A new symmetry underlies the search for new materials

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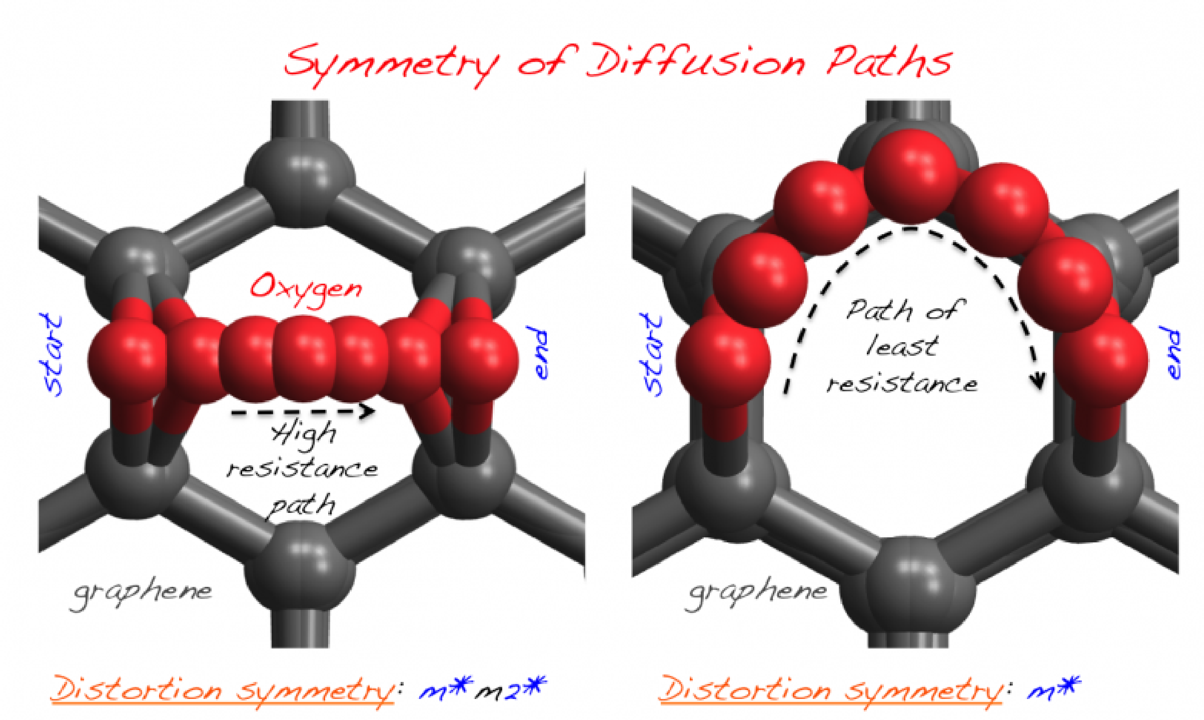

Each diffusion path for an oxygen atom (red) moving across a graphene ring composed of carbon atoms (gray) is considered a 'distortion' and is indexed by a unique 'distortion symmetry group' indicated below each image. The symmetry group contains all the essential information about the properties of the material system as the diffusion occurs, including the ability to help determine the minimum energy pathway. In this case, the minimum energy pathway is when oxygen moves around the ring (right image) rather than across it (left image). Credit: Venkat Gopalan, Penn State

A new symmetry operation developed by Penn State researchers has the potential to speed up the search for new advanced materials that range from tougher steels to new types of electronic, magnetic, and thermal materials. With further developments, this technique could also impact the field of computational materials design.

"In the physical sciences, making measurements can be time consuming and so you don't want to make unnecessary ones," said Venkat Gopalan, professor of materials science and engineering. "This is true for any material property—mechanical, electrical, optical, magnetic, thermal or any other. Knowing the symmetry group of a material can greatly reduce the number of measurements you have to make. "

Symmetry is pervasive throughout the physical universe and underlies the basic laws of physics. Gopalan gives a simple but scientifically accurate definition. "Symmetry is when doing something looks like doing nothing."

A circle has perfect symmetry, because if you rotate it by any number of degrees, it will look the same. Similarly, rotating a hexagon by sixty degrees leaves it exactly the same, but rotating it by a different amount does not. Anything that can be done that leaves an object looking the same is a symmetry operation.

In crystals, atoms are arranged in symmetrical patterns, like a cube of salt or a crystal of sugar or quartz. Symmetry groups tell scientists in how many different ways atoms can arrange in repeating patterns. If they know which symmetry group a material falls into, they already know a great deal about the properties—mechanical, thermal, electrical and so forth - that material will have. There are precisely 230 groups that explain how atoms can be arranged in space. These are symmetry "boxes" a material will fit into. If scientists are looking for a material with a certain property, such as the ability to be electrically polarized, they can look at materials only in that symmetry box and ignore all the boxes that cannot possibly contain polar materials.

Another symmetry operation, called time reversal, adds to the number of symmetry boxes available, and applies specifically to magnetic materials. This simply says that if time runs backwards, a material will either look the same or it won't.

In a paper published online in the journal *Nature Communications*, Gopalan and his coauthor and former Ph.D. student Brian VanLeeuwen report a new set of boxes called distortion symmetry groups that describes what happens when physical systems are perturbed by stresses, electric and magnetic fields or other forces, and change from one state to another.

"Distortions are the most common phenomenon in nature," Gopalan said. "A chemical reaction is a distortion, diffusion is a distortion, and a change in the atomic positions and electronic clouds within a material is a distortion. The symmetry that Brian and I discovered is like recording a movie of atoms and looking at its symmetry, whereas most symmetry operations are looking at one frame of a movie.

"We show that there is a huge family of problems that this will apply to, such as phase transitions—for example, water changing from a liquid to a solid or vibrations in molecules and solids. You will see symmetries you couldn't easily see before. Then we can quickly reduce the number of experiments we have to run or the number of computations that have to be done to find how a material will change under the effect of distortions."

VanLeeuwen and Gopalan's operation is already being applied by colleagues at Penn State working in computational materials design. One group is using the technique to understand and model the diffusion of hydrogen atoms in steel. Another group is incorporating it into a powerful computer code called Quantum Espresso, used by modelers around the globe.

"The first question we like to ask when a new material is discovered is how the atoms are arranged in space," said Ismaila Dabo, assistant professor of materials science and engineering, and one of the developers of Quantum Espresso. "Symmetries provide a powerful language to explain such atomic arrangements and their distortions close to equilibrium. But when the distortions are so large that they bring the atoms far away from equilibrium, there was no clear way to describe materials transformation, making it difficult to classify critical phenomena like phase transitions or grain boundary motions. This work gives an admirably elegant and much needed answer to that question."

Proteins are complex crystals that change when a drug molecule attaches to them. But current drug discovery is very computationally and experimentally intensive. Gopalan feels this technique might someday be useful for reducing the number of trials required.

"Biology is all about distortions of biomolecules towards performing a biological function," he said. "This will be worthwhile knowledge to them. Someday this could be very useful, but biology is highly complex involving hundreds of atoms in a unit cell. We are not yet sure if these ideas could make an impact there, but we plan to try. My goal is to take this and apply it to a variety of simpler problems first."

VanLeeuwen said that many technologies that are limited by materials properties could benefit by applying this method to find new materials. This includes stronger and lighter alloys for space exploration and fuel efficiency, better sensors for healthcare and greater performance from turbines for more energy production.

"Nature always takes the path of least resistance. Knowing this path allows us to calculate tremendously important materials properties. These properties are critical to the function of a very wide range of technologies, from making it possible for an ultrasound to detect a life-threatening heart condition to preventing nuclear reactors from melting down," VanLeeuwen said.

Provided by Pennsylvania State University

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