Comment on "Realization of a Metallic State in 1*T*-TaS_2 with Persisting Long-Range Order of a Charge Density Wave"

In a recent Letter, Zhu *et al.* [1] investigated the evolution of electronic states of the Mott and charge-density-wave (CDW) insulator 1*T*-TaS_2 with potassium adsorbates. They measured scanning tunneling spectroscopy (STS) spectra at different K coverages and argued the metallization of the whole system by K adsorbates. In this Comment, we argue that the experimental evidence of the metallization is not clear and the unconventional mechanism of the metallization proposed is not justified when the experimental and theoretical data are properly compared.

The first issue of Zhu *et al.*'s measurement is that the spectral weight at the Fermi energy is marginal [Fig. 2(a) of Ref. [1]] and the spectra have a V-shaped feature at the Fermi level. Thus, it is not clear whether the system is indeed metallic or not. Furthermore, no information is provided on where the STS data were taken. Since the STS measurement inherently has subatomic resolution and the system becomes inhomogeneous with K adsorbates, this information is crucial to understand the data. As Zhu *et al.*'s own theoretical calculation shows, the K adsorption bifurcates the unit cells into two groups, those with and without K adsorbates, which also have distinct spectral features. The experiment, however, does not tell where the very weak metallic spectral weight observed at the Fermi level comes from, making the discussion on its origin obscure. When the spectra are averaged over an area, one should consider the possible inclusion of the defective sites and areas with in-gap states [2,3]. When the spectra are obtained on specific points, one has to prove that those points properly reflect the global metallization of the system.

The second issue is that the authors' calculation does not provide any sign of the metallic state while it shows the formation of a new in-gap state away from the Fermi level [Fig. 4(a) of Ref. [1]]. Namely, the very weak spectral weight at the Fermi level is not explained in the authors' theory. Moreover, the theoretical and experimental data were not properly compared in the Letter. As Zhu *et al.* observed, the system is obviously doped by the K adsorption and the spectra have strong overall shifts. When this shift is considered as shown in Fig. 1, the corresponding in-gap state (the arrow) deviates farther away from the Fermi level. Theoretically speaking, the evolution of this in-gap state for such a high doping is not clear at all, making its relationship with the observed metallization, if any, totally uncertain.

Finally, we note that the spectra for the metallic state, claimed by the authors, show almost no spectral weight for the upper Hubbard band with the lower Hubbard band only broadened. This indicates that the Mottness of the system is apparently collapsed. Therefore, the spectral behavior observed cannot be properly termed as the "filling up of the Mott gap by the in-gap state." We thus argue that the experimental evidence of the metallization needs to be refined and that the proposed theory does not explain the observed spectral behaviors.

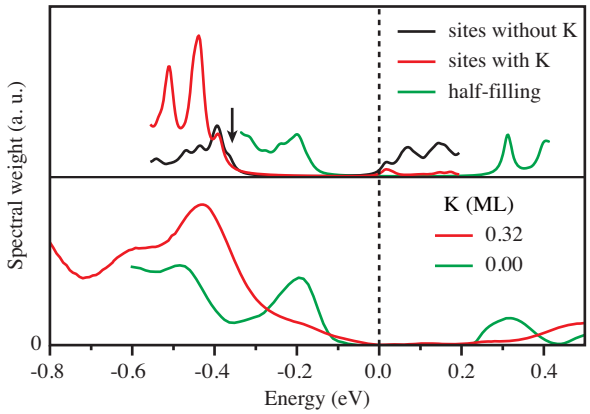

FIG. 1. Comparison between the theoretical calculations (upper) and experimental results (bottom) redrawn from Ref. [1]. An energy of the theoretical results for the K adsorption case (red and black curves) is adjusted to match the spectral features of the experiments, which accounts for the doping.

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