Study reveals breach of 'dancing' barrier governs crystal growth

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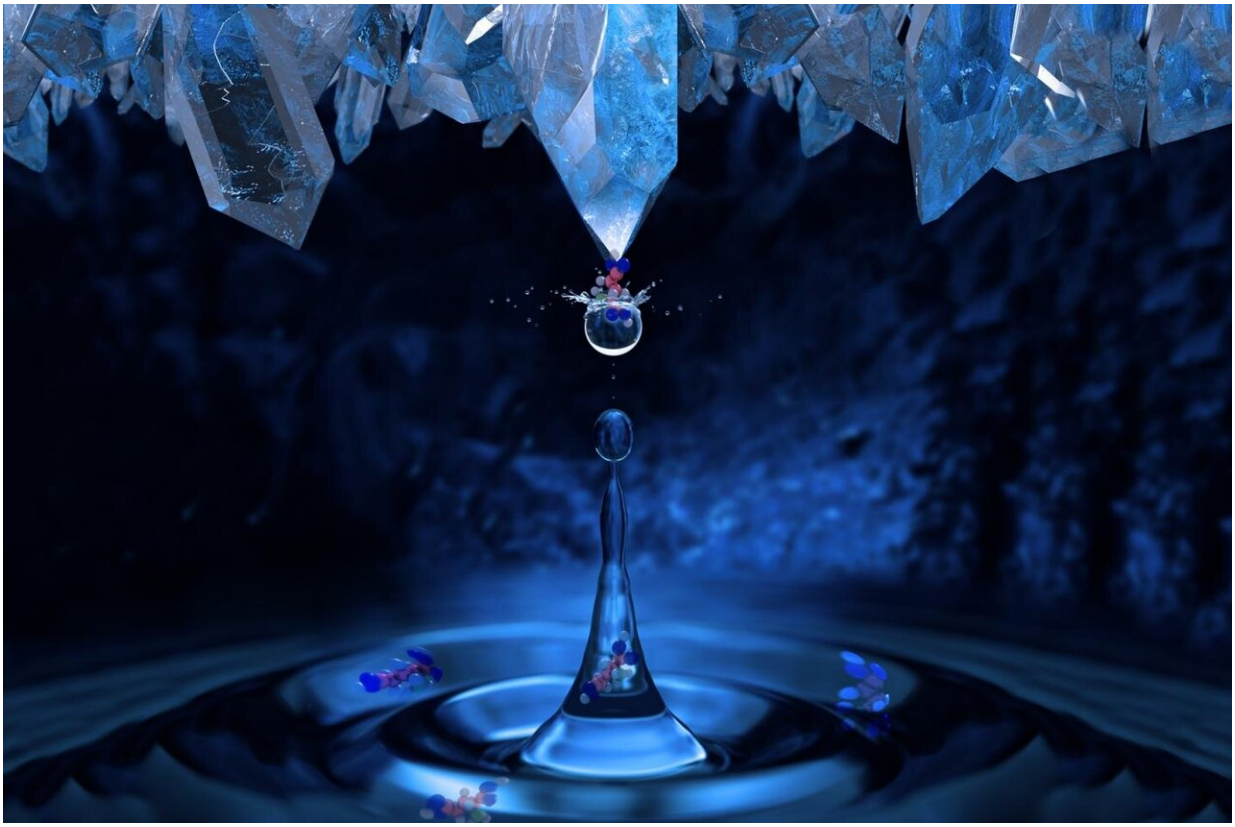

Local fluctuations allow molecules to leave the solvation shell and integrate into the crystal surface Credit: Meenesh Singh

While crystals have been studied for centuries and are ubiquitous in daily life—they are in our bones, the food we eat and the batteries we

use—scientists still don't fully understand how crystals grow or how to efficiently manufacture them. As a result, scientific efforts to improve a wide range of crystalline materials, from self-healing biomaterials to solar panels, have been limited.

Researchers at the University of Illinois at Chicago have unlocked part of this mystery. By using computer-based simulations to analyze how atoms and molecules move in a solution, the UIC team has identified a general mechanism governing crystal growth that scientists can manipulate when developing new materials.

Specifically, they found that when crystal-forming molecules are surrounded by a solvent, like water, the solvent molecules form a shield that they call a solvation shell. When this shield fluctuates, molecules can break free to form crystals. They also showed that temperature, solvent type and the number of solvent molecules all affect the shell's fluctuation.

Their findings are reported in the journal *Proceedings of the National Academy of Sciences*.

"For the first time, we have shown what happens when a molecule leaves a solvent to form a crystal," said Meenesh Singh, senior author and assistant professor of chemical engineering at the UIC College of Engineering. "Under the right conditions, the shield 'dances' around and allows molecules to break free and integrate into the crystal surface. The fluctuations in the solvation shell are key molecular events that explain how crystals form—knowledge of this mechanism has been missing since the inception of crystallization research."

Singh said understanding this mechanism will provide scientists with greater ability to direct molecules to form crystals for specific structure, shape and size. "This will allow us to make better materials for a wide

class of products used in daily life," he said.

Some examples, he said, are bone implants to promote biomineralization, better drug delivery systems, more stable lithium batteries, and improved semiconductors and agricultural chemicals.

"The molecular insight gained from this study will also help save money in various chemical industries by reducing the need for hit or miss techniques in thousands of trials," said UIC graduate student Anish Dighe, co-author of the paper. "With the help of this study, we can now design systems that can crystallize the desired solute molecule without so many trials."

More information: Anish V. Dighe et al, Solvent fluctuations in the solvation shell determine the activation barrier for crystal growth rates, *Proceedings of the National Academy of Sciences* (2019). DOI: 10.1073/pnas.1910691116

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