Crystal growth, ARPES and DFT studies of topological nodal line semimetal $ZrAs_2$

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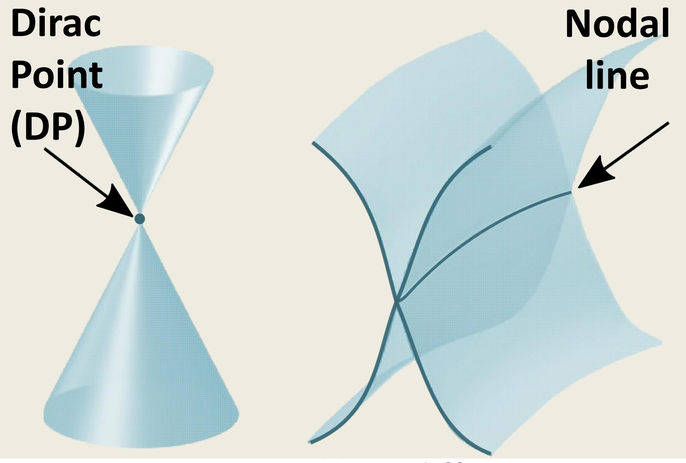
Motivation:

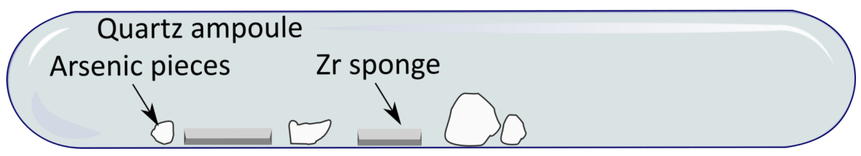
In nodal line semimetals, conduction and valence bands intersect along a one-dimensional path within the three-dimensional Brillouin zone. Furthermore, any external influence or perturbation applied to the system maintains a specific symmetry group [1, 2]. $ZrAs_2$ possess the non-symmorphic symmetry along with the inversion and time reversal symmetry (TRS).

Nodal lines give rise to extremely large magnetoresistance, SdH oscillations and symmetry enforced band crossings [3, 4]

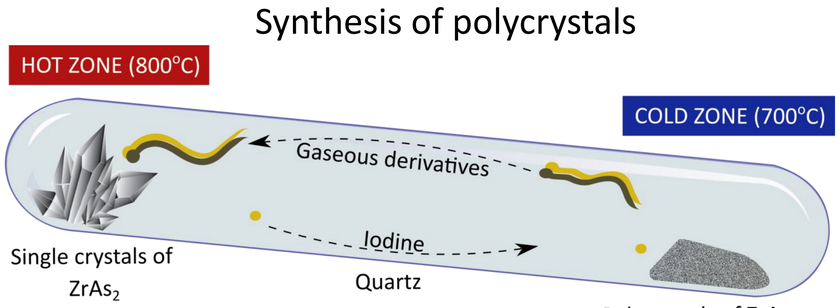
Studying the single crystals of $ZrAs_2$ by angle-resolved photoemission spectroscopy (ARPES) with DFT support helps us understand better how various symmetries are structured and impact the topological properties.



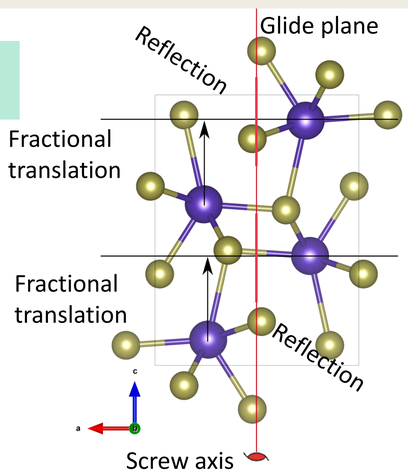
Crystal growth: Chemical Vapor transport (CVT)



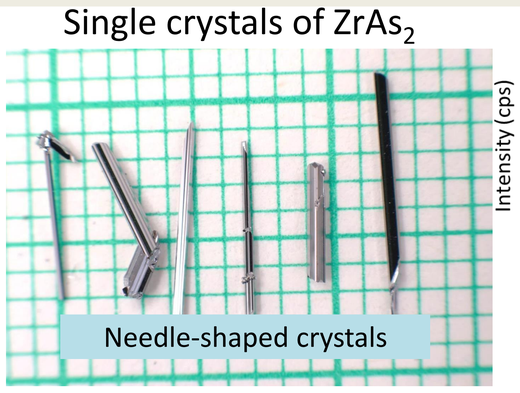
Synthesis of polycrystals



Single crystal growth

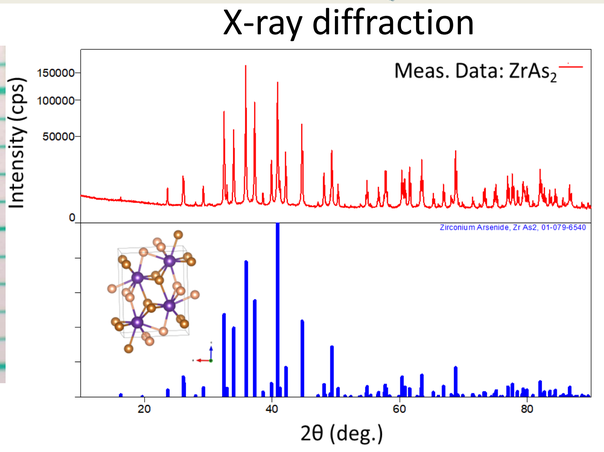


Single crystals of $ZrAs_2$

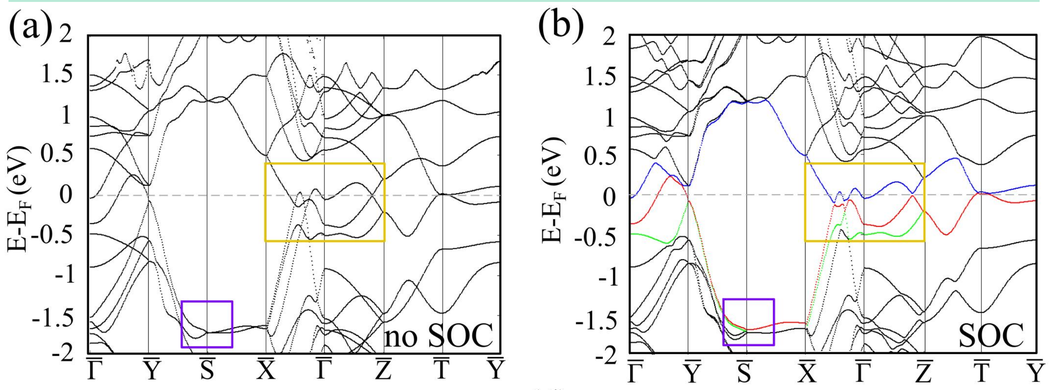


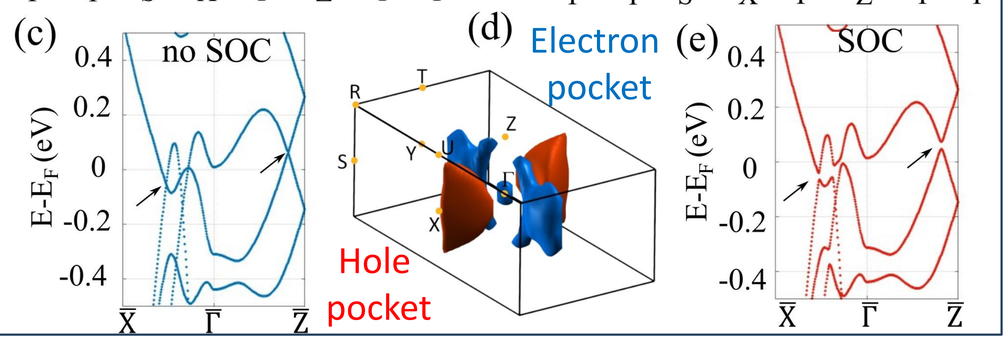
Orthorhombic (Pnma 62)

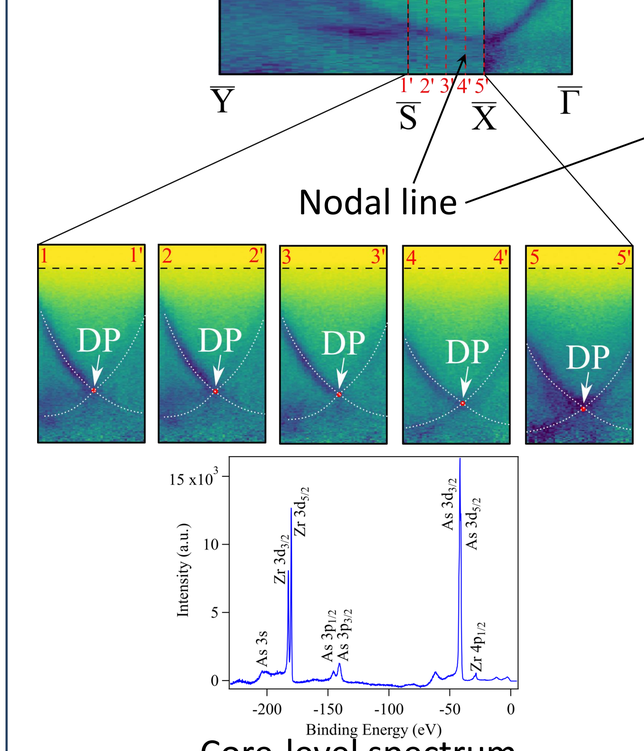
X-ray diffraction

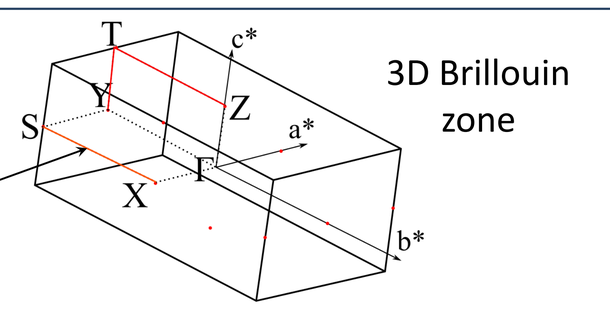


DFT calculations:

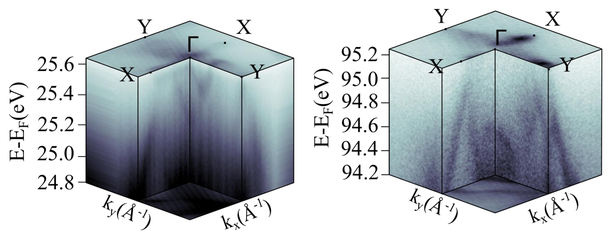




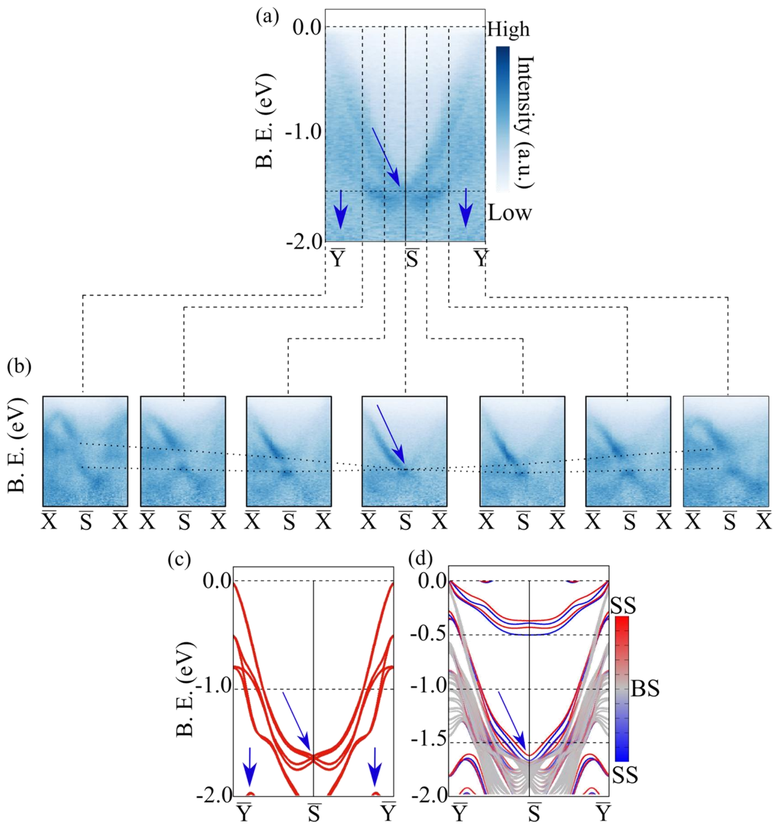




Core-level spectrum

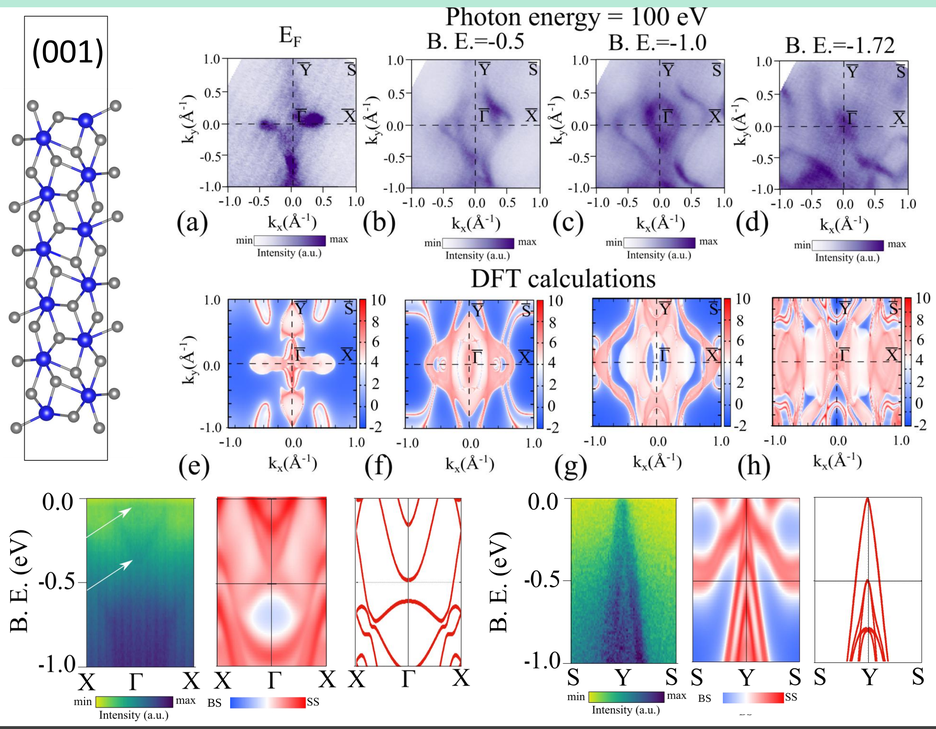


3D ARPES spectra



Non-symmorphic symmetry protected band crossing

ARPES:



Summary

- High-quality needle shaped-crystals: orthorhombic (Pnma 62)
- We observed band structure of $ZrAs_2$ with bulk dominant bands at lower photon energies associated with nodal lines
- Inversion, TRS and non-symmorphic symmetry protected
- Robust band crossing against gap opening at S point (with SOC)

References

[1] Phys. Rev. B **84**, 235126 (2011).
[2] Nat. Commun. **7**, 11696 (2016).
[3] Phys. Rev. B **103**, 245104 (2021)
[4] Rev. B **109**, 075155 (2024)

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