X-RAY PEAKS POINT THE WAY TO UNDERSTANDING HELICAL BEHAVIOR

Titanium diselenide (1*T*-$TiSe_2$) consists of hexagonal layers of titanium (Ti) lying between similar layers of selenium (Se), thus forming Se-Ti-Se sandwiches separated by relatively large gaps. Despite this simple lattice structure, 1*T*-$TiSe_2$ exhibits complex behavior at low temperatures due to the emergence of charge-ordered states resulting from electron shifts that give rise to a chiral (helical) charge density distribution. To learn more about the transition from the normal state to the chiral charge-ordered state, researchers subjected single crystals of $TiSe_2$ to 80-keV x-rays at the XSD 6-ID-D beamline of the APS and followed up with analyses of the temperature dependences of the specific heat, resistivity, and resistance anisotropy of the crystals. The research indicated that the normal state gives way to a nonchiral charge density wave state at about 190K, before transforming to a chiral charge-ordered state at about 183K.

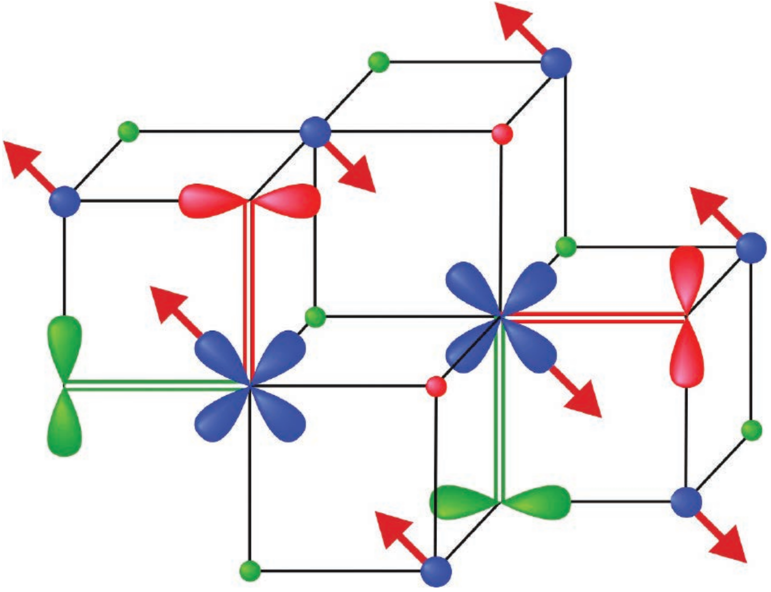

Fig. 1. One of the three components contributing to the proposed chiral CDW state in $TiSe_2$. The specific orbitals involved in the charge transfer process for this component are indicated (in blue for Ti and red and green for Se). The combination of orbital order and CDW formation allows the formation of the chiral charge and orbital ordered state.

$TiSe_2$ has long intrigued scientists because it exhibits so-called charge density waves (CDWs) at low temperatures, whose origin is still being debated. In the CDW phase, a three-component variation in the charge density occurs, with each component being related to a charge transfer process between one particular Ti-3*d* orbital and two Se-4*p* orbitals (Fig. 1). This charge ordering is accompanied by lattice distortions. If the three components of the variation superimpose without any relative phase differences between them, a nonchiral CDW state is produced. When there are phase shifts, the three components superimpose to form chiral lattice distortions.

Detailed order parameter measurements of the transition from the normal state to the charge-ordered phase showed that a nonchiral CDW phase transition occurs at T_{CDW} = 190K. The researchers then discovered previously unobserved x ray diffraction peaks having intensities about fifty times weaker than the primary CDW peaks, while searching for evidence of the emergence of helical ordering below T_{CDW}. Measurements of one of the weak peaks indicated that it evolved differently with decreasing temperature than the primary CDW peaks, suggesting the onset of a different type of order at $T_{chiral} \approx$ 183K.

The temperature dependence of the specific heat of $TiSe_2$ crystals cut from the same samples used in the x-ray diffraction experiments showed an anomaly around 190K related to the nonchiral CDW transition. Below this temperature, the specific heat changed linearly with temperature until about 182K, when a change in slope was seen, indicating a change in the thermodynamic state of the sample.

The two principal components of the resistivity were also measured as a function of temperature. The derivatives of both curves displayed sharp minima at T_{CDW}. Moreover, the resistivity anisotropy showed a sharp peak at 183K.

The researchers in this study, from the University of Bristol (UK), Drexel University, Cornell University, and Argonne concluded that the low-temperature chiral charge-ordered state in 1*T*-$TiSe_2$ arises in a sequence of two

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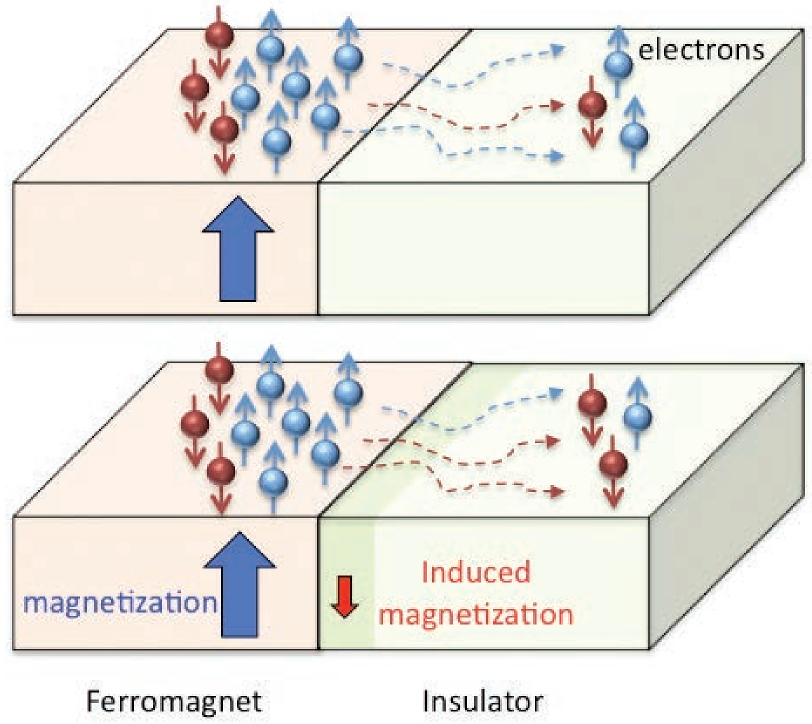

Fig. 2. The effect of induced magnetization on electron tunneling. (Top) The populations of spin-up and spin-down electrons are reduced as electrons tunnel from the ferromagnetic manganite layer on the left into the insulating cuprate layer on the right. (Bottom) The ratio between spin-up and spin-down is strongly affected by the induced magnetization at the cuprate's interface and can even be reversed, as shown here.

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magnetization is antiparallel to the magnetization of the manganite.

The cuprate's antiparallel magnetization makes it harder for the manganite's majority-spin electrons to tunnel through, so more minority-spin electrons reach the other side (Fig. 2). By acting as a negative spin filter, the interfacial region of the cuprate comes into competition with the manganite's high positive spin polarization. This competition gives the magnetoresistance of the magnetic tunnel junction a more complex temperature dependence than had previously been suspected, causing an overall decrease at low temperatures.

Knowing how the induced magnetization affects the transport of electrons may have valuable spintronic applications. By tuning the interface's magnetization, researchers can construct oxide structures with desirable electronic properties. *— Sophie Bushwick*

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closely separated phase transitions. The first transition, at $T_{CDW} \approx 190$K, involves the onset of a nonchiral charge-ordered state. The second transition, which the researchers identified to occur at $T_{chiral} \approx 183$K, is characterized by the emergence of previously unobserved diffraction peaks, a sudden change in slope of the specific heat, and a sharp peak in the resistivity anisotropy.

This sequence of two transitions leading first from the normal state to the nonchiral CDW state and only then to the chiral charge-ordered state agrees with theoretical predictions put forward previously by one of the authors. In that theoretical model, the possibility of forming the novel chiral CDW state in TiSe$_2$ is explained by the simultaneous formation of orbital order. A direct prediction of the theory of coupled charge and orbital order is that the chiral state cannot emerge directly from the disordered state, but rather has to go through a sequence of two closely separated phase transitions, as observed in the current experiments.

— Vic Comello

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