Structural evolution of the kagome superconductors through charge density wave order

Linus Kautzsch, Brenden R Ortiz, Krishnanand Mallayya, Jayden Plumb, Ganesh Pokharel, Jacob PC Ruff, Zahirul Islam, Eun-Ah Kim, Ram Seshadri, and Stephen D. Wilson

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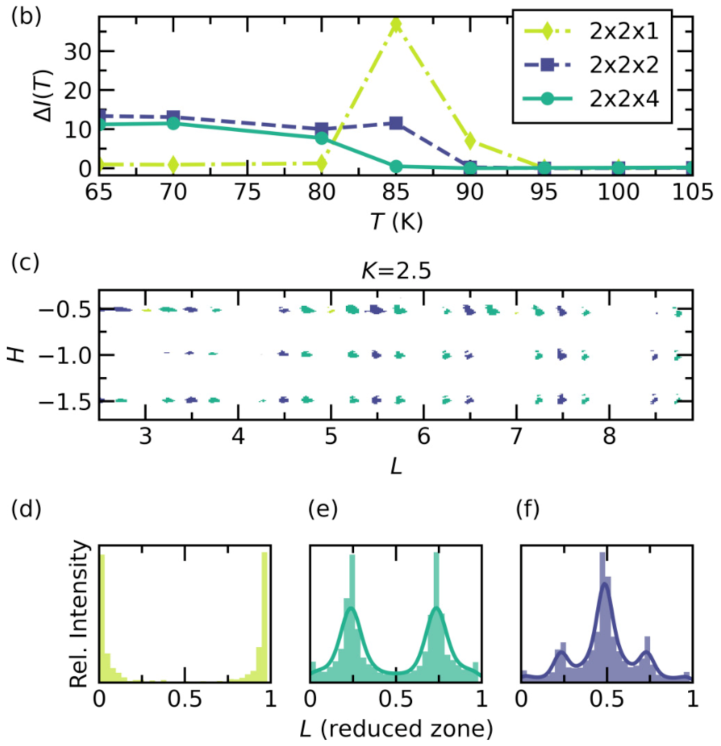
What is the discovery?

The charge density wave (CDW) instability is implicated in the unusual properties of many unconventional superconductors. This is particularly true for three newly discovered kagome superconductors, with chemical formula AV_3Sb_5, (A=K, Rb, or Cs). These materials have been under intense scrutiny by researchers at the Quantum Foundry at UCSB and elsewhere over the past 4 years. Now, a new paper appearing in *Physical Review Materials,* by a team from UCSB, Argonne National Lab, and Cornell, sheds new light on the structural evolution of kagome superconductors during CDW formation. Pristine crystals prepared at the Quantum Foundry were comprehensively characterized with x-rays over a wide range of temperatures at the QM2 beamline at CHEXS. The resulting trove of data was analyzed using a Cornell-developed unsupervised machine learning algorithm know as XTEC. Samples were also studied at the Advanced Photon Source using a unique pulsed-magnet system, to evaluate the response of the CDW state in high magnetic fields. This work reports definitive refinements of the CDW "supercell" in all three compounds. It also resolves a complex temperature evolution of ordering in the Cs compound. Finally, the team determines that the CDW state is robust in magnetic fields as high as 28 Tesla.

Why is this important?

The kagome metals offer a new playground for quantum materials research. Despite having a relatively simple and well-ordered high-temperature structure, the variety and complexity of competing quantum states at low temperatures is rich and surprising. A large community of researchers is assembling to study these effects. The goal is to understand, manipulate, and eventually exploit these new states for new quantum technologies. In order to do that, high-fidelity experimental measurements of high-quality samples are essential. Understanding the complex superstructure modulations is necessary for understanding the unconventional superconducting state which emerges in these materials, as well as other unexplained phenomena such as the observed large anomalous Hall effect.



Comprehensive data collection – measuring wide regions of reciprocal space for many different temperatures and chemical compositions – reveals subtle phenomena in the kagome SCs that would otherwise be overlooked. The XTEC machine-learning algorithm discovers signatures of 3 different CDW supercells (blue, green, and yellow clusters above) with unique temperature dependences in CsV_3Sb_5.

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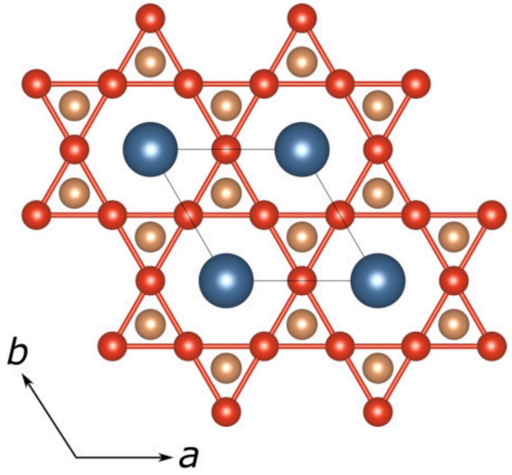
Why did this research need CHEXS?

Detailed studies of subtle structural distortions arising from CDW phases are a core capability of the QM2 beamline at CHEXS. Identifying the CDW superstructures in all 3 kagome SC materials required comprehensive diffraction data, collected at low temperature and with sensitivity to weak scattering features. All this is enabled by the high-dynamic-range mapping capabilities of QM2 (high energy x-rays with helium cryocoolers, large photon-counting area detectors and very low background). The high throughput capabilities at QM2 allow for screening large numbers of crystals quickly, which is essential for researchers who are developing & discovering new materials. These capabilities anchor a successful partnership between QM2 and researchers at the Quantum Foundry at UCSB. Furthermore, access to the XTEC unsupervised learning algorithm via collaboration with the E-A Kim group at Cornell was essential for unravelling the complex evolution of ordered states in CsV_3Sb_5. Finally, close collaboration demonstrated here between users of CHEXS (the future home of the High Magnetic Field beamline currently under construction) and Z Islam's group at the Argonne (home of the APS pulsed magnets) is critical for CHEXS long-term strategic mission to advance x-ray science at the high magnetic field frontier.

How was the work funded?

Q-AMASE-i: Quantum Foundry at UC Santa Barbara, NSF (DMR-1906325)
Materials Research Science and Engineering Center at UC Santa Barbara, NSF (DMR-1720256)
The Center for High Energy X-ray Sciences (CHEXS), NSF MPS/BIO/ENG (DMR-1829070)
The Center for Scientific Computing at UC Santa Barbara, NSF (CNS-1725797)
Gordon and Betty Moore Foundation's EPiQS Initiative (GBMF10436)
US Dept of Energy, BES (Advanced Photon Source & X-TEC Development)



Reference

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Physical Review Materials 7, 024806 (2023); https://doi.org/10.1103/PhysRevMaterials.7.024806