

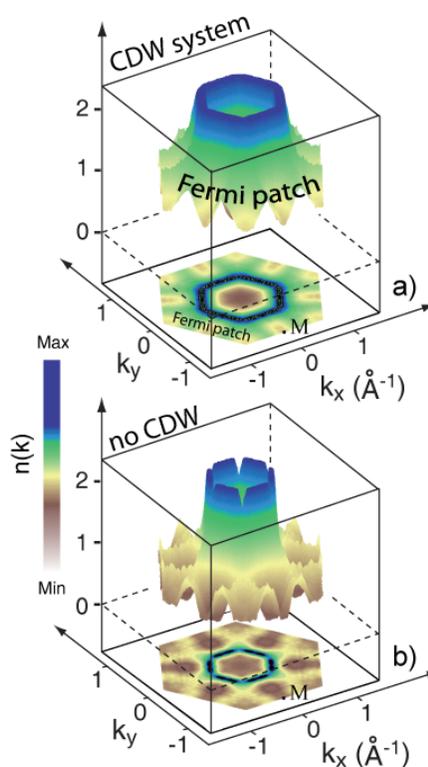
## A New Mechanism of Charge Density Wave Discovered in Transition Metal Dichalcogenides

Charge density waves (CDW) are a type of coupled electronic-lattice instability found in quasi-low dimensional materials. The driving force behind the instability is the reduction in energy of electrons in the material as a consequence of establishing a spontaneous periodic modulation of the crystalline lattice with an appropriate wave vector. The symmetry of the CDW state is very sensitive to the electronic structure of the host material. Charge density wave has been observed in quasi-one dimensional compounds, high temperature superconductors, manganites and many others.<sup>1-4</sup> Conventionally, Fermi surface nesting is the dominant and textbook mechanism for CDW. However, it fails to explain the CDW in the 2H-structured transition metal dichalcogenides (2H-TMD's), which is actually the first two-dimensional CDW materials discovered in 1975.<sup>5</sup> Even after three decades of intensive research on this subject, the CDW mechanism of 2H-TMD's remain mysterious and controversial.

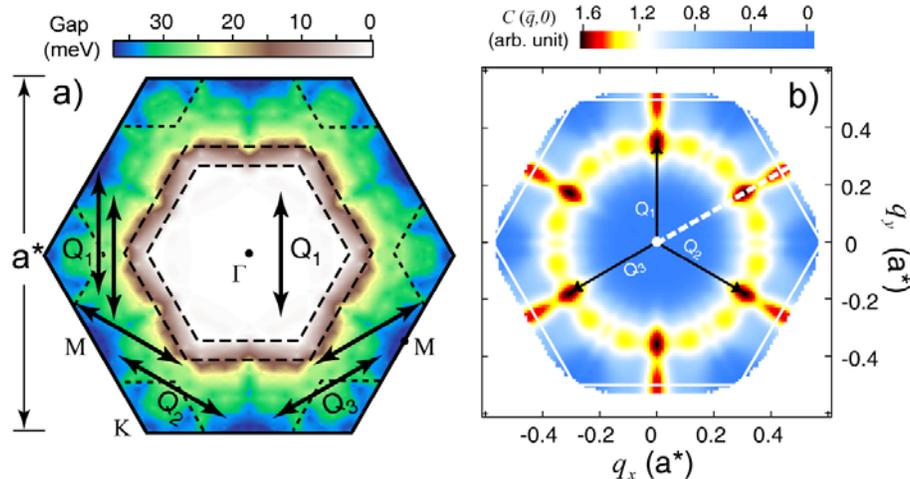
To understand the unusual CDW transition, it is crucial to obtain a comprehensive picture of the subtle low energy electronic structure changes upon the CDW transition. Combining the state-of-the-art electron analyzer and the intense photon beam from a synchrotron accelerator or a high flux helium discharge lamp, modern angle-resolved photoemission spectroscopy (ARPES) can now reach sufficiently high energy and momentum resolutions to address this issue.

Utilizing the high-resolution ARPES apparatus at beamline 5-4 of SSRL, scientists from the Department of Physics at Fudan University and SSRL have recently successfully resolved this long-standing mystery. They investigated the evolution of electronic structures of the 2H- $\text{Na}_x\text{TaS}_2$  compounds, where the strength of CDW can be tuned upon adjusting the doping concentration of the alkali metal elements.

They found that the strong electron-phonon coupling in this system makes the electrons widely spread in the momentum space. At the Fermi energy, the states locate not only at the conventional Fermi surfaces, but also over other large regions in the Brillouin zone for the CDW samples, forming the so-called "Fermi patches" (Figure 1); and the system with CDW order has more states over the Fermi patches than the system without CDW order. Further experiments revealed that a CDW gap opens over the Fermi patches, but not at the Fermi surfaces around  $\Gamma$  as shown in Figure 2(a). This undoubtedly indicates that the electronic states over the Fermi patches are responsible for the CDW.



**Figure 1.** The photoemission intensity map taken at 15K for (a)  $\text{Na}_{0.05}\text{TaS}_2$  with CDW order below 65K, and (b)  $\text{Na}_{0.1}\text{TaS}_2$  without CDW order.



**Figure 2.** (a) The distribution of the CDW gap in the first Brillouin zone of  $\text{Na}_{0.05}\text{TaS}_2$ . The dashed lines are the conventional Fermi surfaces. (b) The two-dimensional joint density-of-states of the ARPES intensity in the normal state of  $\text{CDW}^{65\text{K}}$ .  $Q_1$ ,  $Q_2$ , and  $Q_3$  are the ordering wave-vectors.

To explain the  $3 \times 3$  CDW ordering in this material, the joint density-of-states over the entire Brillouin zone was estimated [Figure 2(b)], which reflects the phase space for charge instabilities.<sup>6</sup> The peaks at the right ordering wave-vectors prove that such charge ordering is indeed favored by the collective behavior of all the states at the Fermi patches. In this way, they resolved previous controversies and unveiled a new CDW mechanism in this material, namely, the Fermi-patch mechanism.

Because many complex materials bare similar electronic properties, such as Fermi patches and broad lineshapes, this Fermi-patch driven CDW mechanism may be a general theme for charge ordering in the strong electron-phonon coupling regime.

### Primary Citation

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