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Comparison between isovalent substitution and electron donor intercalation doping effects on the 1*T*-TiSe₂ charge density wave instability: A combined ARPES and STM study.

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This work presents an experimental study of the impact of isovalent substitution and donor intercalation on the charge density wave (CDW) instability of 1*T*-TiSe₂, with scanning tunneling microscopy (STM) and angle resolved photoemission spectroscopy (ARPES). In the quasi-two-dimensional layered material 1*T*-TiSe₂, a phase transition occurs around 200 K and results in a commensurate 2×2×2 CDW accompanied by a small periodic lattice deformation (PLD). In addition to this transition, this material becomes superconducting in the presence of copper intercalation or under pressure, which makes it particularly interesting in solid state physics and motivates the study of its behavior in the presence of various modifications.

Here, two types of doping are examined: sulfur atoms that replace selenium and have the same open shell structure, and titanium atoms intercalated between two Se-Ti-Se sandwiches which give extra electrons to the system. Although TiS_2 does not show any evidence of a phase transition, the 1*T*-TiSe₂ CDW seems robust against a relatively high sulfur concentration. On the contrary, only a small amount of intercalated titanium drastically affects the CDW coherence length and its appearance.

To understand and analyze the effects of these different types of doping, two experimental measurement methods were utilized: a STM that allows the imaging and characterization of the surface of samples in real-space and an ARPES experiment that probes the electronic band structure of 1*T*-TiSe₂ in reciprocal-space. STM images were obtained at 4.5 K, whereas ARPES measurements were obtained in the range between room temperature and 13 K. By characterizing samples with STM and then measuring them as a function of the temperature in ARPES, this work provides a complete and systematic study of the 1*T*-TiSe₂ behavior in the presence of intercalated titanium and sulfur substitutions and enhances our understanding of the CDW formation.

Jury:

Prof. Dr. Philipp Aebi (Thesis Supervisor)Prof. Dr. Christian Bernhard (Internal Expert)Prof. Dr. Hans Beck (External Expert)Dr. Matthias Hengsberger (External Expert)Prof. Dr. Joseph Brader (President of the Jury)