

Ferroelectric materials react unexpectedly to strain

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Up until recently, researchers thought they had the behaviors of ferroelectric materials mostly figured out.

"The conventional wisdom is that you can put almost any material under mechanical stress, and provided the stress is coherently maintained, the material will become ferroelectric or exhibit an <u>electrical polarization</u>," said James Rondinelli, assistant professor of materials science and engineering at Northwestern University's McCormick School of Engineering. "If you apply similar stresses to a compound that's already ferroelectric, then its polarization increases."

Rondinelli and his team, however, have made a theoretical discovery that flips this widely accepted fact on its head. They found that when a unique class of ferroelectric oxides are stretched or compressed, the polarization does not simply increase as expected. Instead, it goes away completely.

"Based on everything we have known for the past two decades," Rondinelli said, "this is completely unexpected."

Supported by the National Science Foundation, the research is described in the June 13 issue of *Nature Materials*. Xue-Zeng Lu, a PhD student in Rondinelli's laboratory, served as the paper's first author.

Ferroelectrics are found everywhere: in smart phones, watches, and computers. Because they are so technologically useful, researchers have



long been interested in creating new or improved <u>ferroelectric materials</u> —especially in two-dimensional geometries as thin films where they are readily integrated into electronic devices. Ferroelectricity is a property that occurs when a material exhibits a spontaneous electric polarization, which arises from is a shift of positive and negative charges in opposite directions.

When strain is applied to the class of oxides called layered perovskites grown as a thin film, they initially react the same way as other ferroelectrics. Their polarization increases. But if further strain is applied, the polarization completely turns off.

Layered perovskites have recently seen a resurgence of attention because they host functional physical properties like high-temperature super conductivity and support electrochemical or photocatalytic energy conversion processes. Their structures are also much more defect tolerant. Rondinelli's discovery adds a new level of interest to these popular materials.

"You can't strain the material too much because it might lose its functionality," Rondinelli said. "But if you operate near where the polarization turns on and off, you really have a switch. If you're monitoring the <u>polarization</u> for a logic device or memory element, you can apply a small electric field to traverse this boundary and simultaneously read and write the on-and-off state."

Rondinelli's team made this discovery using a theoretical materials tools and quantum mechanical simulations and is now working with experimental collaborators to validate the finding in the laboratory. Another next step is to better understand how this new functionality could help or hinder ferroelectric applications.

In the meantime, Rondinelli said researchers will now need to be careful



when applying <u>mechanical stress</u> to layered perovskite ferroelectrics. Applying too much strain could have unintended consequences.

"This finding motivates us to recalibrate our intuition regarding what interactions are expected between mechanical forces and dielectric properties," Rondinelli said. "It requires us to think more carefully, and I suspect there is much more to learn."

More information: Epitaxial-strain-induced polar-to-nonpolar transitions in layered oxides *Nature Materials* (2016) DOI: 10.1038/nmat4664, www.nature.com/nmat/journal/va t/full/nmat4664.html

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