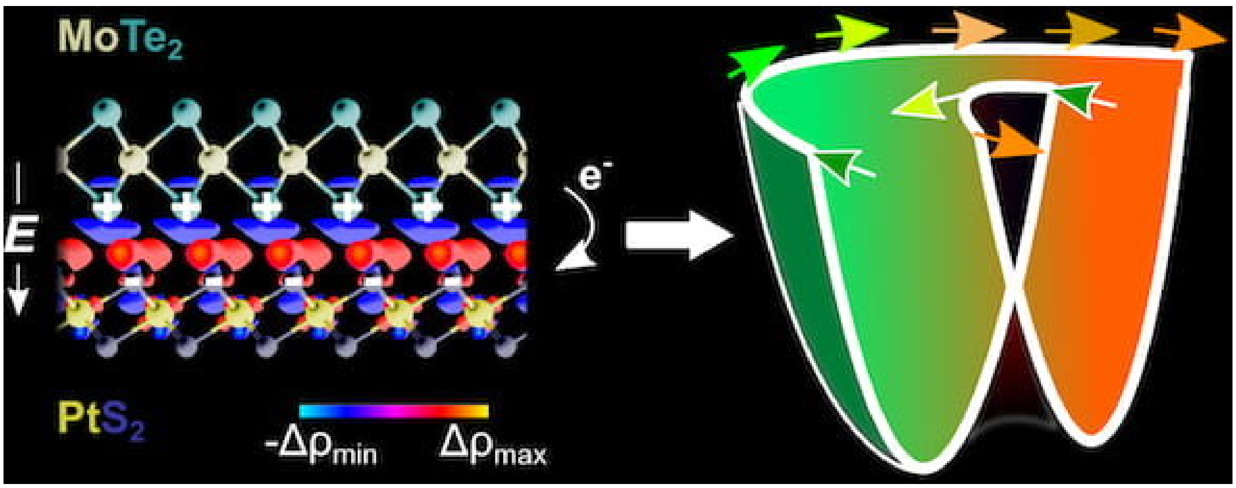
Theory could accelerate push for spintronic devices

February 25 2021



he image at left shows the crystal structure of a MoTe2|PtS2 heterobilayer with isocharge plots from a model created at Rice University. When the materials are stacked together, mirror symmetry is broken and there is a charge transfer that creates an intrinsic electric field. This field is responsible for Rashba-type spin-splitting shown by the band structure at right, where the spin is perpendicular to momentum. Credit: Sunny Gupta

A new theory by Rice University scientists could boost the growing field of spintronics, devices that depend on the state of an electron as much as the brute electrical force required to push it.

Materials theorist Boris Yakobson and graduate student Sunny Gupta at

Rice's Brown School of Engineering describe the mechanism behind Rashba splitting, an effect seen in crystal compounds that can influence their electrons' "up" or "down" spin states, analogous to "on" or "off" in common transistors.

'Spin' is a misnomer, since quantum physics constrains electrons to only two states. But that's useful, because it gives them the potential to become essential bits in next-generation quantum computers, as well as more powerful everyday electronic devices that use far less energy.

However, finding the best materials to read and write these bits is a challenge.

The Rice model characterizes single layers to predict heteropairs—two-dimensional bilayers—that enable large Rashba splitting. These would make it possible to control the spin of enough electrons to make room-temperature spin transistors, a far more advanced version of common transistors that rely on electric current.

"The working principle behind information processing is based on the flow of electrons that can be either off or on," Gupta said. "But electrons also have a spin degree of freedom that can be used to process information and is the basis behind spintronics. The ability to control electron spin by optimizing the Rashba effect can bring new functionality to electronic devices.

"A cellphone with spin-related memory would be much more powerful and much less energy-consuming than it is now," he said.

Yakobson and Gupta would like to eliminate the trial and error of finding materials. Their theory, presented in the *Journal of the American Chemical Society,* aims to do just that.

"Electron spins are tiny magnetic moments that usually require a magnetic field to control," Gupta said. "However, manipulating such fields on the small scales typical in computing is very difficult. The Rashba effect is the phenomenon that allows us to control the electron spin with an easy-to-apply electric field instead of a magnetic field."

Yakobson's group specializes in atom-level computations that predict interactions between materials. In this case, their models helped them understand that calculating the Born effective charge of the individual material components provides a means to predict Rashba splitting in a bilayer.

"Born effective charge characterizes the rate of the bond polarization change under external perturbations of the atoms," Gupta said. "When two layers are stacked together, it effectively captures the resulting change in lattices and charges, which brings about the overall interlayer polarization and interface field responsible for the Rashba splitting."

Their models turned up two heterobilayers—lattices of $MoTe_2|Tl_2O$ or $MoTe_2|PtS_2$—that are good candidates for the manipulation of Rashba spin-orbit coupling, which happens at the interface between two layers held together by the weak van der Waals force. (For the less-chemically inclined, Mo is molybdenum, Te is tellurium, Tl is thallium, O is oxygen, Pt is platinum and S is sulfur.)

Gupta noted the Rashba effect is known to occur in systems with broken inversion symmetry—where the spin of the electron is perpendicular to its momentum—that generates a magnetic field. Its strength can be controlled by an external voltage.

"The difference is that the magnetic field due to the Rashba effect depends on the electron's momentum, which means the magnetic field experienced by a left-moving and right-moving electron is different," he said. "Imagine an electron with spin pointing in the z-direction and moving in the x-direction; it will experience a momentum-dependent Rashba magnetic field in the y-direction, which will precess the electron along the y-axis and change its spin orientation."

Where a traditional field-effect transistor (FET) turns on or off depending on the flow of charge across a barrier with gate voltage, spin transistors control the spin precession length by a gate electric field. If the spin orientation is the same at the transistor's source and drain, the device is on; if the orientation differs, it's off. Because a spin transistor does not require the electronic barrier found in FETs, it needs less power.

"That gives spintronic devices an enormous advantage compared to conventional charge-based electronic devices," Gupta said. "Spin states can be set quickly, which makes transferring data quicker. And spin is nonvolatile. Information sent using spin remains fixed even after a loss of power. Moreover, less energy is needed to change spin than to generate current to maintain electron charges in a device, so spintronics devices use less power."

"To the chemist in me," Yakobson said, "the revelation here that spin-splitting strength depends on the Born charge is, in a way, very similar to the bond ionicity versus the electronegativity of the atoms in Pauling's formula. This parallel is very intriguing and deserves further exploration."

More information: Sunny Gupta et al, What Dictates Rashba Splitting in 2D van der Waals Heterobilayers, *Journal of the American Chemical Society* (2021). DOI: 10.1021/jacs.0c12809

Provided by Rice University