Long-living metastable electronic states in substituted *1T*-TaS_2

G. Reecht[1], J. Jayabalan[1], R. Knipsis[2], V. Mondal[1], F.K. Diekmann[3], W. Schnelle[4], P. Zhou[1], K. Rossnagel[3], F. Queisser[2], R. Schützhold[2], M. Gruber[1], U. Bovensiepen[1]

[1]University of Duisburg-Essen, Fakultät für Physik and CENIDE
[2]Helmholz-Center Dresden-Rossendorf,
[3]Christian-Albrechts-University of Kiel and DESY
[4]MPI for Chemical Physics of Solids, Dresden

1T-TaS_2 is a prototypical strongly correlated material that has been extensively studied for its rich electronic phases [1]. At low temperature, it develops a commensurate charge density wave with a $\sqrt{13} \times \sqrt{13}$ superlattice, known as the "Star of David" (SD) structure, in which 12 Ta atoms contract slightly toward a central Ta atom. Each SD hosts a single valence electron at equilibrium; and owing to a strong on-site Coulomb repulsion exhibit a Mott insulating phase. Adding or removing electrons from individual SDs creates many-body excitations — doublons and holons, respectively—whose relaxation timescales lie in the tens of femtoseconds [2].

Here, combining time-resolved photoemission with low-temperature scanning tunnelling microscopy and spectroscopy (STM and STS), we investigate the impact of low-concentration substitution of Ta with an electron-richer element. Both techniques reveal the presence of long-lived metastable electronic states persisting up to hours. STM/STS measurements further evidence the localized nature of these excitations, while also showing that the substitution introduces disorder visible in both the structure of the charge density wave and the local density of states.

A theoretical description based on a Fermi-Hubbard model produces excitation spectrum in good agreement with the STS results. More strikingly, the disorder induced by the random substitution is shown to strongly spatially localize holons and doublons, prohibiting their annihilation and thereby rationalizing the very-long doublon lifetimes observed experimentally.

REFERENCES

1. Y Fei *et al.*, *AAPPS Bulletin*, **32**, 20 (2022)
2. M. Ligges *et al., Phys. Rev. Lett.*, **120**, 166401 (2018)