NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Revealing the magnetism of Weyl semimetal CeAlGe

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SURF Fellowship 2022 - NIST Center for Neutron Research
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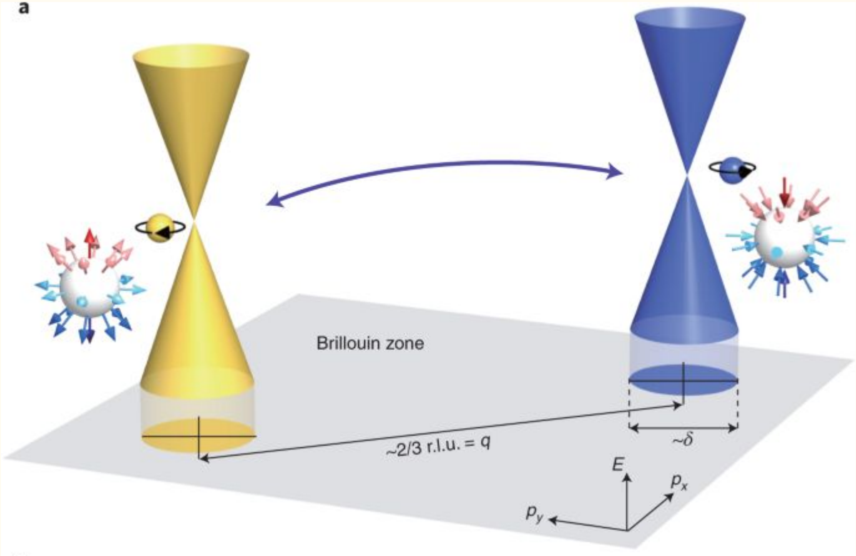
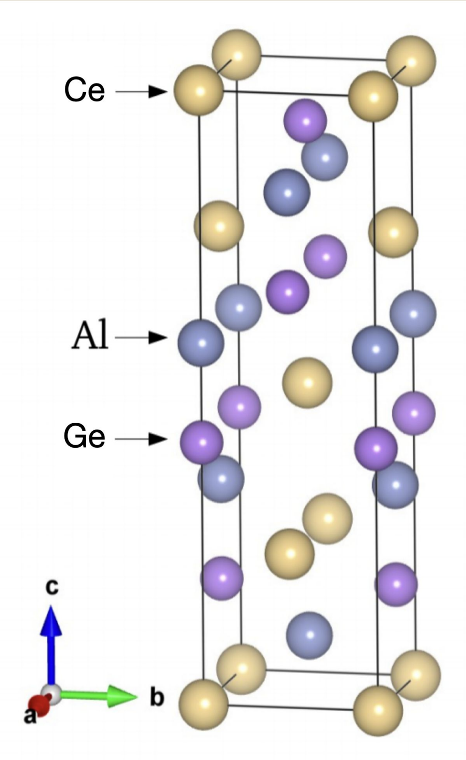
Weyl fermions are massless particles that possesses a high degree of mobility and chirality

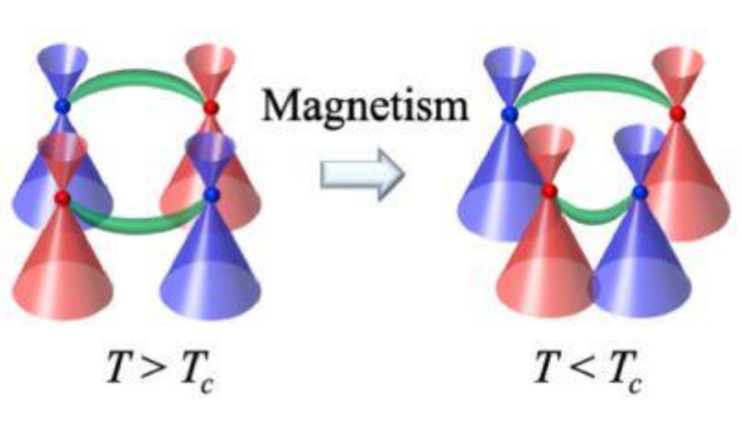


- Weyl Fermions move rapidly in the surface of the single crystal with no backscattering that inhibits efficiency (spin-momentum locking)

CeAlGe is a unique template to study Weyl fermions



- Weyl fermions are not naturally present in nature but in CeAlGe, they emerge as effective charge carriers that arise from breaking inversion and time-reversal symmetry.



Bulk heat capacity and magnetic susceptibility measurements both show the presence of a magnetic phase transition temperature at approximately 5K.

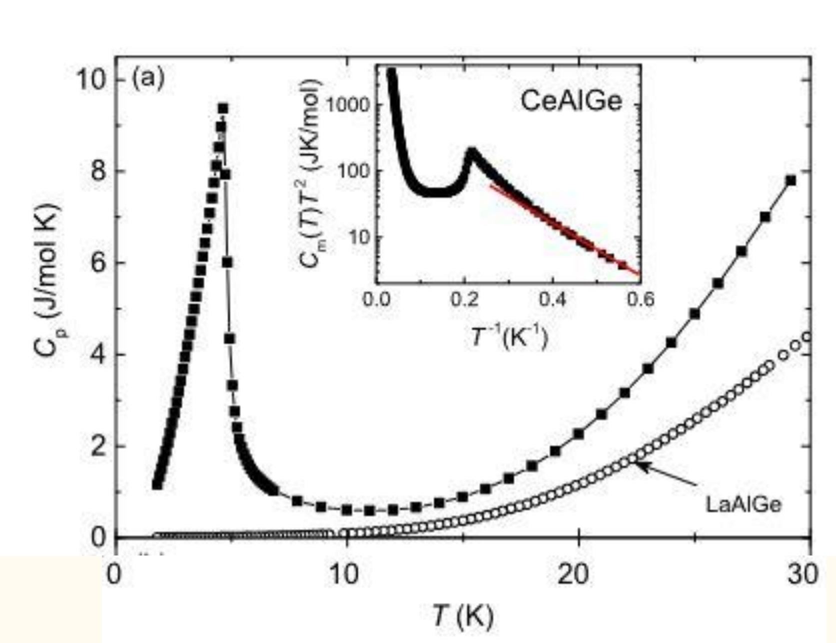
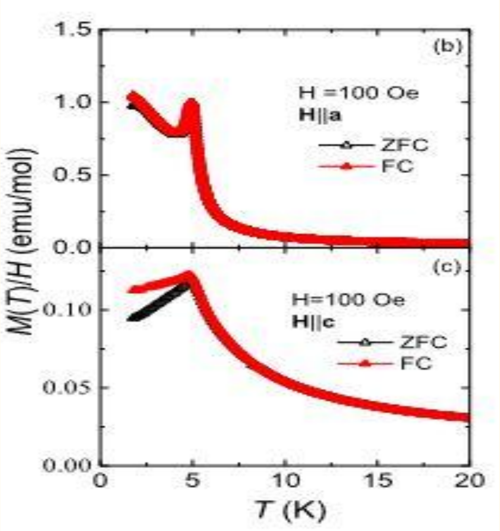


Figure 1: Heat Capacity Measurement

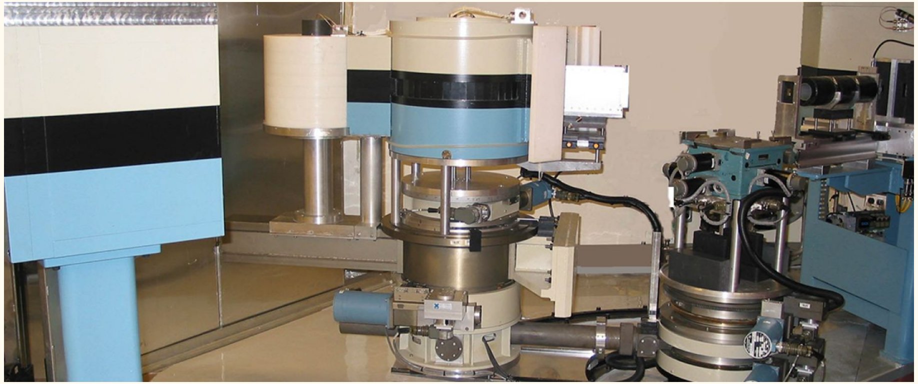


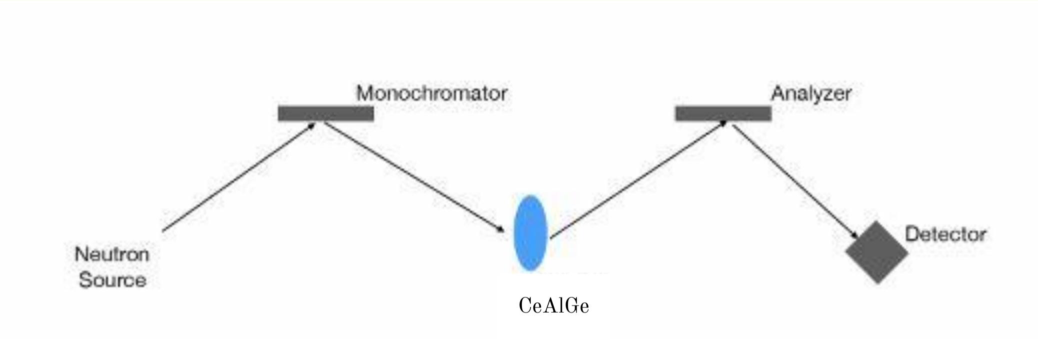
- 2nd Order Phase Transition - (No thermal hysteresis)

Figure 2: Magnetic Susceptibility

Reference: Hodovanets, H., et al. "Single-Crystal Investigation of the Proposed Type-II Weyl Semimetal Cealge." *Physical Review B*, vol. 98, no. 24, 2018, https://doi.org/10.1103/physrevb.98.245132.

Analysis of neutron diffraction data and calculation of theoretical nuclear structure factor, magnetic form factor and spin correlations through MATLAB





$$2d \sin\theta = n\lambda \ .$$

Nuclear Bragg scattering

$$I(\mathbf{Q}) = \mathbf{NV} * |\mathbf{F_N}(\mathbf{Q})|^{\mathbf{2}} \sum_{\mathbf{\Gamma}} \delta(\mathbf{Q} - \mathbf{\Gamma})$$

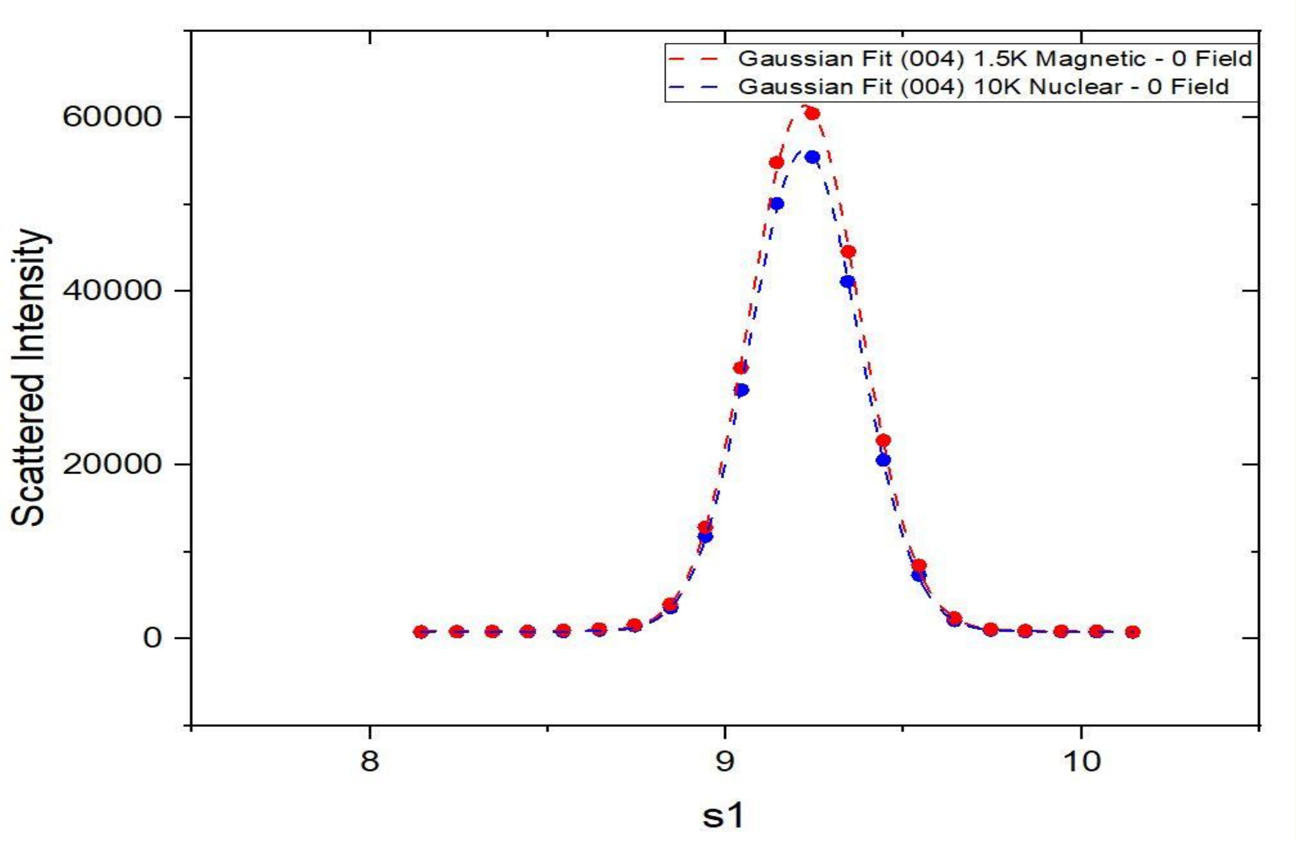
$$F_N(\mathbf{Q}) = \sum_{\mu} \mathbf{b}_{\mu} \mathbf{e}^{\mathbf{iQ\cdot r}}$$

Magnetic Bragg scattering

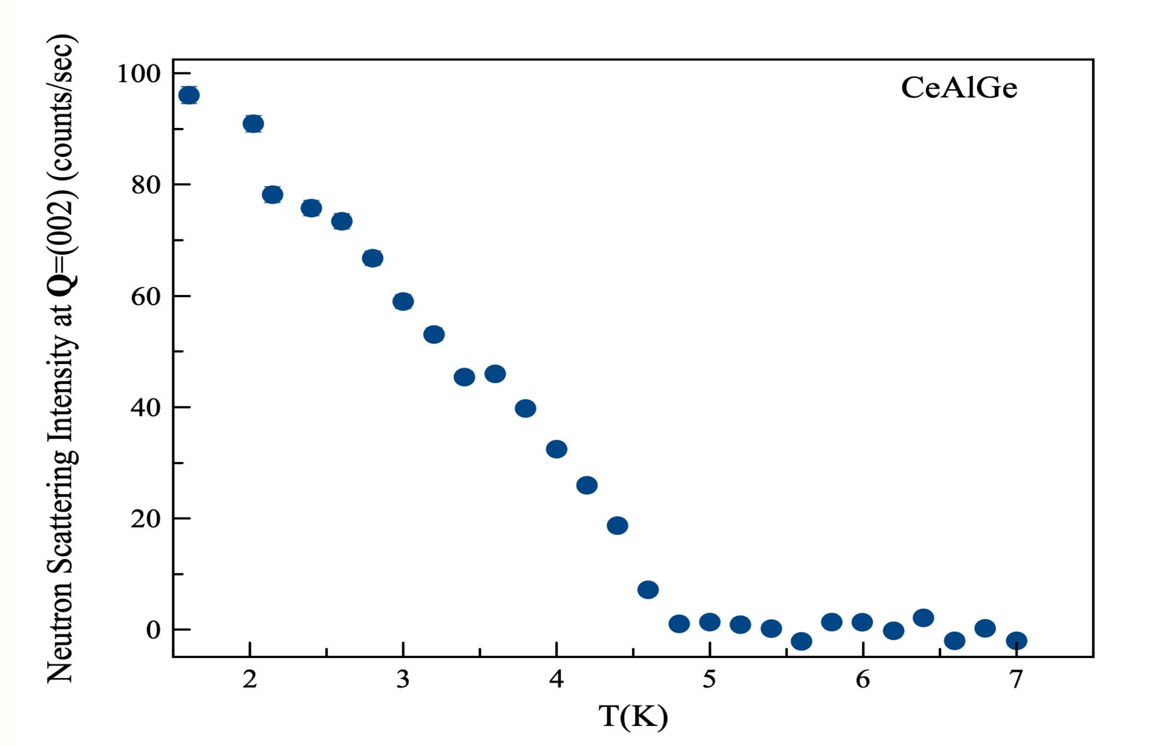
$$I(\mathbf{Q}) = |\mathbf{f}(\mathbf{Q})|^{\mathbf{2}} \frac{\mathbf{r_m^2}}{(\mathbf{2}\mu_{\mathbf{B}})^{\mathbf{2}}} \sum_{\mathbf{\Gamma_m}} |\mathbf{M}_{\perp}(\mathbf{Q})|^{\mathbf{2}} \delta(\mathbf{Q} - \mathbf{\Gamma_m})$$

$$M_{\perp}(\mathbf{Q}) = \sum_{\mu} \mathbf{m}_{\mu} \mathbf{e}^{-\mathbf{iQ\cdot r}_{\mu}}$$

Magnetic scattering lies on top of nuclear bragg peak positions, indicating that the magnetic unit cell is the same size as its nuclear counterpart

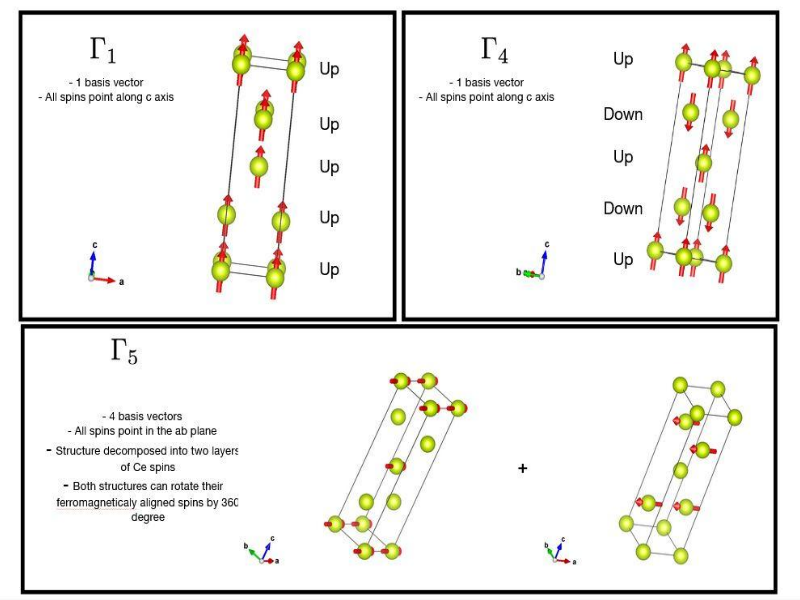


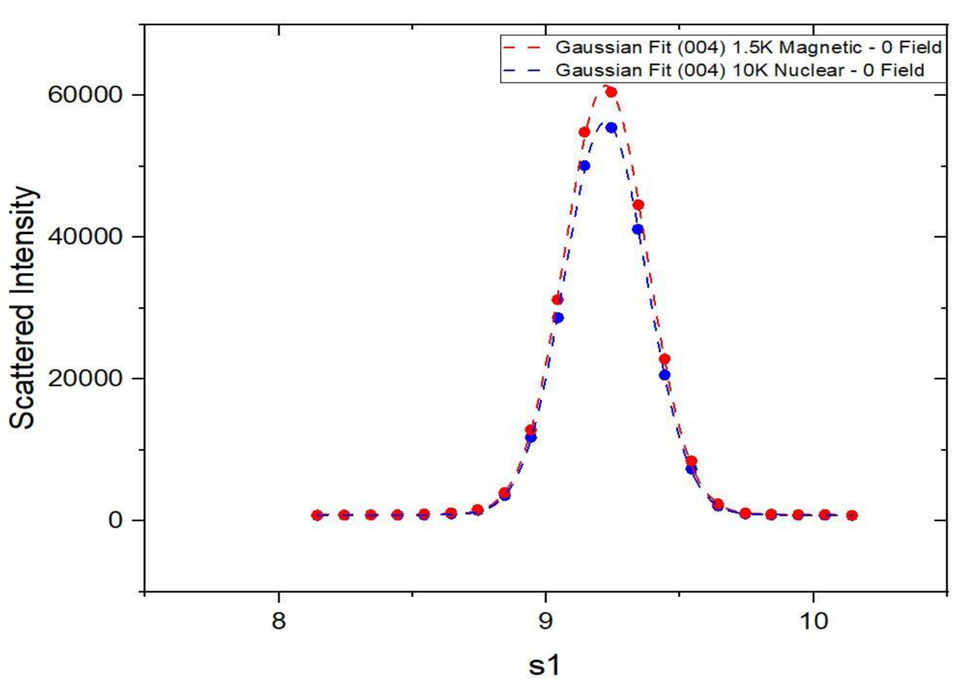
The increase of Bragg scattering onsets around 5K, which is consistent with the critical temperature of the magnetic transition observed in bulk thermodynamic measurements.



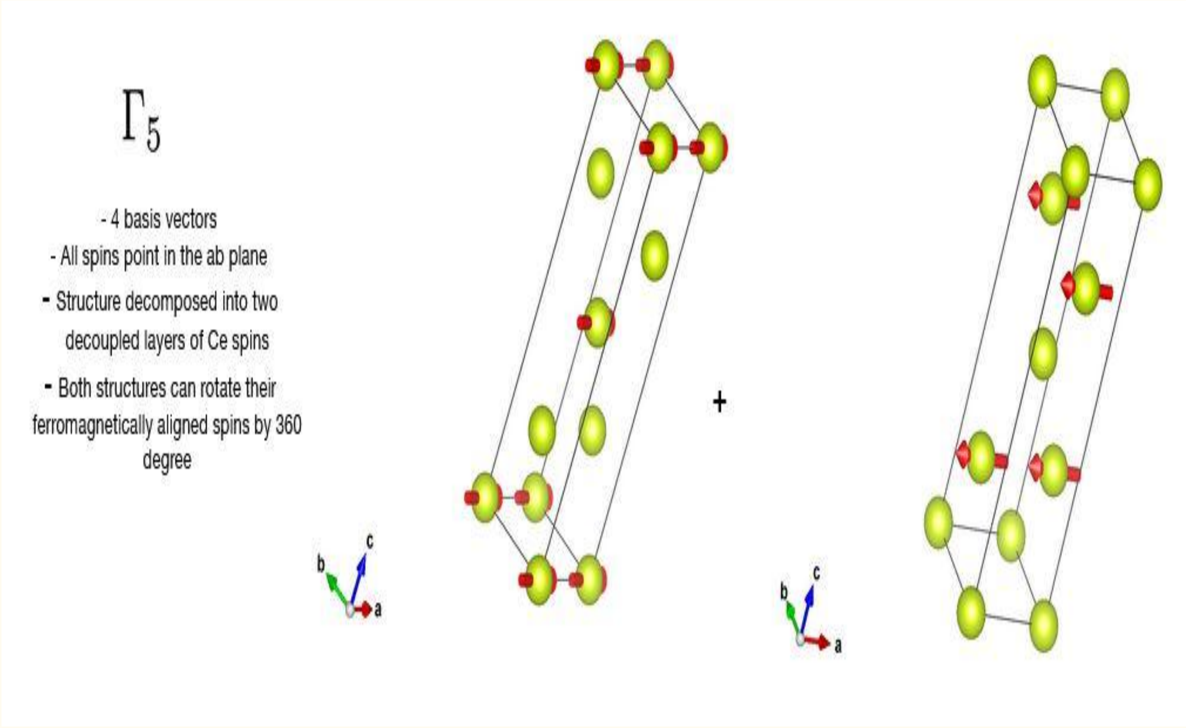
Symmetry analysis of the possible magnetic structures of the Ce spins reveals three different types

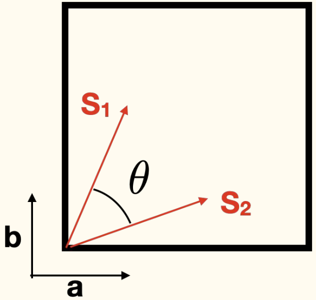
- Can rule out spin structures with purely out-of-plane spin component due to observation of magnetic scattering at (00L) reflections such as **Q**=(004)



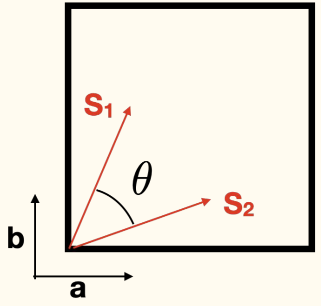


Symmetry analysis of the possible magnetic structures of the Ce spins reveals three different types

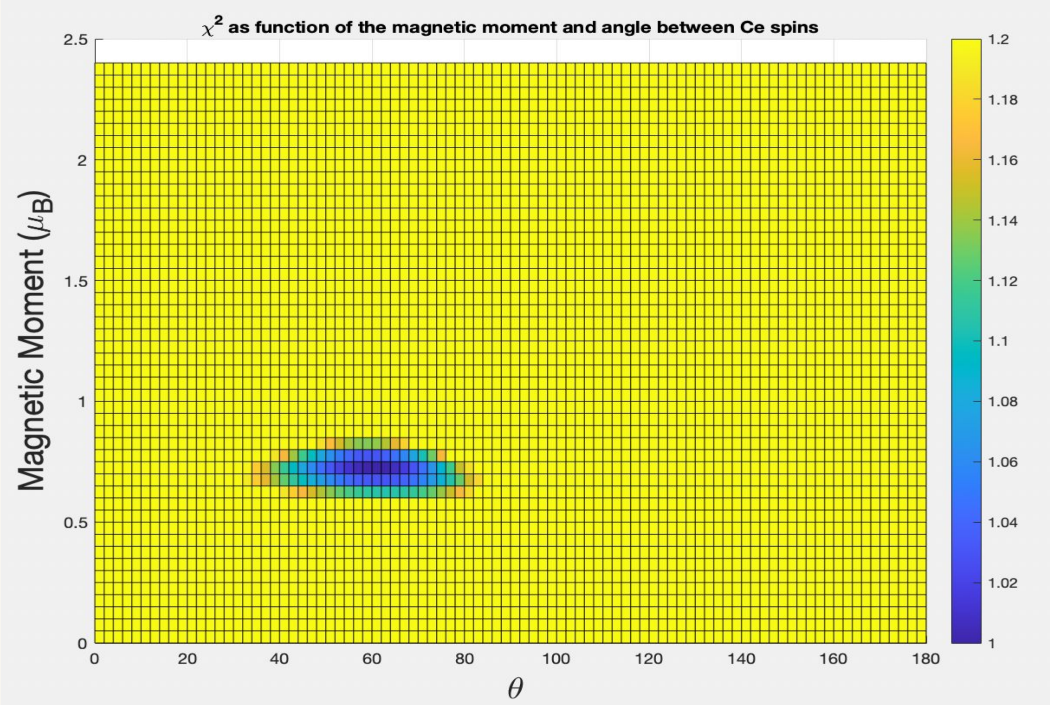




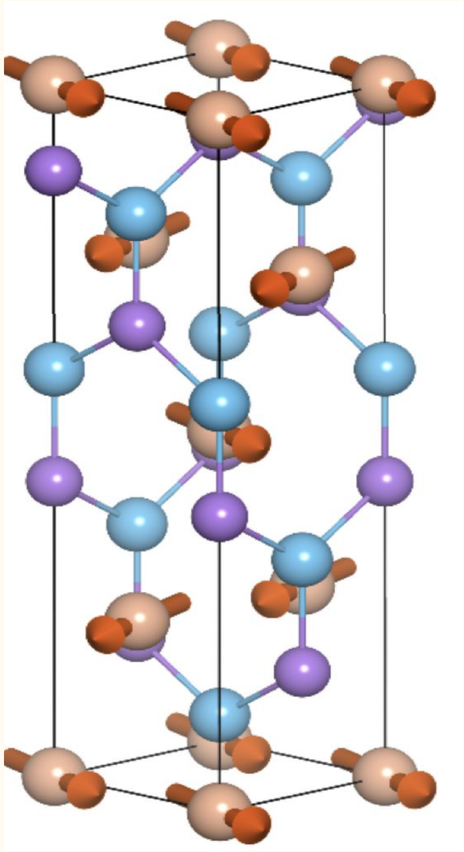
Chi-squared refinement of the magnetic moment and the angle (theta) between the Ce spins



$$\chi_c^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$



Conclusion & Future Work



- The crystal structure of CeAlGe breaks inversion symmetry and also has collective magnetism (interplay of magnetism and weyl fermions can be studied)
- We probed the magnetism of CeAlGe through neutron diffraction and we found that the spins are forming an in-plane collinear structure (see structure on the left).
- In-field neutron diffraction will be used to determine the exact spin orientation and Density Functional Theory will be performed to look at the influence of the magnetism on the electronic band structure of CeAlGe.

Acknowledgements

CHRNS
CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING
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NIST | SUMMER UNDERGRADUATE RESEARCH FELLOWSHP
SURF

- Mentor: Jonathan Gaudet
- NCNR: Susana Teixeira, Joseph Dura, Julie Borchers
- SURF: Brandi Toliver