Superproperties in 2D

Simulations suggest that new nanostructured materials capable of storing information can be developed

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Calculations performed by a team of theoretical physicists working in São Paulo and Singapore suggest that a one-atom-thick tin oxide film (SnO) can have extraordinary mechanical and magnetic properties. Materials consisting of a single layer of atoms are called two-dimensional because they have width and depth, but negligible height. In recent years, such materials have attracted the interest of theoretical and experimental researchers because of the electrical, magnetic, mechanical and optical properties they can display. Tin oxide, for example, whose atomic structure is shown on the left of this page, could become an exciting new nanotechnology if its recently-discovered properties are confirmed in laboratory tests. For example, it may be possible to use tin oxide to manufacture nanometer scale devices for storing data.

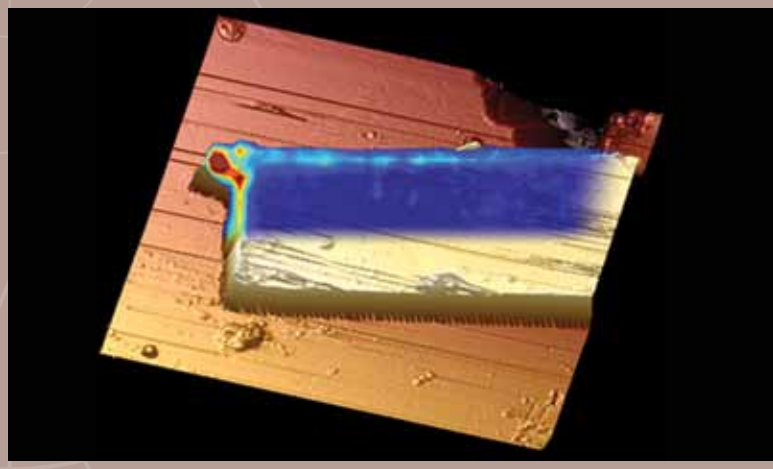
"The mechanical and magnetic properties of a monatomic layer of tin oxide depend on its electric charge," explains physicist Leandro Seixas, professor at the Center for Graphene, Nanomaterials and Nanotechnologies Research Center (MackGraphe) at Mackenzie Presbyterian University, which was officially inaugurated in March 2016 in São Paulo. Seixas is the lead author of a theoretical study that was published in May 2016 in the *Physical Review Letters* journal, which shows that by altering the electric potential of this material, one can control its atomic arrangement and the degree of magnetization. "This is the first time that the existence of a two-dimensional material with this behavior has been predicted," says Seixas, who conducted the study together with Aleksandr Rodin, Alexandra Carvalho and Antônio Castro Neto, all physicists at the 2D Advanced Materials Center and the Graphene Research Center at the National University of Singapore (NUS). In addition to directing these centers, Castro Neto is the principal investigator of the "Graphene: Photonics and optoelectronics. UPM-NUS Collaboration" project, which is part of the FAPESP São Paulo Excellence Chair (SPEC) program, based at MackGraphe.

A great transformation occurs when blocks of certain solid materials are sliced in the laboratory into finer and finer layers until the smallest possible thickness is reached. This is what physicists Andre Geim and Konstantin Novoselov discovered in 2004 when they exfoliated graphite, the mineral used in pencils, until they produced a sheet with a single layer of carbon atoms: this layer is called graphene. Although graphene is flexible and smooth like a sheet of paper, it is stronger than steel. It can also conduct electricity thousands of times more efficiently than silicon, the raw material in all current electronic technology, although

graphene does not allow good control of electrical current flow. This characteristic makes it difficult to manufacture a computer transistor using graphene. Since 2004, however, other materials have been identified that, under special conditions, are able to overcome these limitations. Ways to improve the fit between graphene sheets and other two-dimensional structures are also being studied in order to combine the advantageous properties of various materials.

One of the most widely studied alternatives to graphene is a layer of molybdenum sulfide (MoS_2) that is three atoms thick and was discovered in 2005. More recently, in 2014, researchers also discovered that black phosphorus, a synthetic material composed solely of phosphorus atoms, can be exfoliated until it forms a monatomic layer known as phosphorene. Similar to MoS_2, both phosphorene and black phosphorus, composed of only a few atomic layers, have some optical and electronic properties that are superior to those of graphene.

The differences between black phosphorus and graphene have not yet been completely uncovered. Experiments carried out in 2016 at MackGraphe by the group led by physicist Christiano de Matos, together with researchers at the Theoretical Physics Institute at São Paulo State University (Unesp), the Physics Department of the Federal University of Minas Gerais (UFMG), and the NUS 2D Advanced Materials Center, revealed that the atoms along the edge of black phosphorus layers can vibrate in a manner quite different from the edge atoms of graphene. Described in an article published in July 2016 in *Nature Communications*, these edge vibrations affect how black phosphorus dissipates heat and scatters light. It is difficult to say whether the changes in vibration would aid or inhibit the design of nanotechnological devices such as transistors or light sensors. "What is clear," says Matos, "is that the design of any device has to take these edge vibrations into consideration."



A crystal of black phosphorus: the colors on the upper edge indicate the intensity of vibrations (*greater intensity in the red regions*)

TWO-DIMENSIONAL MEMORY

Experimental physicists have obtained increasingly thinner layers of SnO in the laboratory, demonstrating that the material, depending on its thickness, can be an excellent semiconductor or an electrical insulator. "The hope is that some experimental group will develop a monatomic layer of SnO before the end of 2016, which will allow us to confirm our predictions," says Seixas.

Tin oxide has magnetic properties when sliced to atomic thickness

Supercomputer simulations of the behavior of the atoms show that, depending on the amount of electric charge on a monatomic layer of SnO, the material becomes a magnet whose poles can be controlled. If this control is feasible in experiments, it is possible that the magnetism can be used to store information in a tin oxide surface, similar to what occurs in the hard drive of current computers. Seixas and his colleagues also demonstrated that this property is not necessarily exclusive to SnO. They predict that other materials, such as gallium sulfide (GaS) and gallium selenide (GaSe), could also be magnetized in a similar way if they are produced with two-dimensional layers.

"The magnetization of two-dimensional materials is unusual," says Seixas. He explains that, although the edge atoms in the layers of pure materials such as black phosphorus and graphene can be magnetized under special circumstances, the center of these layers can be magnetized only through the addition of impurities, such as cobalt atoms.

The calculations performed by Seixas' team also suggest that, depending on the amount of electric charge circulating in the two-dimensional material, the atomic arrangement of the SnO layer could sustain spontaneous deformation, which could also lead to some technological applications. The squares formed by the arrangement of tin and oxygen atoms can be stretched, forming rectangles. "As with magnetization, these deformations can become controllable by changing the electric charge density of the material," he explains. "However, unlike with magnetization, we do not know how to explain the origin of these deformations, nor if they will appear in other materials." ■

Projects

1. Graphene: Photonics and optoelectronics. UPM-NUS Collaboration (No. 2012/50259-8); **Grant Mechanism:** SPEC program; **Principal Investigator:** Antonio Helio de Castro Neto (Mackenzie Presbyterian University); **Investment:** R$13,110,474.99 (for the entire project).
2. Plasmonic and nonlinear effects in graphene coupled to optical waveguides (No. 2015/11779-4); **Grant Mechanism:** Research grant—Thematic Project; **Principal investigator:** Christiano José Santiago de Matos (Mackenzie Presbyterian University); **Investment:** R$832,300.86
3. ICTP South American Institute for Fundamental Research: a regional center for theoretical physics (No. 2011/11973-4); **Grant Mechanism:** Research grant—Thematic Project; **Principal investigator:** Nathan Jacob Berkovits (Unesp); **Investment:** R$5,393,992.00.

Scientific articles

SEIXAS, L. et al. Multiferroic Two-Dimensional Materials. **Physical Review Letters**, V. 116, p. 206803. May 20, 2016.
RIBEIRO, H. B. et al. Edge phonons in black phosphorus. **Nature Communications**. July 14, 2016.

IMAGES 1 LEANDRO SEIXAS / MACKGRAPHE **2** CHRISTIANO DE MATOS / MACKGRAPHE