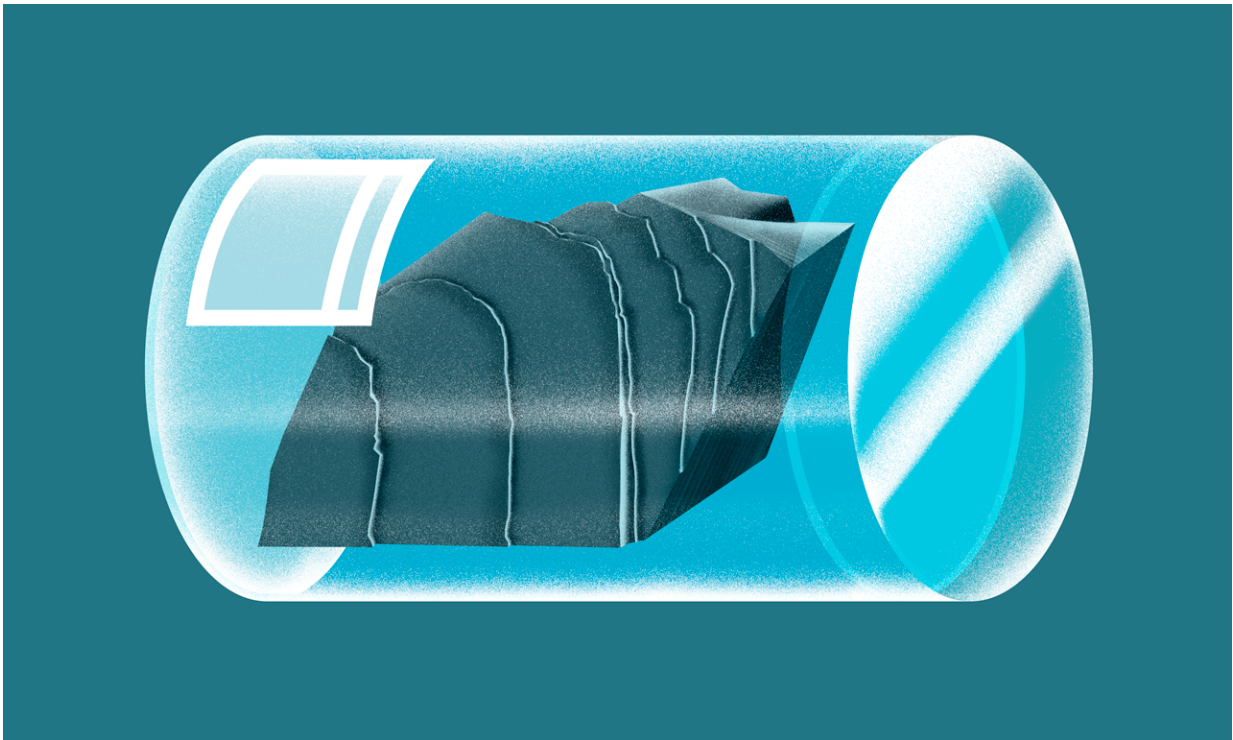


# Physicists predict nonmetallic half-metallicity

September 15 2017

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Credit: MIPT

A team of researchers of the Russian Academy of Sciences (RAS), in collaboration with a colleague from RIKEN (Institute for Physical and Chemical Research in Japan), has provided theoretical proof of the existence of a new class of materials, spin-valley half-metals. Their paper was published in the journal *Physical Review Letters*. The

discovery has potential applications in implantable electronics and devices based on graphene, nanotubes, and a number of other promising materials.

The microscopic mechanism proposed by the researchers differs significantly from the usual half-metal model based on a strong electron-electron interaction. This might give rise to a new direction in search for "nonmetallic" half-metals, i.e., those that do not contain atoms of [transition metals](#) such as nickel, manganese and lanthanum. Such [materials](#) would be useful in [implantable devices](#) and systems. The authors use the term "spin-valley-tronics" to refer to this possible alternative to traditional electronics.

As electronics become smaller and more densely organized, it is highly challenging to continue increasing the number of transistors or the microprocessor clock rate. So researchers around the globe are exploring new possibilities. One of them is spintronics, which makes use of electron spins and already has some important practical applications. Around the turn of the century, the use of giant magnetoresistance materials in magnetic field sensors (used to read data in hard disk drives) has enabled the storage of much larger amounts of data on HDDs.

Half-metals are believed to have great potential in spintronics. They were first predicted based on computer simulations and later proved to exist experimentally. In a half-metallic material, [electrons](#) of only one spin orientation—e.g., spin up—participate in the electric current. The energy of spin-down electrons is too high, and therefore they cannot carry charge current. This means that when the current is passed through a half-metal, a spin-polarized current is generated, as well. But spin-valley-tronics seeks to manipulate not only a spin-polarized population of electrons in the current but also the so-called valley index.

The term "valley" is borrowed from semiconductor physics.

Mathematically, the excitation energy in a solid is expressed by  $E(k, n)$ , where  $k$  is the momentum of the electron and  $n$  is the zone index, i.e., a discrete quantum property of the state of the electron. This function may look rather odd, and in the case of several minimums with comparable excitation energies, there are multiple "valleys." Essentially, electrons whose states correspond to one of the valleys do not interact with electrons from another valley. Such an ensemble of electrons can carry not only spin and charge, but also a distinct value called the valley index.

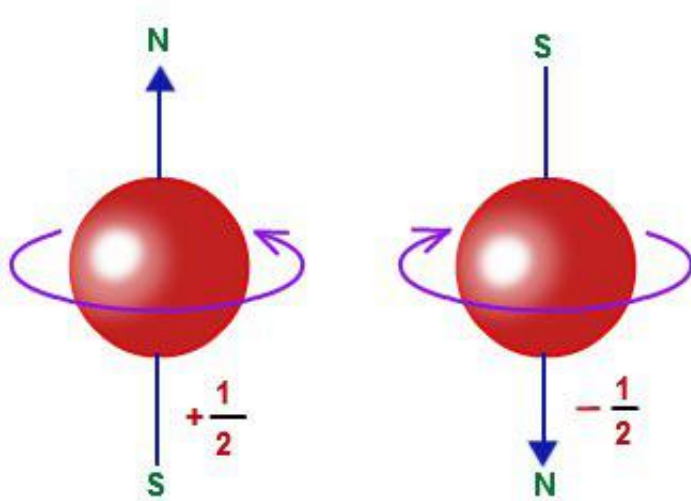


Fig. 1. The term “spin” refers to the intrinsic angular momentum of a particle. The spin of a particle has both a magnitude and a direction. In the case of the electron, the magnitude is  $1/2$  times Planck’s constant, and the direction is either up or down. Credit: 10.1103/PhysRevLett.119.107601

The valley index can be used to transfer information with the help of valley currents—in this regard, the valley index is quite similar to spin. Research in this direction is currently being carried out by several groups. The researchers have now theoretically proved the existence of a novel class of materials for use in spin-valley-tronics.

The half-metals available to the researchers all contain atoms of transition metals: nickel, manganese, lanthanum, etc. The researchers demonstrated a theoretical mechanism for achieving half-metallicity that requires no transition metal atoms. This has a number of useful applications, including in implantable devices.

The physicists suggest that such nonmetallic half-metals be obtained from a special class of dielectric materials called charge- or spin-density wave insulators. The term refers to a state with periodic microscopic regions with nonzero average charge (spin) in the material. Theorists describe such systems as a quantum condensate of electron-hole pairs. For a pair of this kind to form, two valleys are required: One provides electrons, the other provides holes. It is the presence of two valleys in the original system that gives rise to spin-valley half-metallicity. In semiconductor physics, a "hole" is a quasiparticle that is considered to have a positive charge.

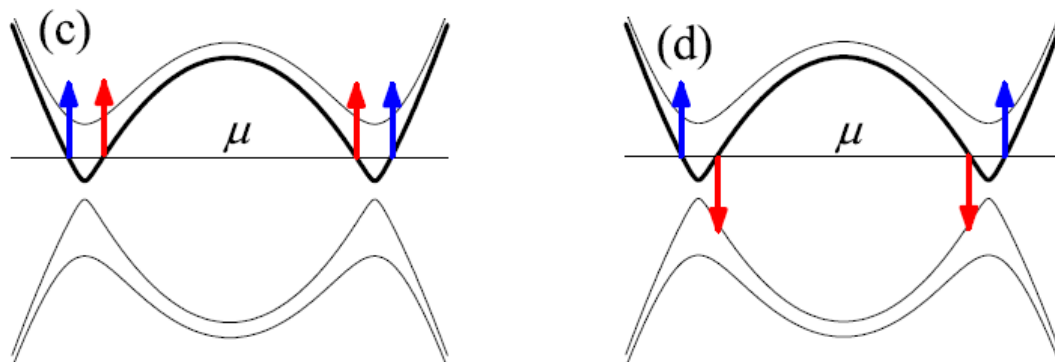


Fig.2. In the figure, electron and hole energy is plotted against momentum. (The four black curves correspond to two projections of electron spin and two projections of hole spin.) The thick curve corresponds to electron states capable of conducting an electric current (forming a Fermi surface). Depending on the mutual orientation of the spins of electrons (blue arrows) and holes (red arrows) on the Fermi surface, the system is either an ordinary half-metal (c) or a spin-

valley half-metal (d). Credit: 10.1103/PhysRevLett.119.107601

For a material with a density wave to become a half-metal, it requires a special treatment known as doping. This involves the incorporation of electrons or holes into the insulator. Alexander Rozhkov, a co-author of the paper and a researcher at MIPT's Department of Problems of Physics and Energetics, explains that a system can be doped by subjecting it to an external electric field or chemical modifications of bulk or surface: "For each system, a suitable type of doping atom—such as nitrogen, phosphorus, or some other element—needs to be selected. By replacing atoms of the host system with impurities donating or accepting conduction electrons, a change in the properties of the original material is induced."

The possibility of doping materials with density waves has been discussed in the literature for a long time. The systems dealt with by the researchers have various phases, including spatially inhomogeneous—for example, states with the so-called electronic phase separation, and the phases with domain walls, often called "stripes." Now, the researchers have made the unexpected discovery of two new phases—regular and spin-valley half-metallicity.

Artem Sboychakov, one of the authors of the paper and a senior researcher at ITAE RAS, said, "In a way, our discovery proved to be a surprise even to ourselves. The physical model that, we found, has a spin-valley half-metallic phase is a classical one—it has been studied for decades. It is now up to the experimenters. There are plenty of materials adequately described by the model we dealt with. I am therefore convinced that the phase we predicted will eventually be discovered, either in a material that is available today or in one that is yet to be synthesized."

**More information:** A. V. Rozhkov et al, Spin-Valley Half-Metal as a Prospective Material for Spin Valleytronics, *Physical Review Letters* (2017). [DOI: 10.1103/PhysRevLett.119.107601](https://doi.org/10.1103/PhysRevLett.119.107601)

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