The exciting story of $TiSe_2$

One of the most beautiful theories of condensed matter is certainly the theory of conventional superconductivity. Called the BCS theory after the names of the creators (Bardeen, Cooper and Schrieffer), it explains the zero resistance appearing in particular materials when their temperature approaches absolute zero. In the BCS theory, electrons are bound together by an attractive interaction and form pairs which will condense into a macroscopic quantum state at low temperature. Since breaking such a pair costs energy, it is more favorable for the system to let them flow without losses, giving rise to conductivity with zero resistance.

Recently, scientists from Neuchâtel in collaboration with the PSI [1] unveiled a similar mechanism in the layered compound $TiSe_2$: here such a pairing is also at play, but between particles of different types. This material has also intrigued scientists for a long time because it exhibits so-called charge density waves (CDWs) at low temperature, the origin of which has held out against a detailed explanation. In a CDW phase, electrons reorganize themselves and deviate from their initial highly uniform density, displaying a new periodicity different than that of the original atomic lattice. In some cases, this rearrangement is accompanied by a periodic lattice deformation, so that the total energy in the system is lowered. The key aspect to understand about a CDW transition is the nature of its driving force. In the case of $TiSe_2$, this issue was under discussion for a long time. Now, strong evidence has been found for the identification of an exotic ground state, the excitonic insulator phase [2].

$TiSe_2$ has an electronic structure near the Fermi energy comparable to that of a semiconductor, but its valence and conduction bands are slightly overlapping through an indirect gap. In the case of the excitonic insulator phase, the Coulomb interaction, weakly screened due to the low free carrier density, is strong enough to bind together an electron in the conduction band and a hole in the valence band. This bound pair is called an exciton. This bond, however, can be easily broken by thermal energies, hence excitons only exist a low temperatures, above which the holes and electrons move independently.

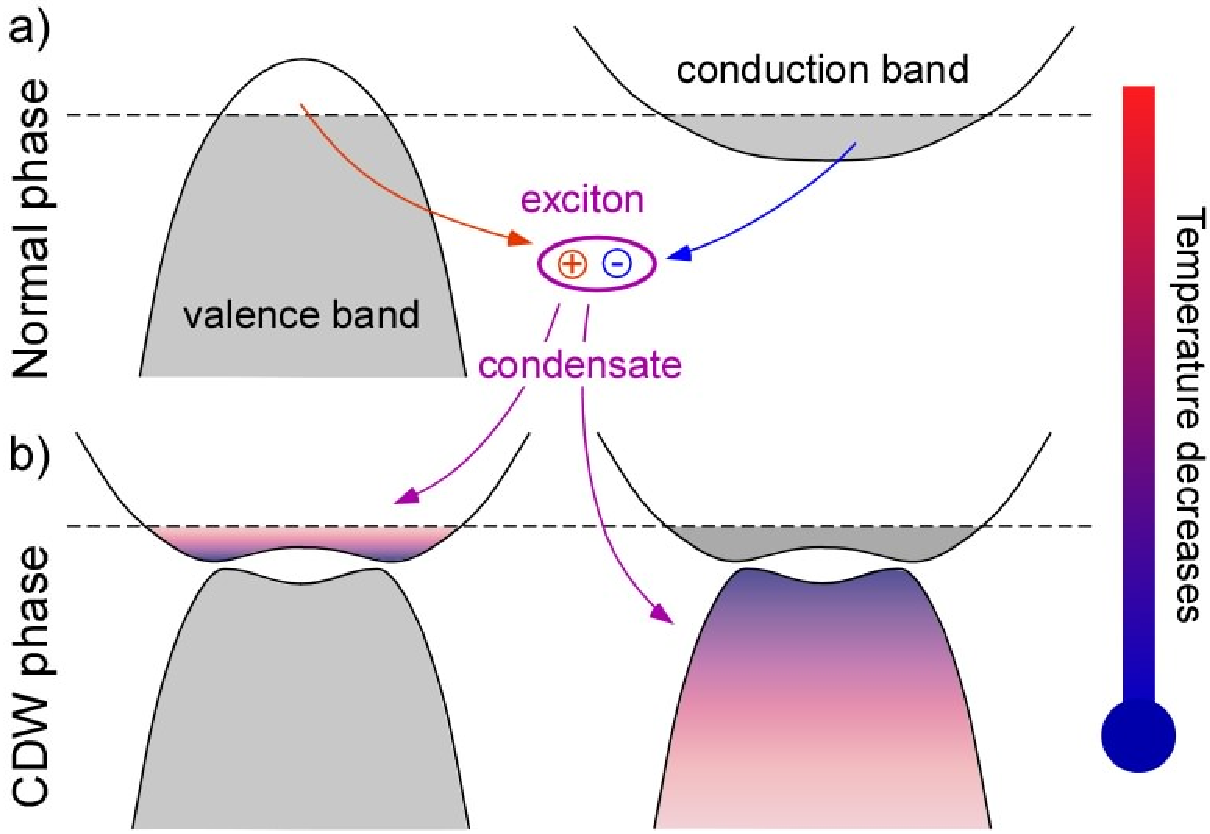

Figure 1: *Schematic picture of the CDW phase transition in the excitonic insulator phase model. At high temperature (a), the electronic structure of $TiSe_2$ near the Fermi energy consists of a valence band and a conduction, which overlap slightly and indirectly. At low temperature (b), excitons, consisting of holes in the valence band and electrons in the conduction band, condense in a macroscopic quantum state, leading to the CDW phase.*

However, once the temperature is lowered, a scenario similar to BCS superconductivity occurs, as illustrated schematically in figure 1. Since the valence and the conduction bands overlap indirectly, excitons will form spontaneously and, under the pressure of their growing population, they will condense into a macroscopic state. Due to the nature of excitons, this state induces a new periodicity in the system arising naturally as the distance between the valence and the conduction bands. In other words, exciton condensation can lead the system towards a CDW phase with a purely electronic origin.

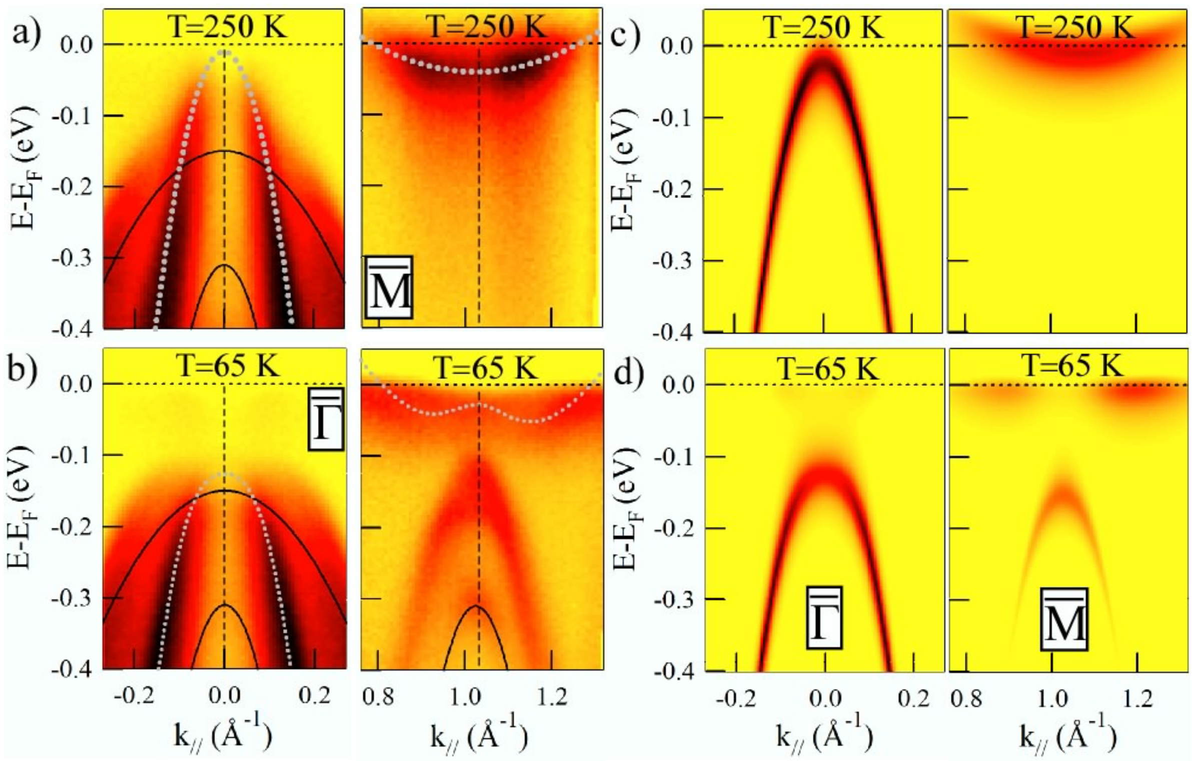

Figure 2: *Figure (a) and (b) show the angle-resolved photoemission spectroscopy data taken at the SIS beamline of the SLS on* 1T-*$TiSe_2$ samples. At a temperature of 250K (a), the system is in the normal phase, above the transition. At 65K (b), it is in the CDW phase where one clearly sees at the border of the Brillouin zone (the so-called M point) replica of the bands originally situated in the center of the Brillouin zone (the Γ point). The right part of the figure shows the simulated intensity maps derived from the excitonic insulator model, above (c) and below (d) the CDW transition. The very good agreement between experiment and simulation gives strongly supports the hypothesis that the low temperature ground state of* 1T-*$TiSe_2$ is the excitonic insulator phase.*

So far, so good. But how can one prove the existence of such a mechanism in $TiSe_2$? At this point, photoemission comes into play. This experimental technique uses the photoelectric effect, whereby the energy gained by absorbing a photon can kick out electrons from a solid. By collecting these electrons and measuring their velocity, one can infer valuable information about the electronic structure of the solid. In the case of $TiSe_2$, excitons leave a particular trace on the spectra, which can be compared to theory by computing the corresponding spectral function, a quantity intimately related to photoemission. Based on the excitonic insulator model, scientists from Neuchatel simulated photoemission spectra, which exhibited a very good agreement with experiment and consequently lent strong evidence for an excitonic origin in the CDW phase of $TiSe_2$. Photoemission data together with their corresponding simulations are reproduced in figure 2.

[1] H. Cercellier *et al.*, Phys. Rev. Lett. **99**, 146403 (2007)
[2] D. Jérome *et al.*, Phys. Rev. **158**, 462 (1967)