The solution to a 7-decade mystery is crystal-clear to FSU chemist

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Ammonium dihyrogen phosphate, or ADP, crystals, which have applications in computer memory, laser and fiber optic technology. Credit: Florida State University

A Florida State University researcher has helped solve a scientific mystery that stumped chemists for nearly seven decades. In so doing, his team's findings may lead to the development of more-powerful computer memories and lasers.

Naresh S. Dalal, the Dirac Professor of Chemistry and Biochemistry at FSU, recently collaborated with three colleagues, Jorge Lasave, Sergio

Koval and Ricardo Migoni, all of the Universidad Nacional de Rosario in Argentina, to determine why a certain type of crystal known as ammonium dihydrogen phosphate, or ADP, behaves the way it does.

"ADP was discovered in 1938," Dalal said. "It was observed to have some unusual electrical properties that weren't fully understood -- and for nearly 70 years, scientists have been perplexed by these properties. Using the supercomputer at SCRI (FSU's Supercomputer Computations Research Institute), we were able to perform in-depth computational analyses that explained for the very first time what causes ADP to have these unusual properties."

ADP, like many crystals, exhibits an electrical phenomenon known as ferroelectricity. Ferroelectric materials are analogous to magnets in that they maintain a positively charged and a negatively charged pole below a certain temperature that is characteristic for each compound.

"Ferroelectric materials can stay in a given state of charge for a long time -- they retain their charge after the external electrical source is removed," Dalal said. "This has made ADP and other materials like it very useful for storing and transmitting data.

ADP is commonly used in computer memory devices, fiber optic technology, lasers and other electro-optic applications."

What researchers found perplexing about ADP was that it often displays a very different electrical phase -- one known as antiferroelectricity.

"With antiferroelectricity, one layer of molecules in a crystal has a plus and a minus pole, but in the next layer, the charges are reversed," Dalal said. "You see this reversal of charges, layer by layer, throughout the crystal."

Using the supercomputer at SCRI enabled Dalal and his colleagues to perform numerous highly complex calculations that couldn't be duplicated in a laboratory environment. For example, they were able to theoretically alter the angles of ADP's ammonium ions and then measure the effects on the crystal's electrical charge. That approach ultimately led to their solution to the seven-decade mystery.

"We found that the position of the ammonium ions in the compound, as well as the presence of stresses or defects in the crystal, determine whether it behaves in a ferroelectric or antiferroelectric manner," Dalal said.

The team's research is important for two main reasons, Dalal said: "First, this allows us to further understand how to design new materials with both ferroelectric and antiferroelectric properties. Doing so could open new doors for computer memory technology -- and possibly play a role in the development of quantum computers.

"Second, our research opens up new ways of testing materials," Dalal said. "Using supercomputers, we can quickly perform tests to see how materials would react under a variety of conditions. Many such tests can't even be performed in the lab."

Source: Florida State University

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