2025 Helmholtz – OCPC – Program

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Substitution- and pressure-dependent tuning of the charge density waves in ScV_6Sn_6

Helmholtz Centre and/or institute:

Karlsruhe Institute of Technology (KIT), Institute for Quantum Materials and Technologies (IQMT)

Project leader:

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Department: (at the Helmholtz centre or Institute)

Karlsruhe Institute of Technology (KIT), Institute for Quantum Materials and Technologies (IQMT)

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Description of the project (max. 1 page)**:**

A primary goal in the study of quantum materials is to identify how exotic quantum phases of matter emerge from the interplay between charge, spin, and lattice degrees of freedom. Especially, transition-metal-based kagome metals are of significant interest due to their potential to host a wide range of electronic instabilities. The unique electronic frustration arising from the triangular and hexagonal atomic arrangements in these systems gives rise to intriguing features such as Dirac nodes, van Hove singularities, and flat bands, which in turn can bring about topological phenomena, magnetism, superconductivity, and charge-density-wave (CDW) induced superstructures.

Among these materials, the hexagonal $RETM_6CG_6$-type (RE=rare earth, TM=transition metal, CG=carbon group) compounds form a large family characterized by two kagome layers per unit cell for which the ScV_6Sn_6 system is a notable exception, as it exhibits a CDW with a 3×3×3 superstructure below 92 K. With our high-resolution x-ray diffraction experiments we found that upon cooling from room temperature, diffuse peaks corresponding to a 3×3×2 superstructure occur and gradually intensify as the system approaches the phase transition. Directly at the phase transition, a competition is observed between the 3×3×2 and a 3×3×3 CDW, with the latter ultimately prevailing below the transition temperature. Preliminary results show that both CDWs are progressively suppressed by substitution, eventually becoming completely incoherent, which ultimately leads to the emergence of a quantum critical point.

The proposal aims to investigate the $RETM_6CG_6$ material group, focusing on how the substitution of various RE, TM, and CG elements affects the structural properties. Specifically, we want to understand how these structural modifications influence the CDW phenomena and the quantum critical behavior. Additionally, we will explore the impact of temperature- and pressure-induced instabilities on the crystal structure and their subsequent effects on the electronic properties of these materials.

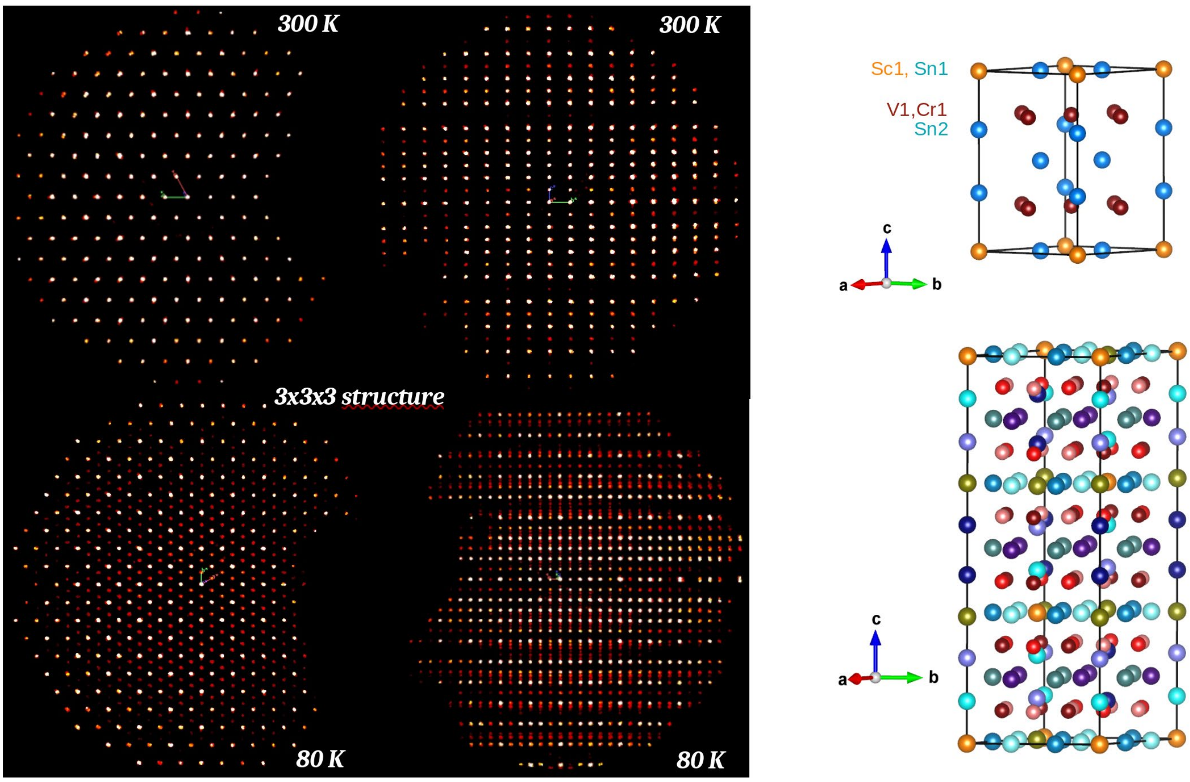

Figure 1: left) Reciprocal lattice of ScV_6Sn_6 along the c* and a* directions showing the 3x3x3 CDW for the low-T phase as derived from our XRD experiments, right) corresponding high- and 3x3x3

low-temperature structure of ScV_6Sn_6 refined from our XRD data.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

We aim to establish a bilateral fundamental research exchange with two different Chinese institutions: (i) the groups led by Profs. Aifeng Wang and Mingquan He at the Low Temperature Physics Laboratory, College of Physics & Center for Quantum Materials and Devices, Chongqing University, and (ii) the research group led by Prof. Guoliang Zhang at the Institute of Oceanology, Chinese Academy of Sciences (IOCAS). We have had a longstanding and fruitful collaboration with the groups at Chongqing University, where especially samples of many kagome systems – among them the substituted ScV_6Sn_6 samples - are prepared and studied using thermodynamic methods in Chongqing, while at the Institute for Quantum Materials and Technologies (IQMT), the samples are characterized using a variety of x-ray diffraction techniques and extensive crystallographic expertise. This collaboration is intended to be expanded further for mutual benefit in the long term within the framework of an OCPC proposal. Additionally, a new collaboration with the group at the Institute of Oceanology, Chinese Academy of Sciences, is to be established. A key focus of this institute is the synthesis of materials under extreme pressures, along with the measurement of their properties using high-pressure experimental techniques. However, the full potential of these synthesized materials can only be realized through precise structural characterization. This is where the XRD facility at the Institute for Quantum Materials and Technologies (IQMT) plays a crucial role. Equipped with multiple state-of-the-art x-ray diffractometers, the group ensures the highest standards in structural analysis. In both collaborations, the combined expertise allows for the identification of phase transitions and electronic properties crucial to understanding the material's behavior under extreme conditions. These partnerships are essential for bridging the gap between synthesis and characterization, aiming to establish a synergistic platform that advances fundamental material discovery and explores their structural and electronic properties under extreme environments.

Required qualification of the postdoc:

- PhD in condensed matter physics, chemistry, or materials sciences
- Experience in solid-state physics, single-crystal and powder x-ray diffraction, and crystallography
- Good knowledge of the English language