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Domain wall fluctuations in 2D materials reveal a new mechanism of superconductivity

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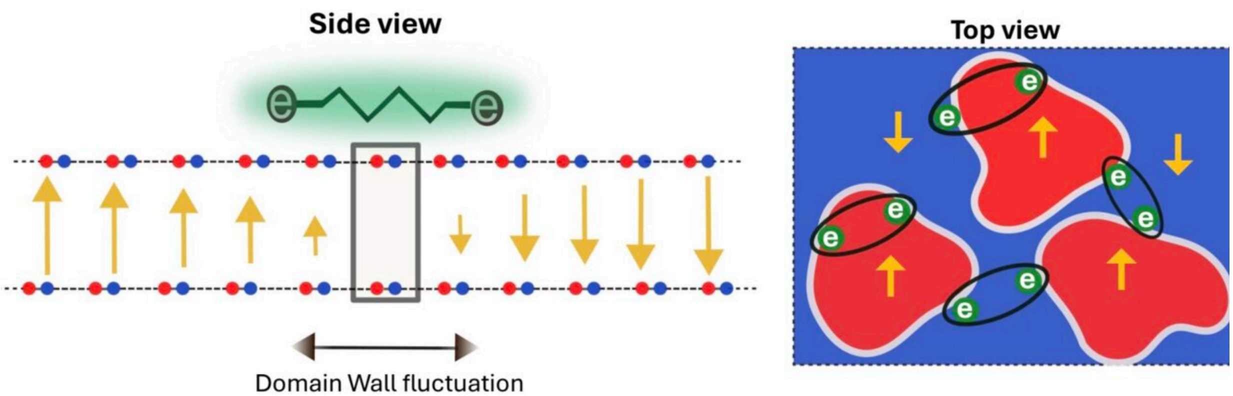

Credit: Chaudhary & Martin.

Two-dimensional (2D) van der Waals are made of atomically thin layers, held together by weak van der Waals forces. These materials have been the focus of numerous studies, as their unique properties make them ideal for studying various exotic and rare physical phenomena.

Gaurav Chaudhary and Ivar Martin, two researchers at the University of Cambridge and Argonne National Laboratory, respectively, set out to further investigate a particular type of 2D van der Waals material, namely 2D materials without an inversion center (i.e., a symmetry in which two halves of a material mirror one another).

Their paper, published in *Physical Review Letters*, unveiled the existence of an intriguing link between ferroelectric domain walls and electron interactions in some of these materials.

"A large number of few-layer van der Waals materials, including boron nitride and transition metal dichalcogenides (TMDs), show the curious phenomenon of sliding ferroelectricity," Chaudhary and Martin told Phys.org.

"Despite being metallic, due to the chemistry and structure of these systems, different layer stackings can have built-in electric polarization, i.e., interlayer electric field and charge imbalance. What is particularly striking is that by applying a moderate external electric field, it is possible to change the stacking on a fairly large scale, thus reversing the direction of polarization."

Different stacks in 2D van der Waals materials affected by this phenomenon, dubbed "sliding ferroelectricity," are related by a large, device-scale shift of two layers by several angstroms. Past studies have shown that this effect can persist at room temperature.

"This phenomenon has attracted the interest of scientists trying to understand the microscopic mechanism of these transformations, as well as engineers eager to find applications of this remarkable phenomenon," said Chaudhary and Martin.

"Just like in ferromagnets and bulk ferroelectrics, an energetically efficient way to reverse polarization is by having a domain wall sweep through the system. The spatial dimensionality of a domain wall is one less than that of the material (a 2D surface in the case of 3D bulk materials and 1D for thin films). "

A domain wall is a boundary or interface separating regions inside a material that exhibit different orientations of ferroelectric polarization or other properties. This unique boundary realizes a saddle point of free energy density, as opposed to a minimum.

As a result of this, the properties of domain walls can differ significantly from those of the original bulk materials they are in and of materials with reduced spatial dimensionality. In particular, these interfaces can exhibit a unique form and large in-strength electron-phonon coupling.

"Our project focusing on the interplay between sliding FE and superconductivity came out in the following way," explained Chaudhary and Martin.

"We were thinking about a number of curious aspects of ferroelectricity in bilayers of van der Waals materials, including graphene, which was completely unrelated to superconductivity. However, as we started to gain some understanding of the so-called 'sliding ferroelectric' phenomena, it occurred to us that there could be an interesting coupling with electrons near the ferroelectric domain walls."

While they were theoretically exploring the underpinnings of "sliding ferroelectricity," the researchers observed hints of this phenomenon in the material $MoTe_2$. Specifically, they found that the superconducting Tc is strongly enhanced in this material at the FE reversal transition.

"The enhancement is 'transient' and it is seen within the hysteresis loop, that is when the system contains domains of both orientations and domain walls separating them," said Chaudhary and Martin.

"So, we followed our curiosity, and luckily, it turned out that the situation near the domain walls is quite suitable for pairing interactions, which are required for superconductivity."

Overall, the findings of the recent work by Chaudhary and Martin demonstrated that the domain wall region in 2D TMD materials is in fact extremely special. In this region, electronic density couples to polarization directly, as it creates a potential drop between the layers of these materials.

"The center of the domain wall is defined by the absence of polarization, and naively, one could expect that there the coupling between polarization and itinerant electrons should vanish," said Chaudhary and Martin.

"This is indeed the case for static coupling; however, superconductivity is driven by dynamical fluctuations. The lattice vibrations in the domain wall region, which affect the relative position of layers (the stacking), lead to fluctuations of polarization (or are equivalent to fluctuations in the position of the domain wall)."

After closely studying 2D TMDs, Chaudhary and Martin were able to better understand the 'sliding ferroelectricity' they exhibit. This allowed them to devise a theoretical methodology outlining the physical processes behind this phenomenon.

"Once we understood this system and had a physical picture of what could be happening, the theoretical methodology was straightforward, from the standard treatment of electron-phonon or electron coupling to a soft boson (some kind of low-energy vibrations) in the many-body physics textbooks," explained Chaudhary and Martin.

"It did take us some time to understand what microscopic interactions can look like. The systems are highly irregular in the physical setup with domain walls compared to standard textbook setups of uniform systems."

Notably, the mechanism that gives rise to superconductivity studied by Chaudhary and Martin is unique to 2D TMDs with a few layers. This is because only these materials can support interlayer ferroelectricity while remaining conductive within 2D planes.

"The physical conditions realized within these domain walls are very special, enabling strong electron-electron interactions even if the dynamical glue is more or less standard lattice vibrations," said Chaudhary and Martin. "This makes for a conceptually new mechanism of superconductivity."

Generally, superconductivity arising from the coupling of electrons and phonons is viewed as a conventional physical mechanism. To characterize unconventional mechanisms, on the other hand, physicists seek strong electron-electron interactions. The superconductivity observed by Chaudhary and Martin sits somewhere in between conventional and unconventional mechanisms.

"We showed that places like domain walls, typically associated with irregularities and potentially harmful for things like superconductivity, can indeed be helpful for superconductivity," said the researchers.

This study could soon inspire other research groups to investigate the emergence of superconductivity in 2D TMDs and other bilayer van der Waals materials. Meanwhile, the researchers plan to continue investigating the domain wall-related superconductivity that they uncovered.

"There are plenty of things that need to be figured out, as well as a lot of new opportunities in applications," they said. "First, we still need to think of more direct ways to establish the validity of our theoretical ideas in real systems. These efforts would benefit from microscopic modeling using first-principles methods."

The researchers suggest that indirect signatures of the domain wall fluctuation-related superconductivity may already exist in a recent experimental study carried out by another team at Columbia, UW Madison and the University of Minnesota, focusing on the material $MoTe_2$.

In their next studies, the researchers also plan to investigate the possibility of leveraging this superconductivity to develop various superconducting devices.

"From the application point, we are exploring whether there is a possibility of highly controllable superconducting devices, where manipulating the ferroelectric order switches superconductivity on and off," added Chaudhary and Martin.

"We also anticipate that new superconductors can be designed systematically by putting polar layers on top of each other. We also expect similar mechanisms to be operational in moiré systems where domain walls form a regular network."

More information: Gaurav Chaudhary et al, Superconductivity from Domain Wall Fluctuations in Sliding Ferroelectrics, *Physical Review Letters* (2024). DOI: 10.1103/PhysRevLett.133.246001.