Study uncovers the fundamental mechanisms underlying the formation of polarons in 2D atomic crystals

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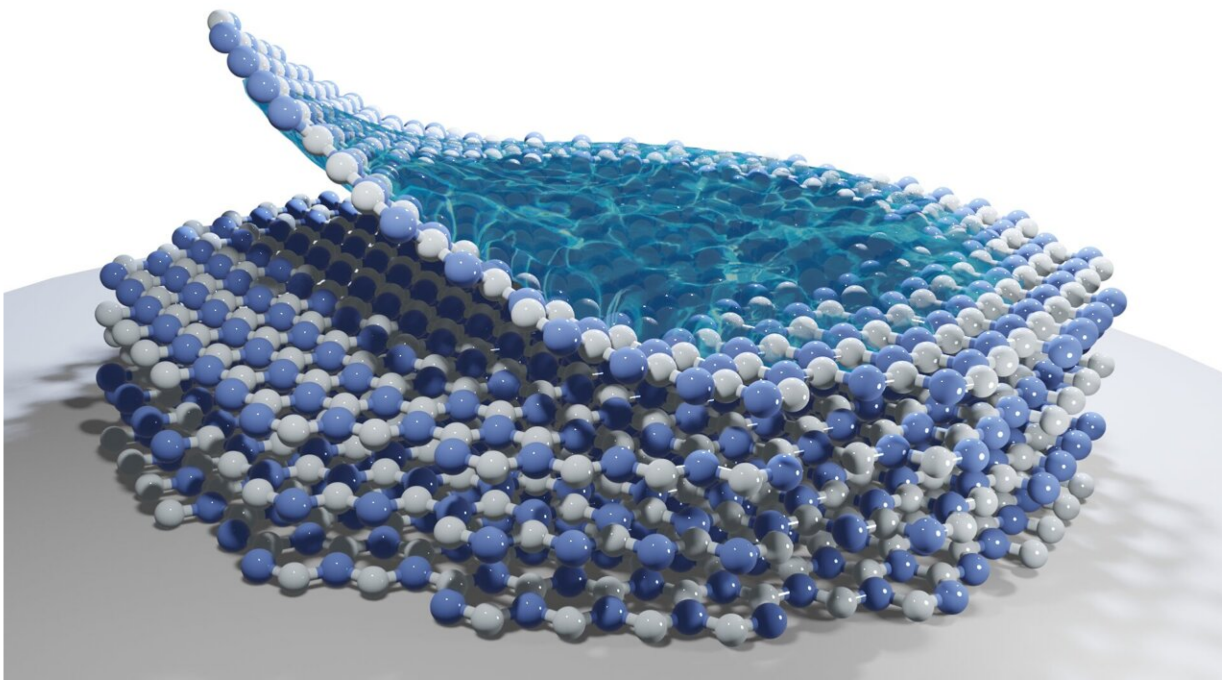


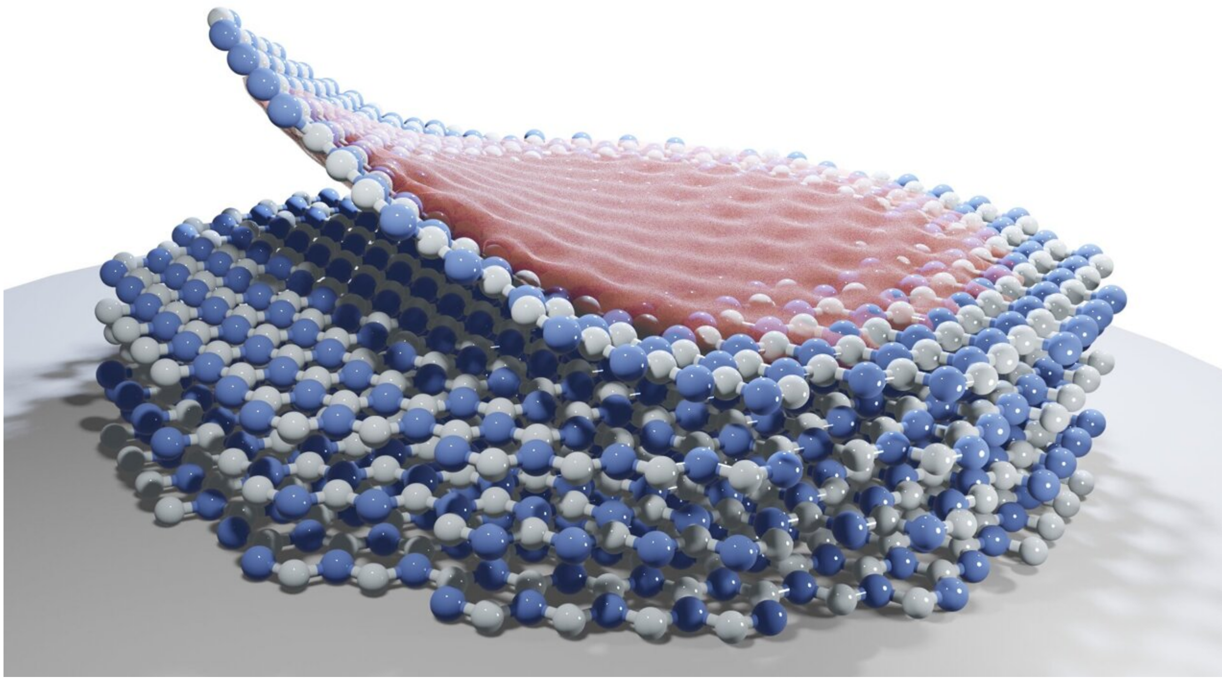
Schematic visualization of a polaron in monolayer hexagonal boron nitride. Credit: Feliciano Giustino

Polarons are localized quasiparticles that result from the interaction between fermionic particles and bosonic fields. Specifically, polarons are formed when individual electrons in crystals distort their surrounding atomic lattice, producing composite objects that behave more like a massive particles than electron waves.

Feliciano Giustino and Weng Hong Sio, two researchers at the University of Texas at Austin, recently carried out a study investigating the processes underpinning the formation of polarons in 2D materials. Their paper, published in *Nature Physics*, outlines some fundamental mechanisms associated with these particles' formation that had not been identified in previous works.

"Back in 2019, we developed a new theoretical and computational framework to study polarons," Feliciano Giustino, one of the researchers who carried out the study, told Phys.org. "One thing that caught our attention is that many experimental papers discuss polarons in 3D bulk materials, but we could find only a couple of papers reporting observations of these particles in 2D. So, we were wondering whether this is just a coincidence, or else polarons in 2D are more rare or more elusive than in 3D, and our recent paper addresses this question."

Initially, Giustino and Sio set out to compute the shape (i.e., wavefunction) and stability (i.e., energy) of localized polarons in 2D materials at the atomic scale. This is a challenging endeavor, as it entails describing all the atoms and electrons involved in the formation of polarons, which cannot yet be efficiently done using computers.



Schematic visualization of a polaron in monolayer hexagonal boron nitride. Credit: Feliciano Giustino

"For example, the polarons considered in this study involve up to 30,000 atoms," Giustino explained. "Our strategy was to reformulate the problem in the language of density-functional perturbation theory, a technique that has successfully been used for many years to study lattice vibrations (i.e., phonons). This technique allows us to capture the physics of polarons while bypassing the need for direct calculations with thousands of atoms. The other important ingredient was to figure out how to describe the interaction between electrons and vibrations in 2D."

In a paper published last year, Giustino and Sio introduced a new approach for describing the interaction between electrons and vibrations in 2D materials, which essentially entails figuring out the electrostatics of point dipoles in 2D. In their recent study, they used this approach along with density-functional perturbation theory to investigate the mechanisms underpinning the formation of polarons in 2D crystals.

"We clarified the fundamental mechanisms whereby a polaron form in 2D materials, so this work will be useful to understand these particles more broadly," Giustino said. "In particular, beyond our heavy-duty quantum-mechanical calculations, we developed a simple model that allows us to draw a map of where to find these particles and what their properties would be."

Using the model they created, Giustino and Sio were able to determine the real-space structure of a hole polaron in hexagonal boron nitride that was reported in recent research. In addition, they uncovered crucial conditions and laws that underpin the formation of polarons to form in 2D crystals.

"Polarons are drawing increasing attention because they are found in materials used for OLED screens, photocatalysis and even materials for future neuromorphic computers, so we hope that this study will help researchers to attain a deeper understanding of these particles and possibly even tune their properties to realize more efficient materials and devices," Giustino added. "We now plan to use these tools to investigate a broader family of materials. We would also like to understand how these particles respond to electric and magnetic fields and how one could leverage their unique properties to realize new functionalities."

More information: Weng Hong Sio et al, Polarons in two-dimensional atomic crystals, *Nature Physics* (2023). DOI: 10.1038/s41567-023-01953-4