest energy state at room temperature.

Quasicrystals are a puzzling intermediate between glass and crystal. They have locally ordered atomic arrangements like crystals, but like glass, they do not form long-range, repeating patterns.

To determine if quasicrystals are enthalpy- or entropy-stabilized, the researcher's method scoops out smaller nanoparticles from a larger simulated block of quasicrystal. The researchers then calculate the total energy in each nanoparticle, which doesn't require an infinite sequence because the particle has defined boundaries.

Since the energy in a nanoparticle is related to its volume and surface area, repeating the calculations for nanoparticles of increasing sizes allows the researchers to extrapolate the total energy inside a larger block of quasicrystal. With this method, the researchers discovered that two well-studied quasicrystals are enthalpy-stabilized. One is an alloy of scandium and zinc, the other of ytterbium and cadmium.

The most accurate estimates of quasicrystal energy require the largest particles possible, but scaling up the nanoparticles is difficult with standard algorithms. For nanoparticles with only hundreds of atoms, doubling the atoms increases the computing time eightfold. But the researchers found a solution for the computing bottleneck, too.

"In conventional algorithms, every computer processor needs to communicate with one another, but our algorithm is up to 100 times faster because only the neighboring processors communicate, and we effectively use GPU acceleration in supercomputers," said study co-author Vikram Gavini, a U-M professor of mechanical engineering and materials science and engineering.

"We can now simulate glass and amorphous materials, interfaces between different crystals, as well as crystal defects that can enable quantum computing bits."

More information: Baek, W et al. Quasicrystal stability and nucleation kinetics from density functional theory. *Nature Physics* (2025). DOI: 10.1038/s41567-025-02925-6, www.nature.com/articles/s41567-025-02925-6

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