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## High Resolution Photoemission Investigation of Phase Transitions in 1T-TaS<sub>2</sub>.

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**Abstract.** Photoelectron spectroscopy with very high energy resolution reveals both dramatic and subtle changes in the electronic density of states of the quasi-2D material 1T-TaS<sub>2</sub>, in coincidence with transitions between different charge density wave phases. Our results are consistent with the occurrence of a zero-gap Mott transition at ~185 K and of a subsequent Anderson localization in the pseudogap between the Hubbard subbands, and provide new insight into the unusual electronic properties of this material.

The layered compound 1T-TaS<sub>2</sub> exhibits unique physical properties which are related to, but are not fully explained by, the presence of a charge density wave (CDW) with a complex phase diagram. Especially the tenfold increase in the resistivity observed at the transition from a *quasi-commensurate* (QC) to a commensurate (C) CDW structure calls for an explanation other than the simple opening of a Peierls gap over portions of the Brillouin zone. Previous photoelectron spectroscopy (PES) studies have provided experimental support to a model predicting the occurrence of a Mott localization in coincidence with the QC-C transition. However, the values of the Mott-Hubbard gap (100-200 meV) estimated from PES data are incompatible with the results of transport measurements, which suggest a gap of the order of 1 meV.

We have addressed this controversial issue by a careful investigation of the temperature dependence of the electronic density of states (DOS) in the various CDW phases. The selected results presented here concern the QC-C transition. Our high resolution ( $\Delta E \sim 15$  meV) PES spectra are very sensitive to small variations of the DOS occurring in the critical energy region, within a few  $k_B T$  of the Fermi level ( $E_F$ ), that determines the low-energy properties of the material. The dramatic effect that the QC-C transition produces on the DOS of 1T-TaS<sub>2</sub> is well illustrated by the valence band spectra of Fig.1, which show that the sample evolves from a metallic to an apparently semiconducting state in less than 5 degrees. The prominent structure observed at a binding energy of 180 meV in the 186 K spectrum corresponds to the occupied Hubbard subband on the nonmetallic side of the Mott-Hubbard transition, and its binding energy is a measure of the on-site Coulomb correlation ( $U$ ) in the Ta 5d band. Our results reveal the details of the growth and shift of this structure throughout the transition. We observe, at the transition temperature, a sharp

increase of the peak intensity, correlated with the resistivity jump, and with the sudden drop of the photoemission intensity at the Fermi level. This drop, reproduced in Fig.2, is a very direct evidence of the abrupt disappearance of most of the Fermi surface in coincidence with the QC-C transition. However, our results make clear that a finite electron density persists at  $E_F$  below the transition temperature and down to the experimental limit of 20 K. The separation of the Hubbard subbands is therefore incomplete and the Fermi level lies in a *pseudogap*. 1T-TaS<sub>2</sub> would therefore remain a metal, if localization due to disorder associated with the random distribution of impurities and defects, for which evidence exists from low-temperature resistivity data, did not occur in this pseudogap<sup>2</sup>, probably around 180 K. Our results show that the relevant energy scale for the transport properties of this material is not defined by the binding energy of the Hubbard subband ( $\sim U$ ) but by the difference between the Fermi energy and the mobility edge (which we estimate at  $\sim 5$ meV). They also demonstrate that PES with state-of-the-art resolution can greatly contribute to our understanding of Fermi surface driven electronic instabilities.

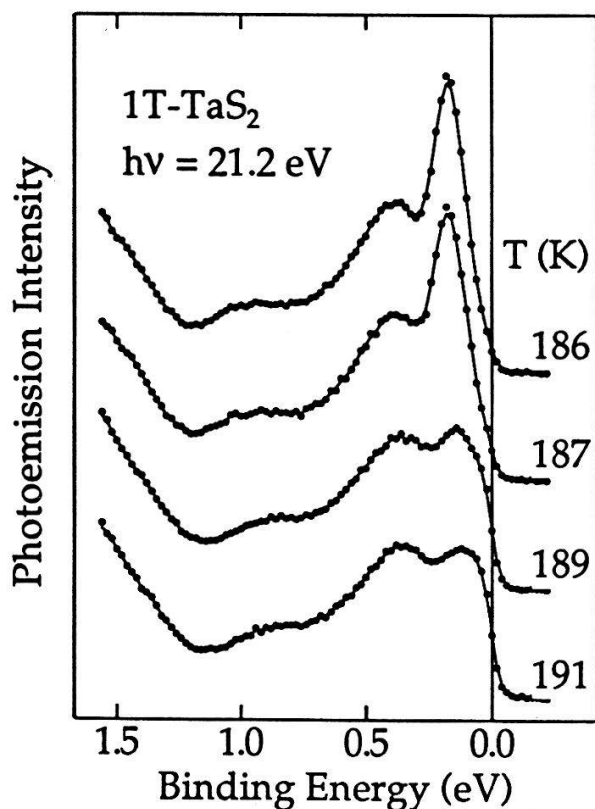


Fig.1. PES spectra of the valence band of 1T-TaS<sub>2</sub> through the QC-C CDW transition.

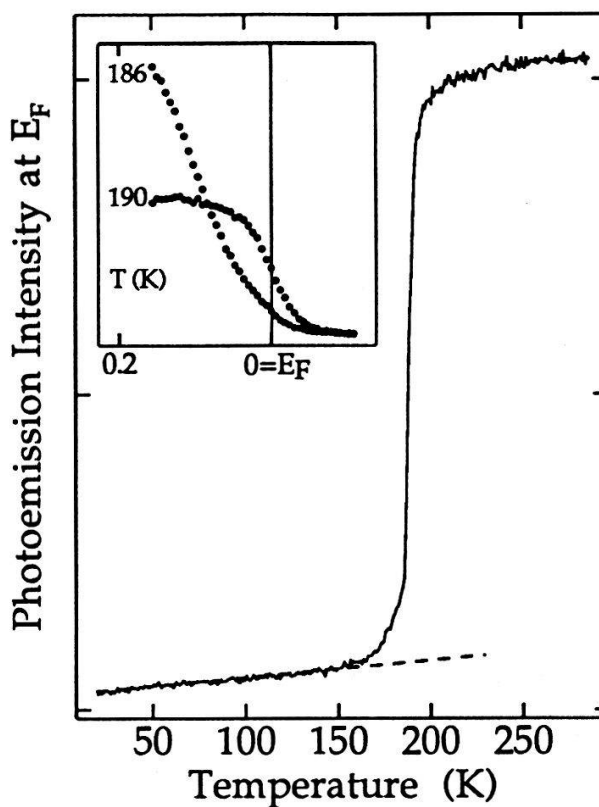


Fig.2. Temperature dependence of the PES intensity at  $E_F$ . Inset: Close-up of PES spectra near  $E_F$ .

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