

# Spin-resolved Fermi Surface of "Half-Metallic" FePd Alloy Monolayers

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Arthur Ernst<sup>3</sup>, Claus M. Schneider<sup>1,2,4</sup>, and Christian Tuschel<sup>1,2</sup>

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<sup>2</sup>Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany

<sup>3</sup>Institute for Theoretical Physics, Johannes Kepler University Linz, Linz, Austria

<sup>4</sup>Department of Physics, University of California, Davis, California 95616, USA



# Ultrathin FePd Ferromagnet

Ferromagnetism in low dimensions /  
Surface ferromagnetism

Reduced Dimensionality

+

Exchange interaction

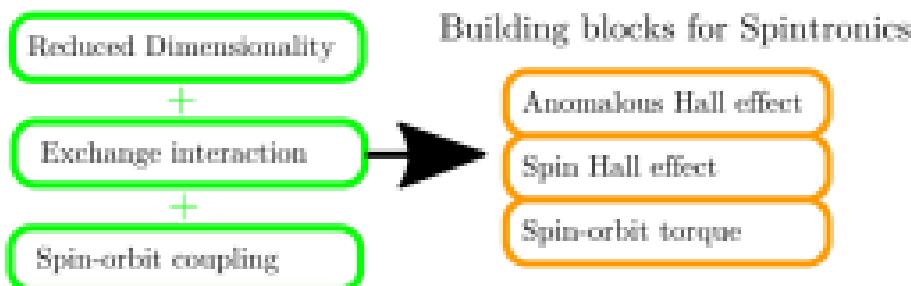
+

Spin-orbit coupling



# Ultrathin FePd Ferromagnet

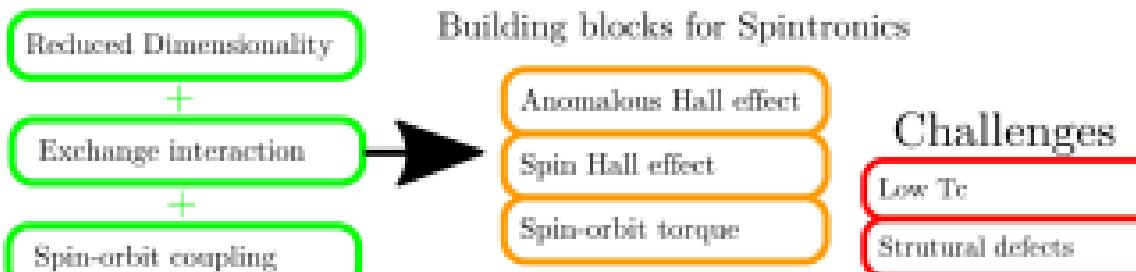
Ferromagnetism in low dimensions /  
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Ferromagnetism in low dimensions /  
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# Ultrathin FePd Ferromagnet

Ferromagnetism in low dimensions /  
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Reduced Dimensionality

+

Exchange interaction

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Spin-orbit coupling

Building blocks for Spintronics

Anomalous Hall effect

Spin Hall effect

Spin-orbit torque

Challenges

Low Tc

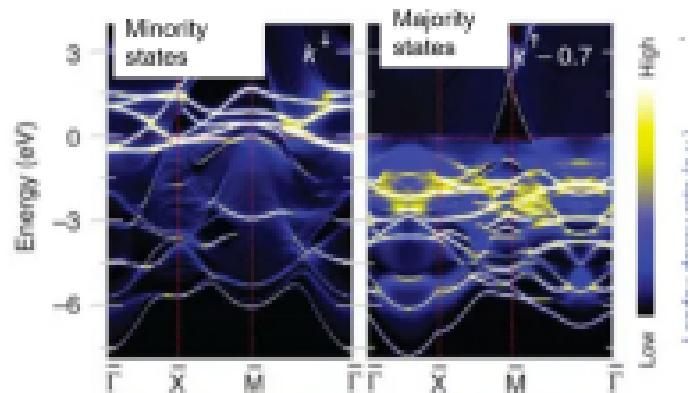
Structural defects

Complex stoichiometry  
Multi-layers



# The Thinnest Known Half Metallic System

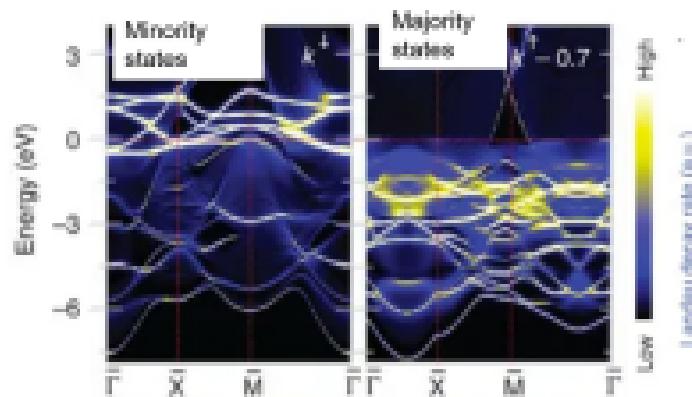
2ML FePd alloy on Pd(100)



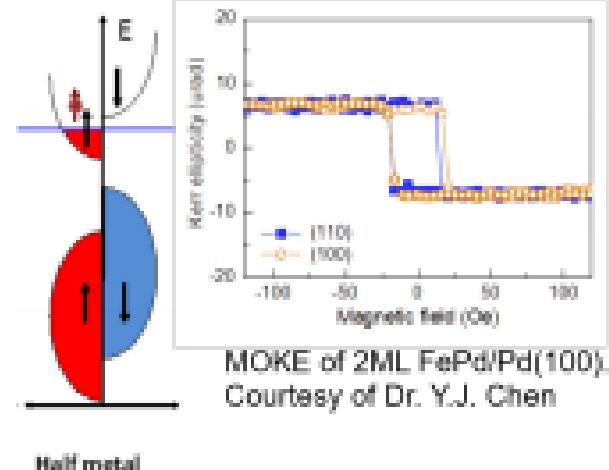
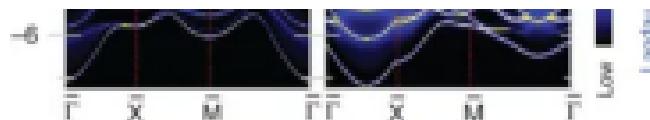


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2ML FePd alloy on Pd(100)



H. J. Qin, J. Kirschner, et al. Nature Communications volume 6, Article number: 6126 (2015)

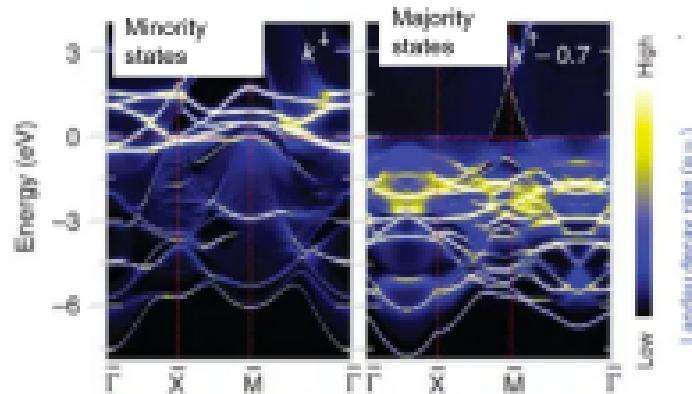


MOKE of 2ML FePd/Pd(100).  
Courtesy of Dr. Y.J. Chen



# The Thinnest Known Half Metallic System

2ML FePd alloy on Pd(100)

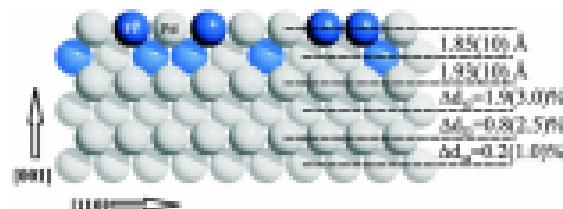


H. J. Qin, J. Kirschner, et al. Nature Communications volume 6, Article number: 6126 (2015)



Highly controllable and tunable

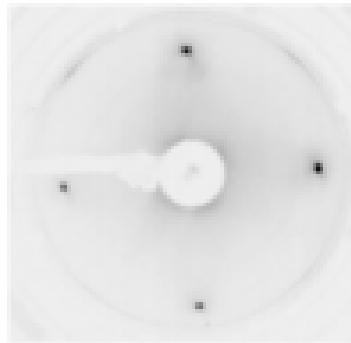
$T_{\text{core}} \sim 370\text{K}$



H. L. Meyerheim, R. Popescu, and J. Kirschner  
Phys. Rev. B 73, 245432 (2006)



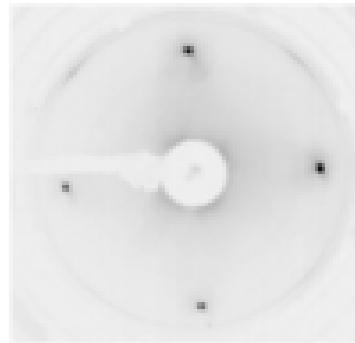
## Preparation of 1.8 monolayers FePd on Pd(100)



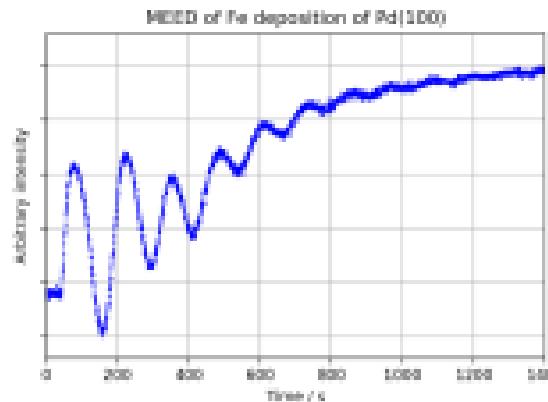
LEED Pd(100) at 56eV



## Preparation of 1.8 monolayers FePd on Pd(100)

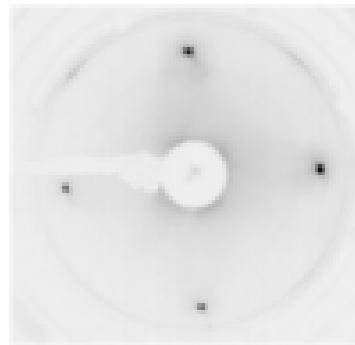


LEED Pd(100) at 56eV

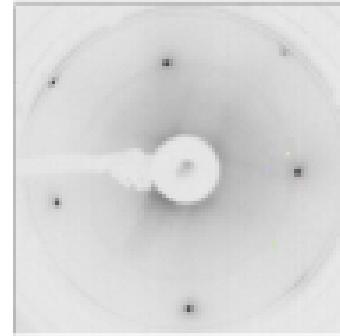
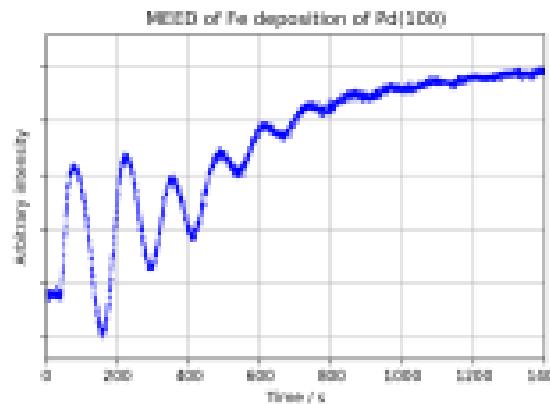




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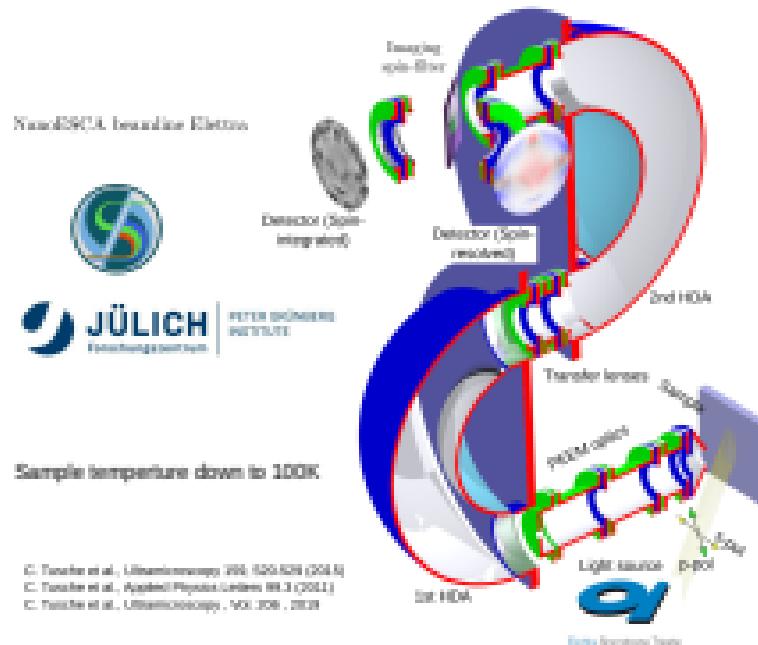
LEED Pd(100) at 56eV



LEED 1.8ML FePd/Pd(100)  
at 70eV



# Spin-resolved Momentum Microscopy



Pseudospin Resolving Electro.



Detector (Spin-  
integrated)

Tilted spin-filter

Detector (Spin-  
resolved)

2nd HOA

Transfer lenses

1st HOA

Light source

Sample

Sample temperature down to 100K

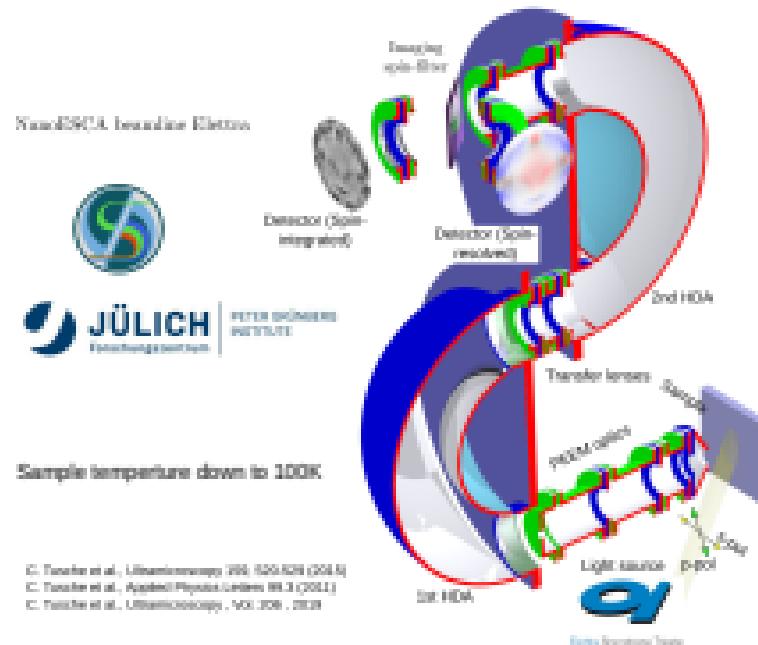
C. Tausch et al., Ultramicroscopy 196, 123-129 (2018)

C. Tausch et al., Applied Physics Letters 109, 3 (2016)

C. Tausch et al., Ultramicroscopy, 203, 206, 2019



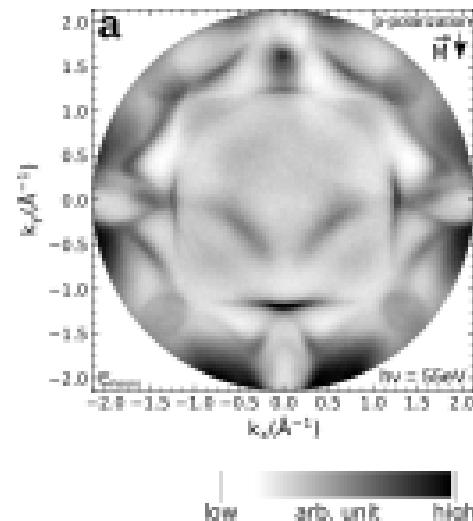
# Spin-resolved Momentum Microscopy



Sample temperature down to 100K

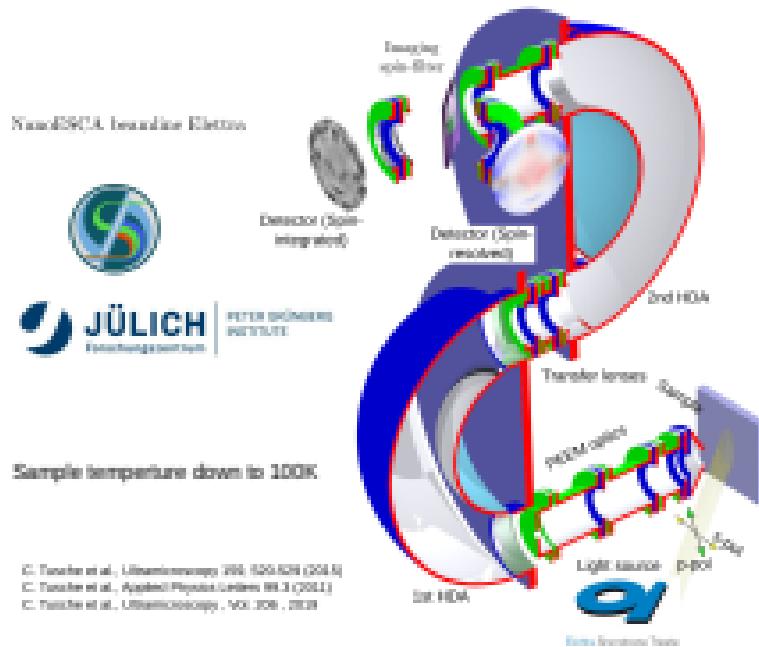
- C. Tausch et al., Ultramicroscopy 196, 123-129 (2018)  
C. Tausch et al., Applied Physics Letters 99(3) (2011)  
C. Tausch et al., Ultramicroscopy, Vol. 209, 2019

Fermi Surface of 12ML Fe/Pd(100)

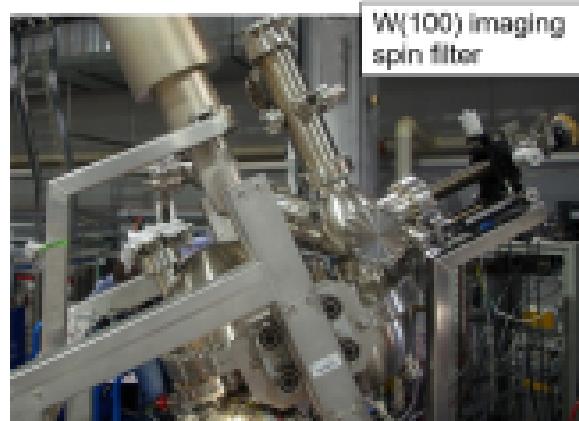




# Spin-resolved Momentum Microscopy

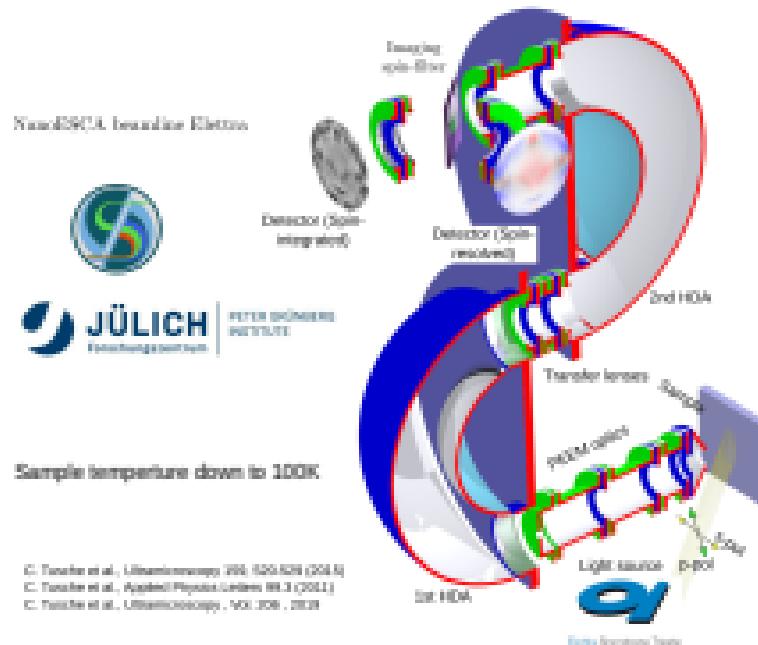


C. Tausch et al., Ultramicroscopy 196, 123-139 (2018)  
C. Tausch et al., Applied Physics Letters 99, 3 (2011)  
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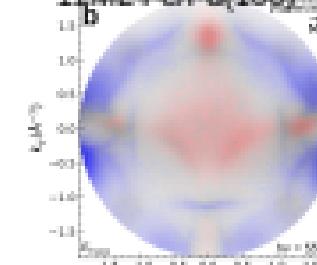
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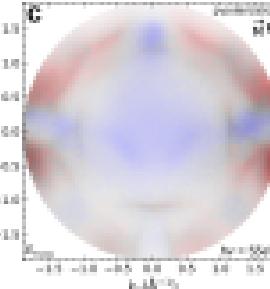
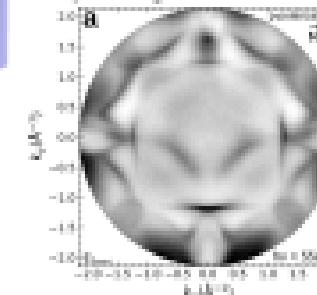
Sample temperature down to 100K

- C. Tacke et al., Ultramicroscopy 196, 120-129 (2018)  
C. Tacke et al., Applied Physics Letters 99(3) (2011)  
C. Tacke et al., Ultramicroscopy, 203, 209 , 2019

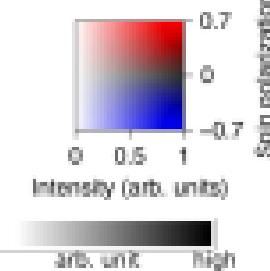
Spin-resolved Fermi Surface of  
12ML-Fe/Pd(100)



Spin-integrated Fermi Surface

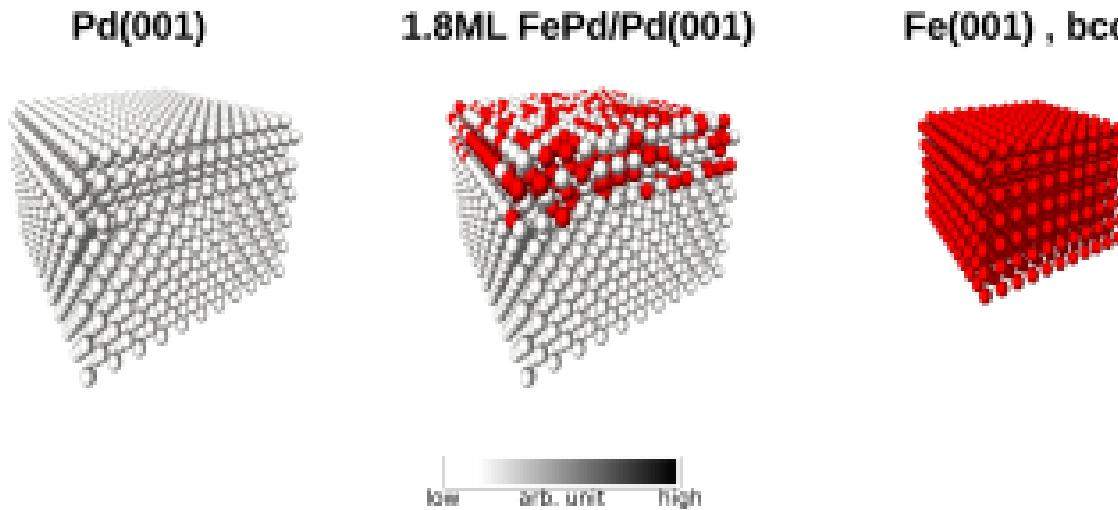


Spin quantization axis





## Fermi Surface of 1.8ML FePd/Pd(100)

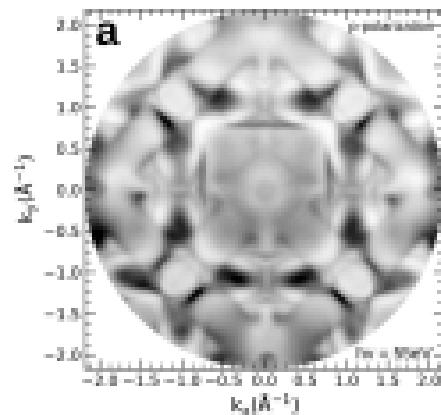




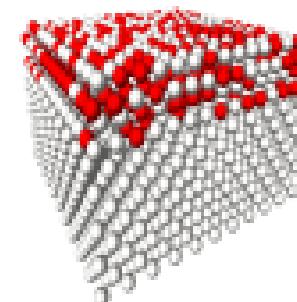
# Fermi Surface of 1.8ML FePd/Pd(100)

Fermi surfaces of Pd, 1.8ML FePd/Pd(100) and Fe

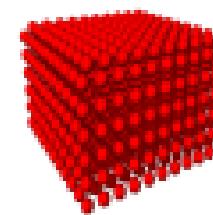
Pd



1.8ML FePd/Pd(001)



Fe(001) , bcc

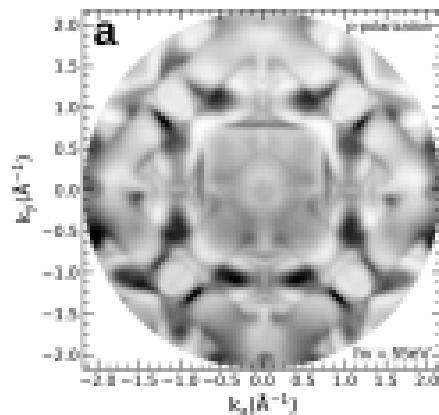




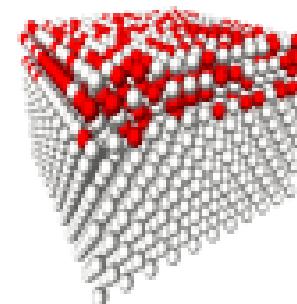
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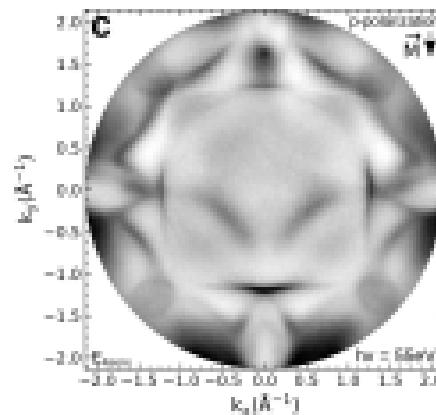
Pd



1.8ML FePd/Pd(001)



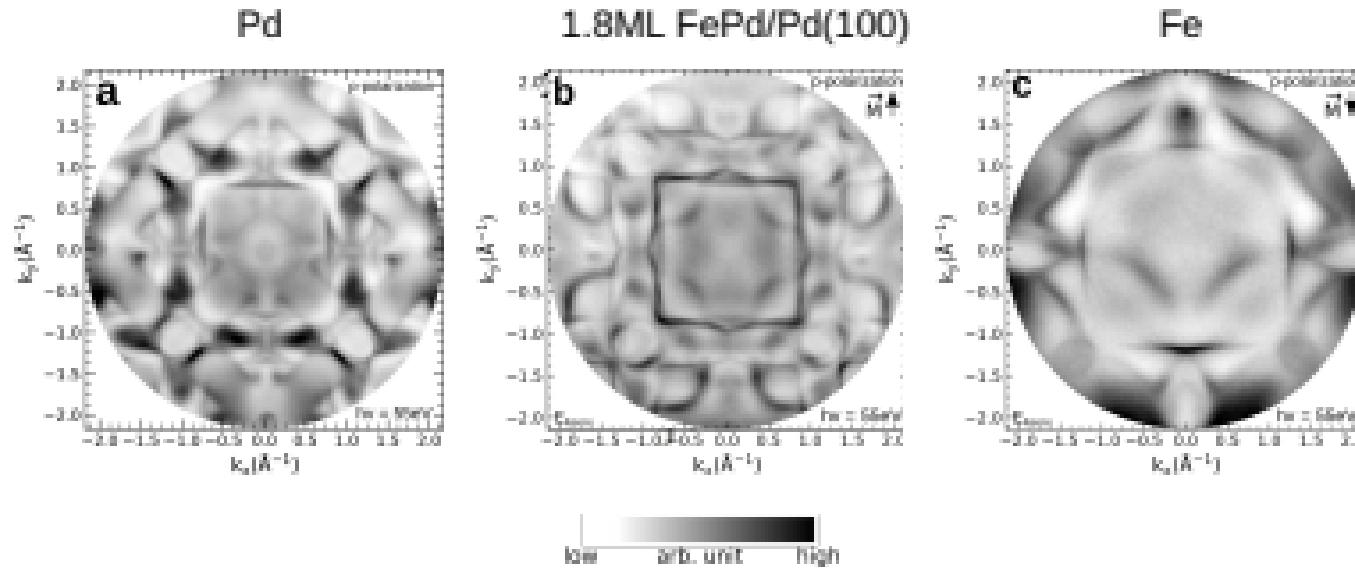
Fe





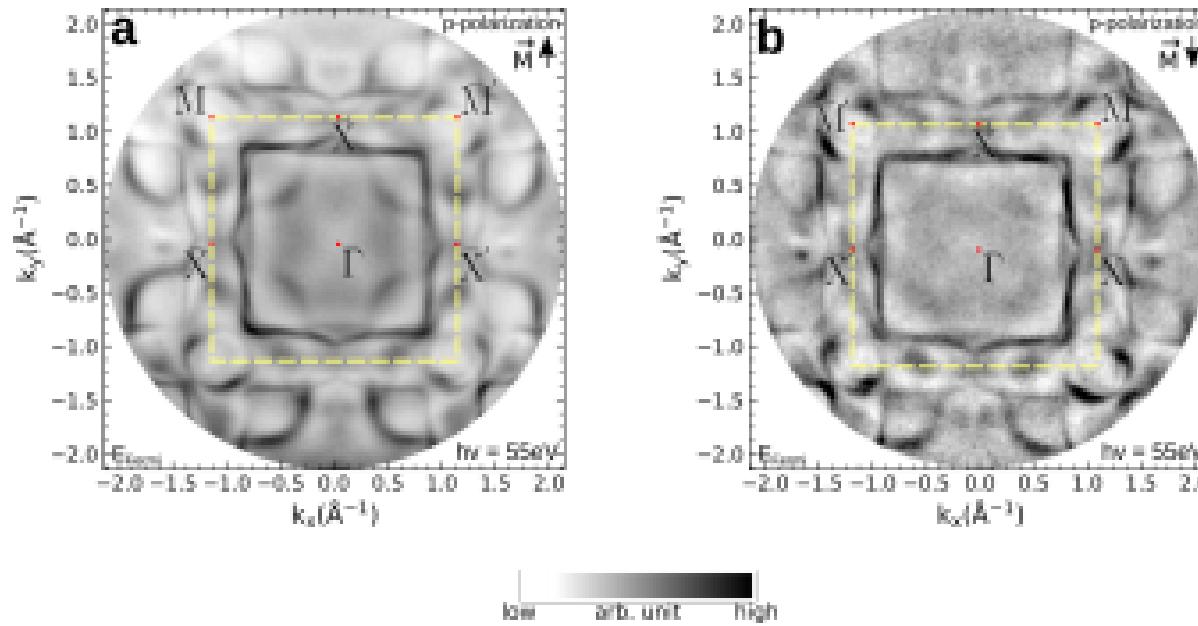
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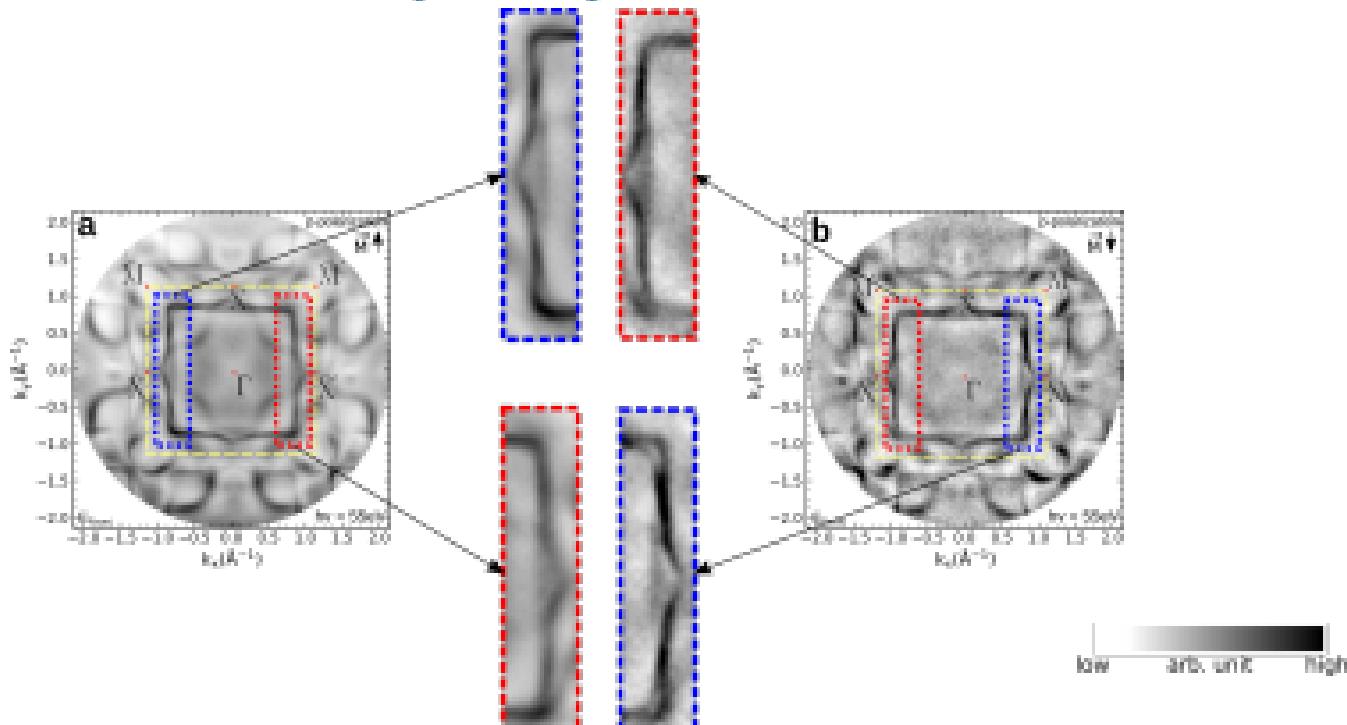


## Broken Time-reversal Symmetry across Fermi Surface



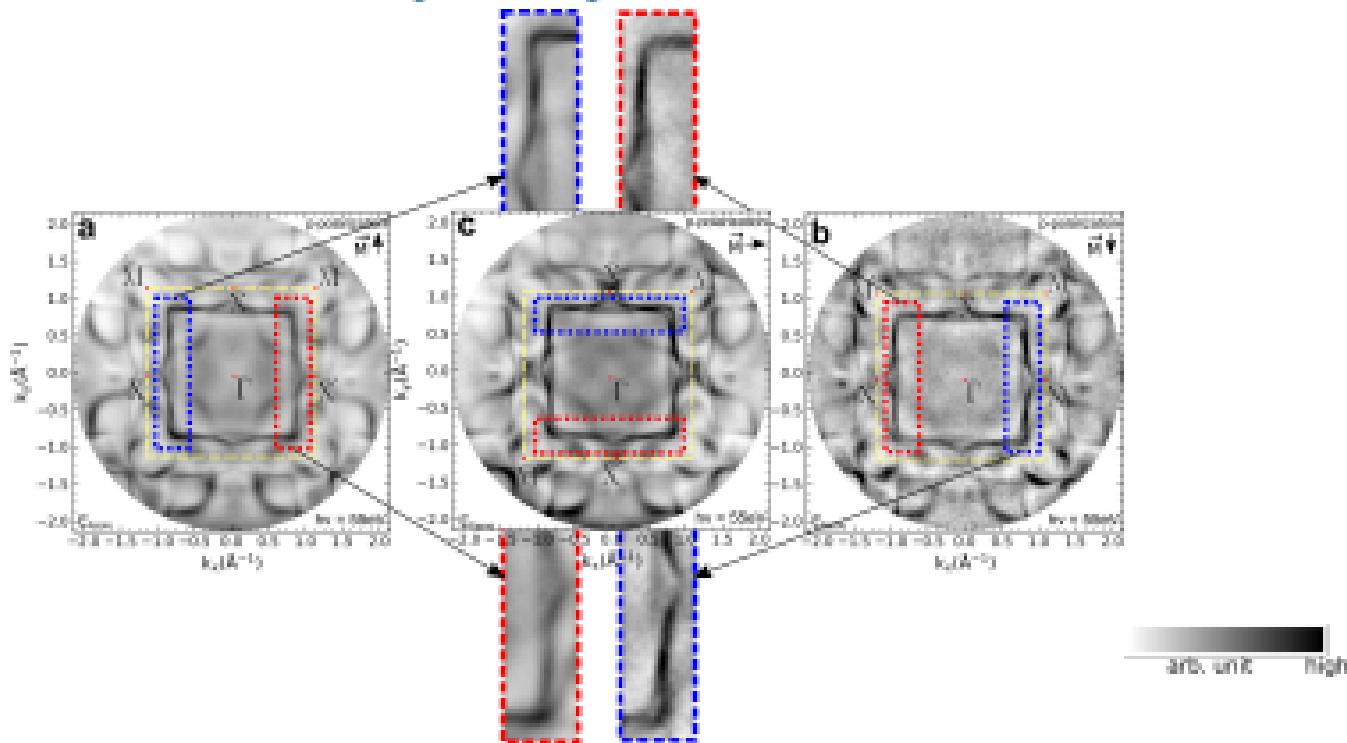


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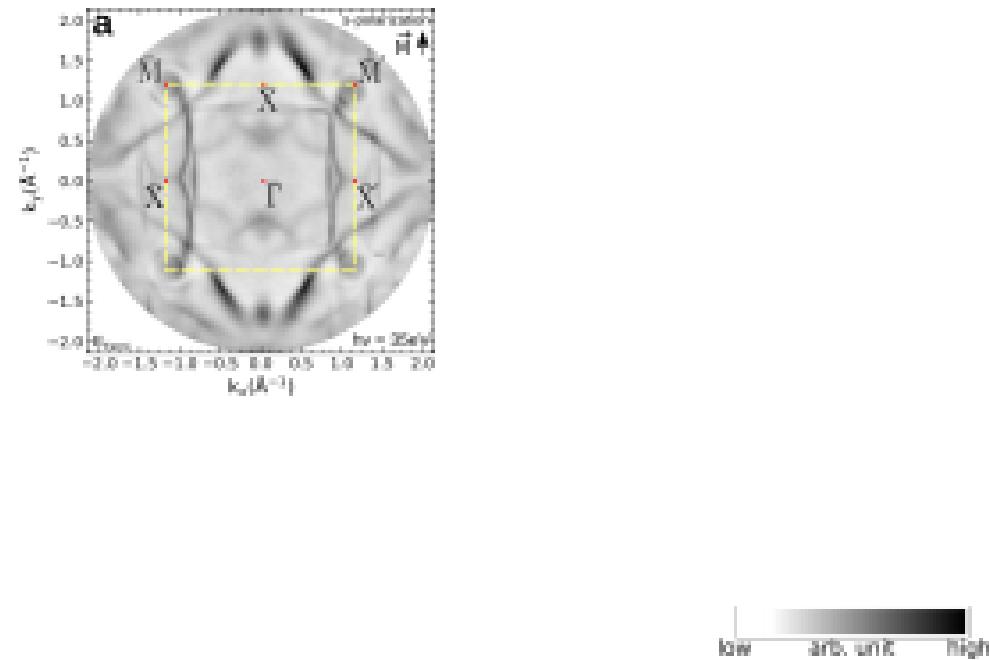


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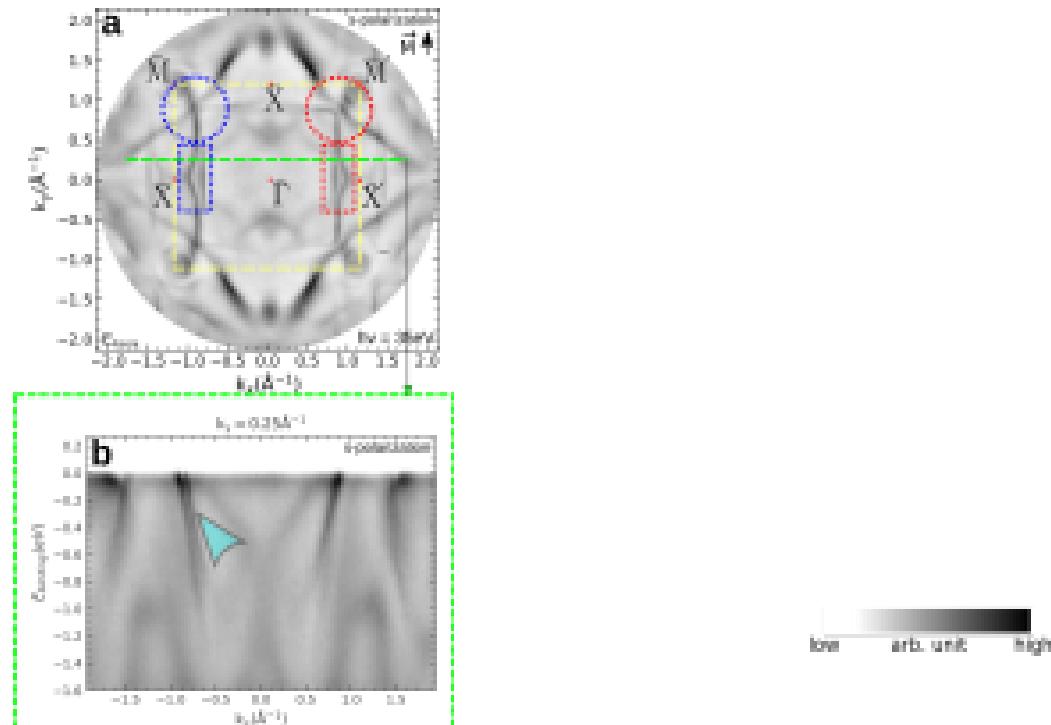


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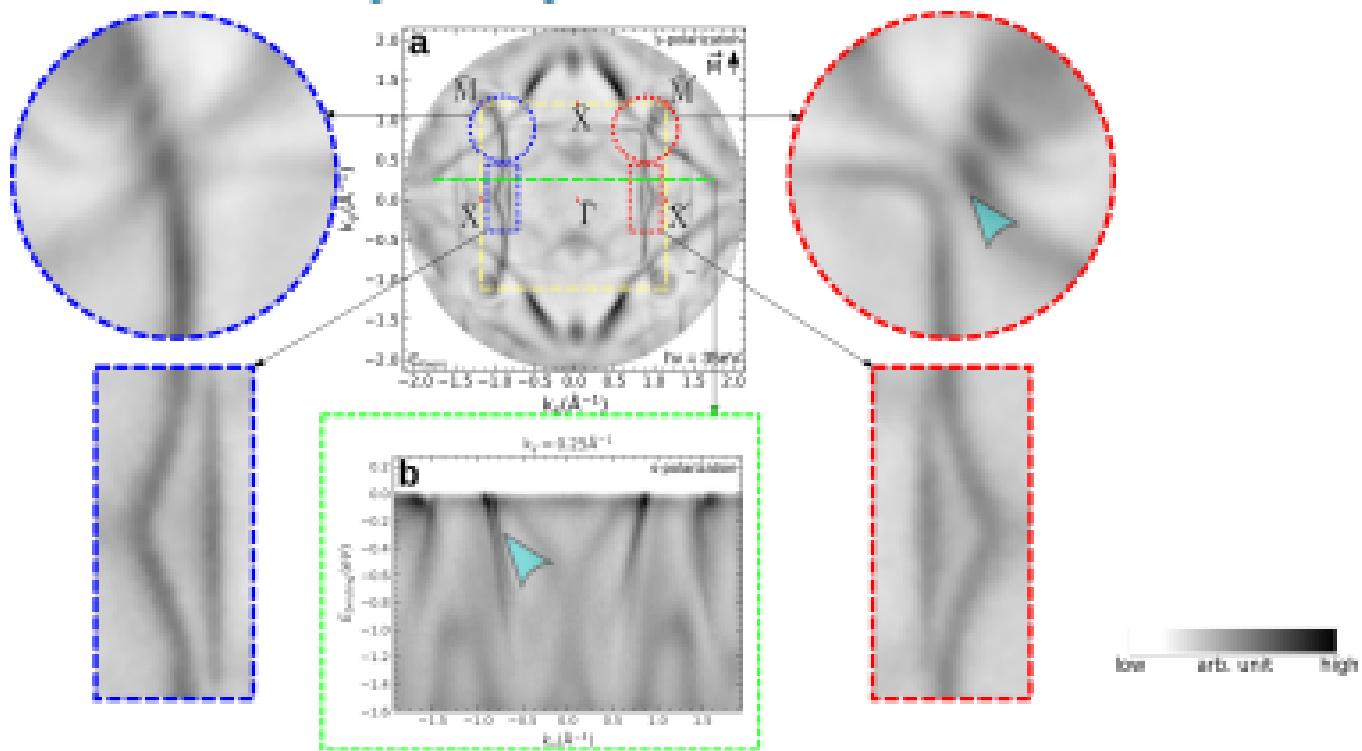


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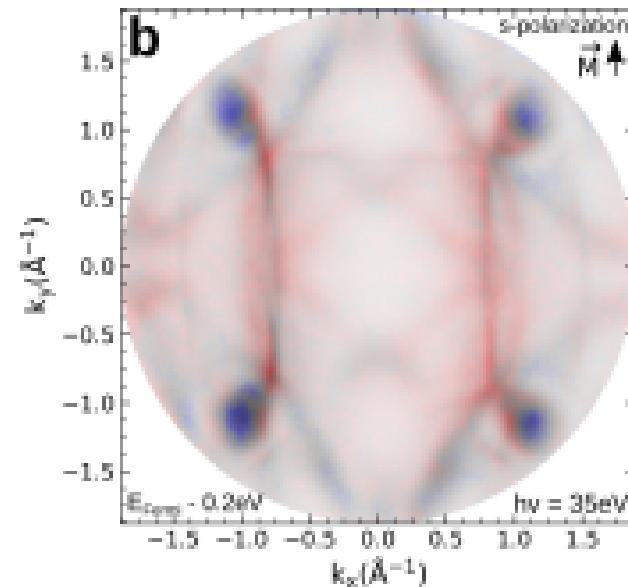
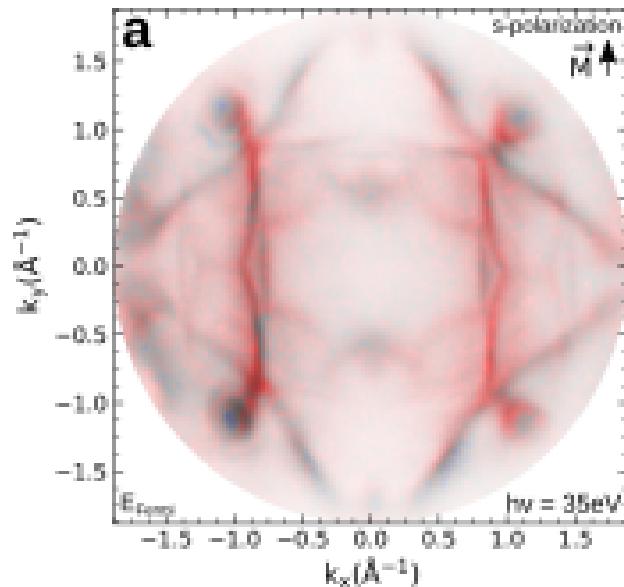


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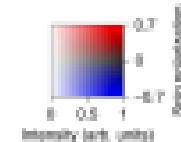




## Band Hybridizations of 1.8ML FePd/Pd(100) Fermi Surface

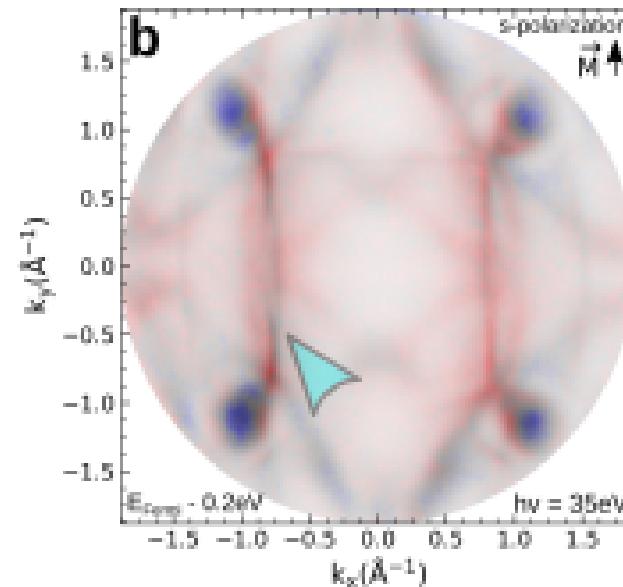
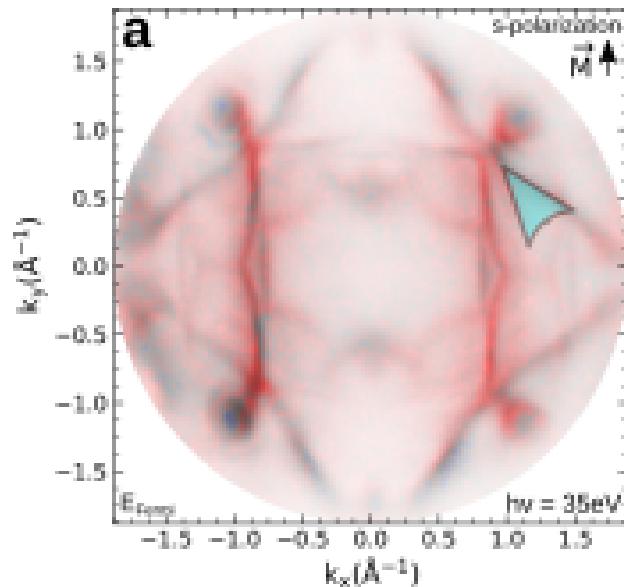


$S$





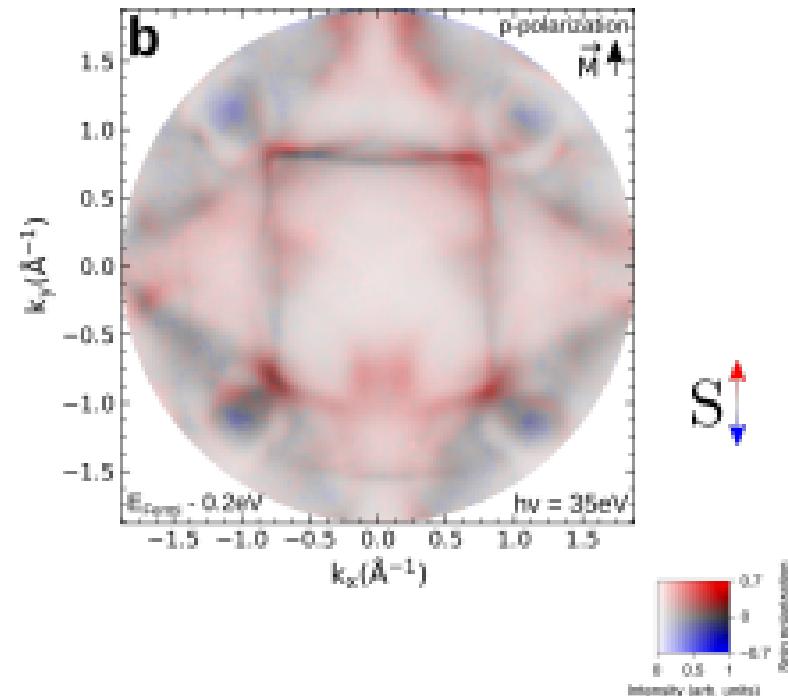
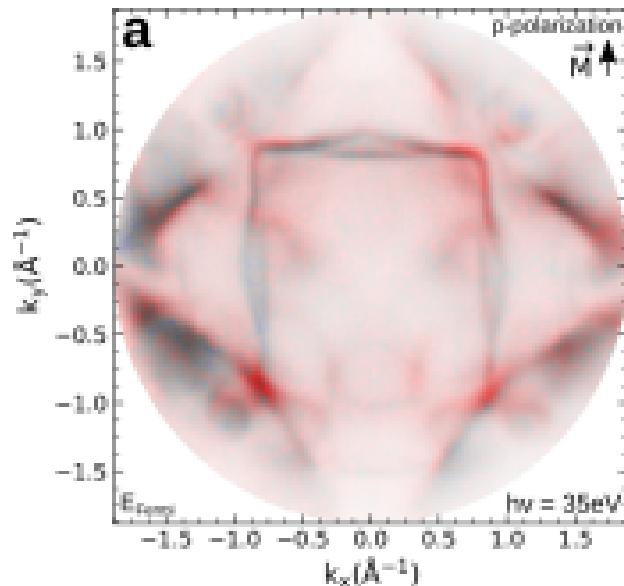
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$S$

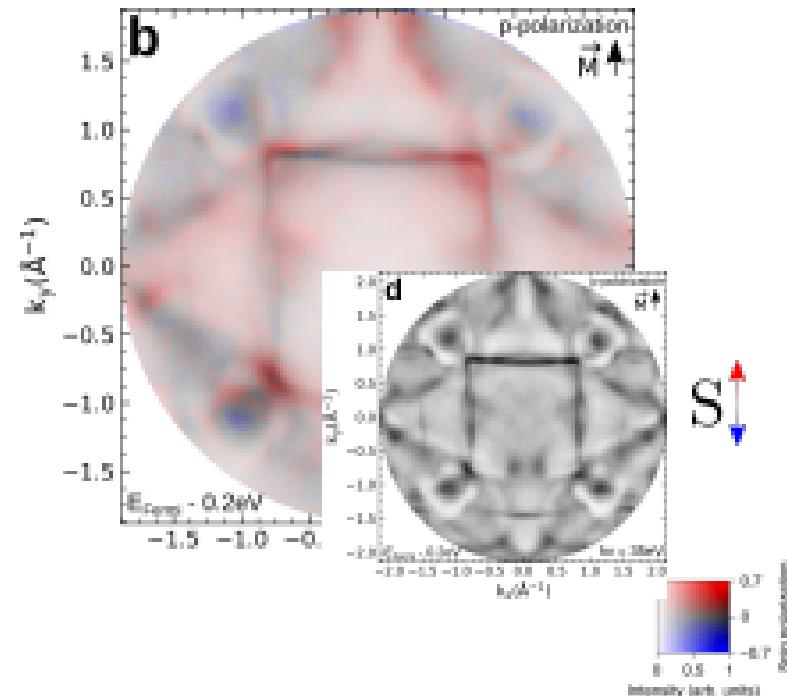
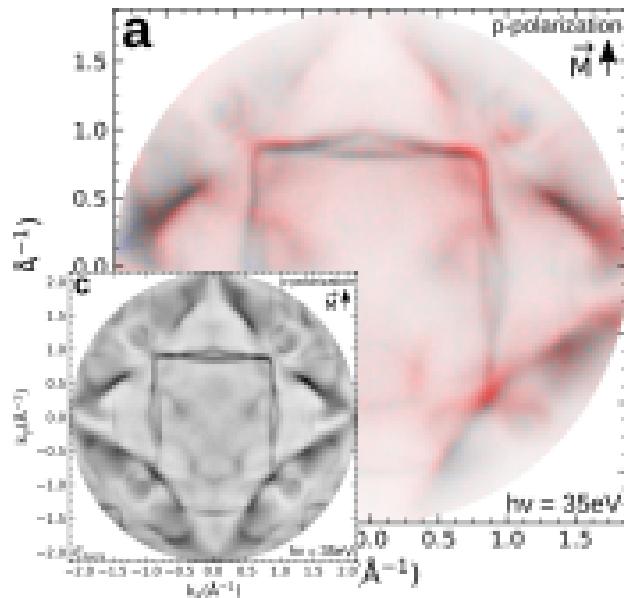


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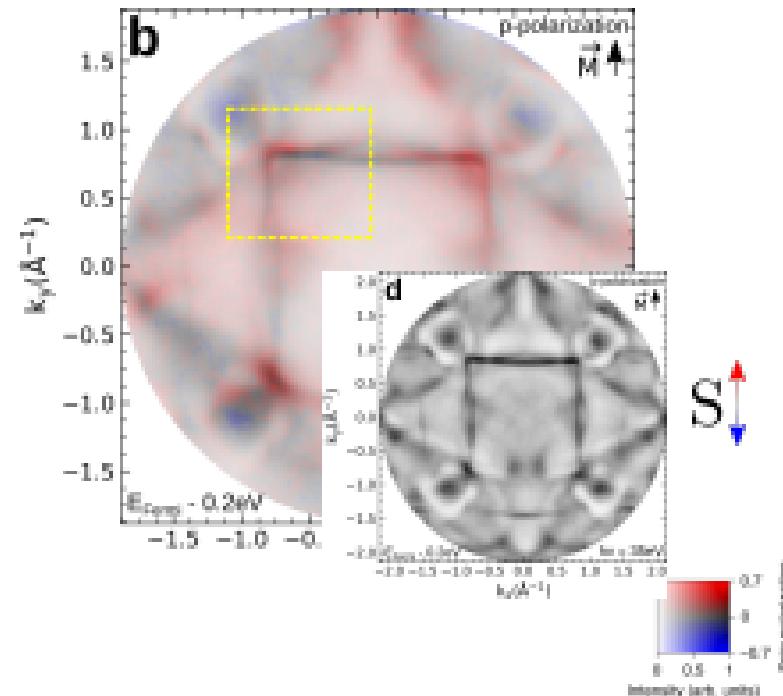
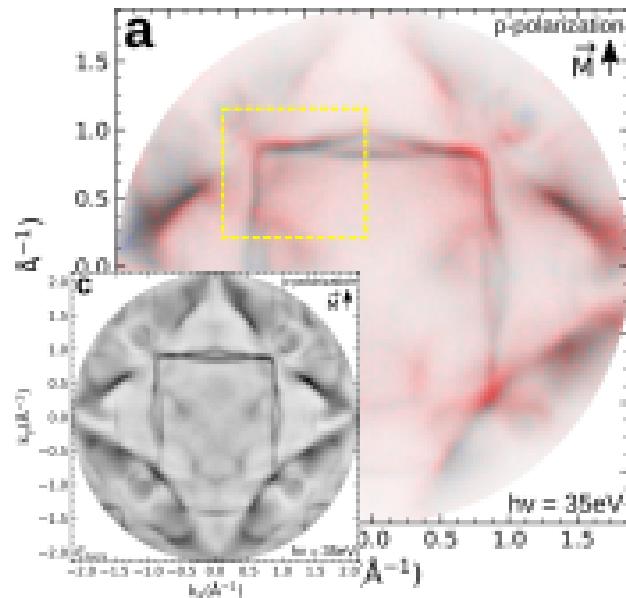


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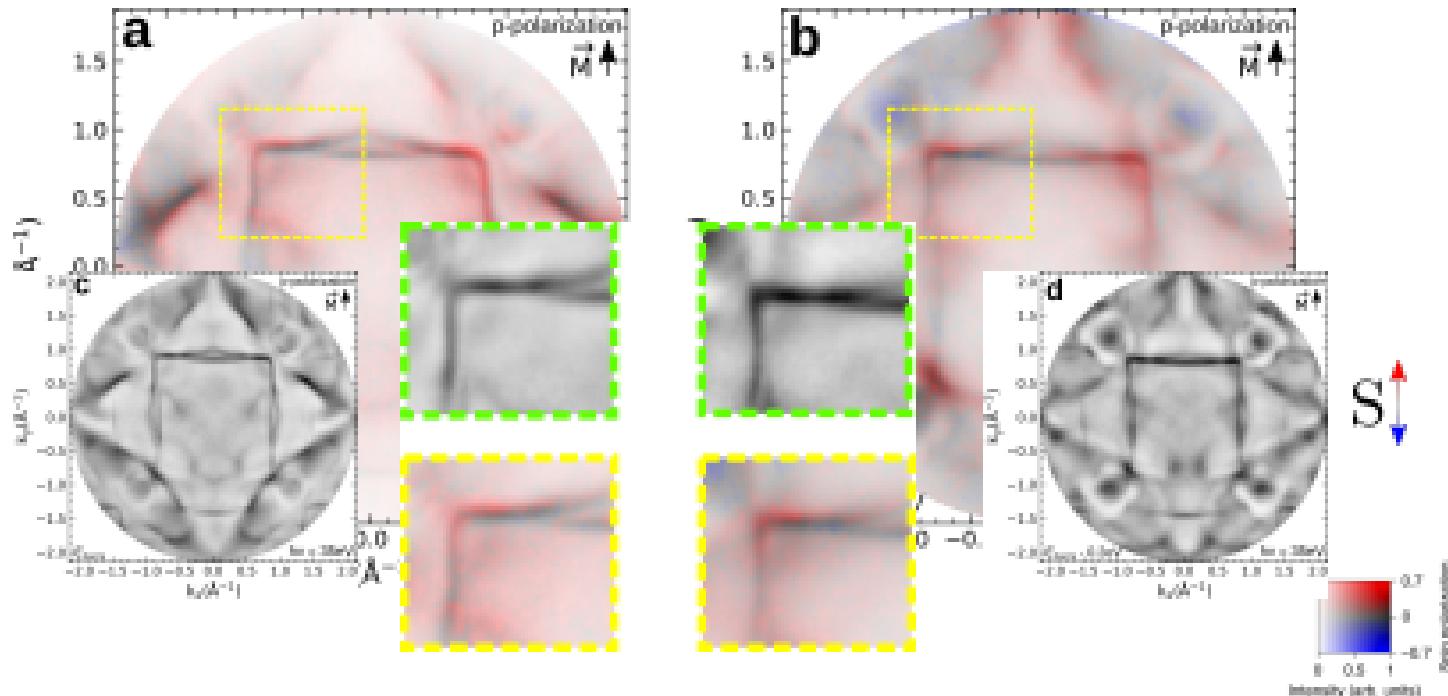


## Band Hybridizations of 1.8ML FePd/Pd(100) Fermi Surface





## Band Hybridizations of 1.8ML FePd/Pd(100) Fermi Surface





## Summary

- Fermi surface Topology of 1.8ML FePd/Pd(100), compared to Pd(100) and bulk Fe.
- Explicit breaking of time-reversal symmetry across FePd Fermi surface.
- Hybridization of electronic states of FePd due to strong spin-orbit coupling.  
Craving for more?



Thank you for your attention!

O: Fachverband Oberflächenphysik

O 94: Overview Talk Claus M. Schneider (joint session OCPP)

O 94.1: Invited talk

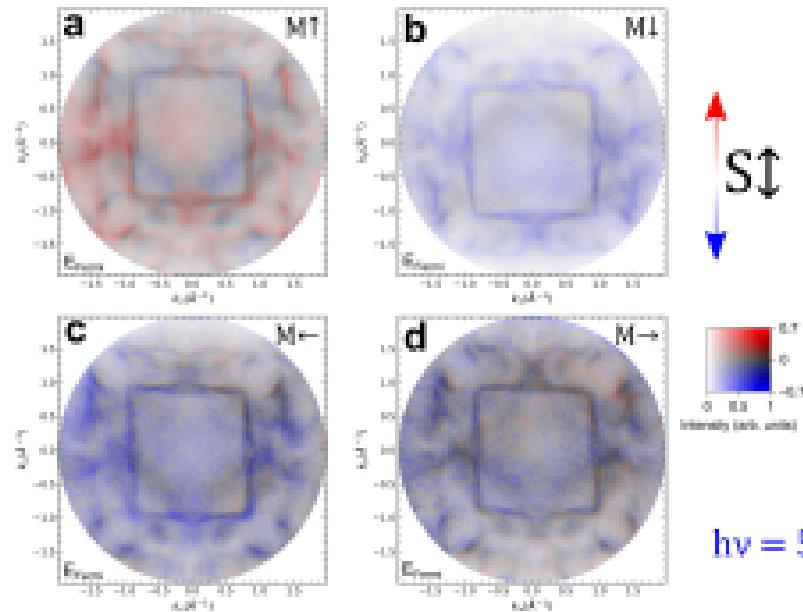
Friday, September 9, 2022, 12:30–14:00, 8001a

<https://momentum-microscopy.tz-juelich.de/>



## Spin-resolved Fermi Surface of 1.8ML FePd/Pd(100)

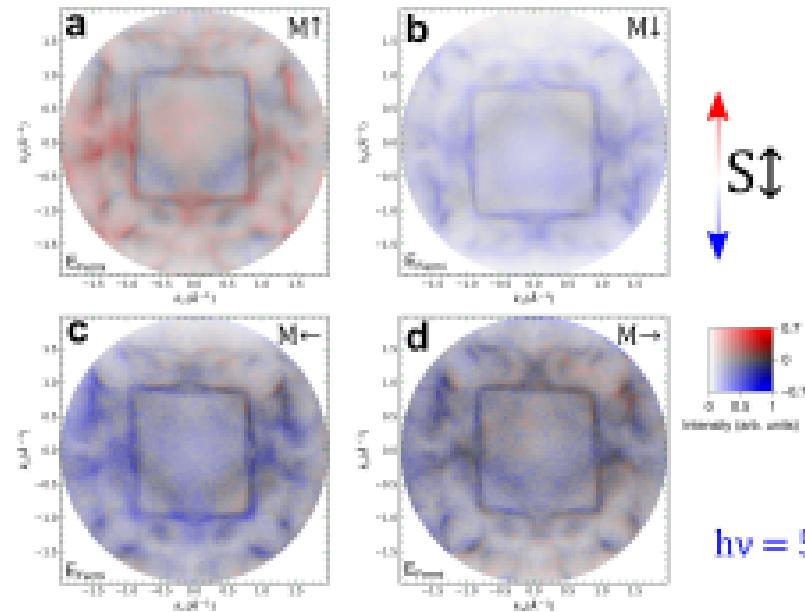
Complex non-collinear Fermi surface spin texture





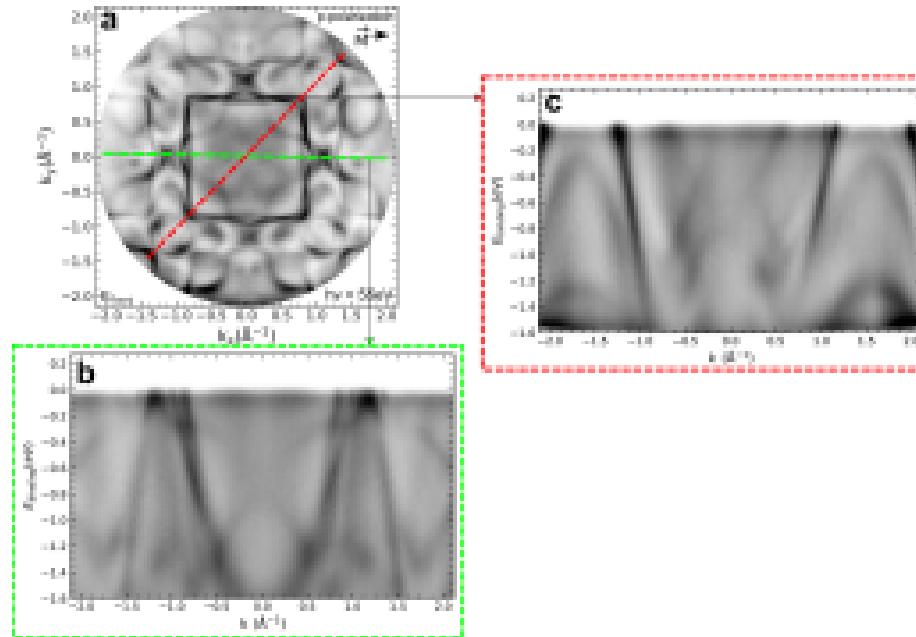
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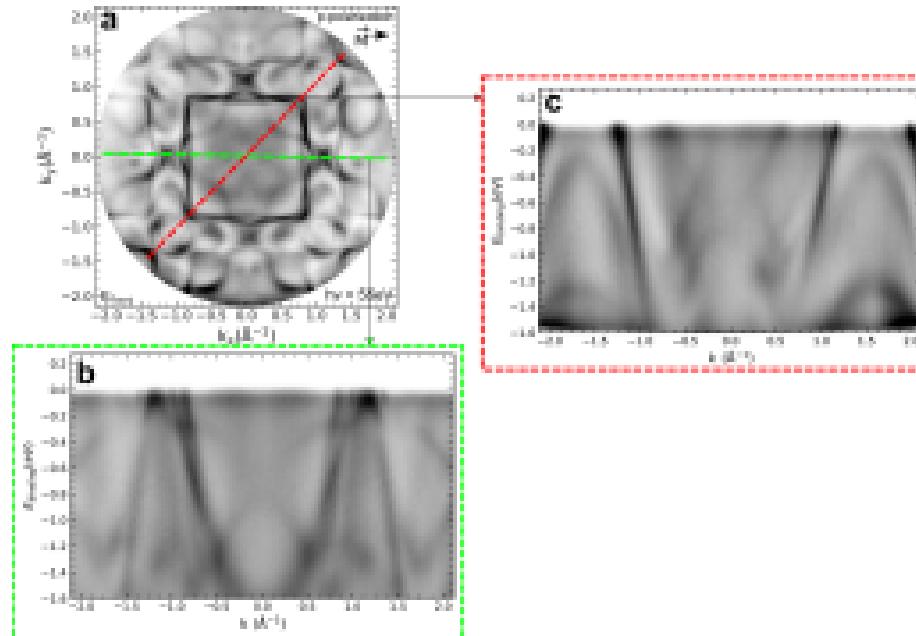


## Other interesting aspects





## Other interesting aspects



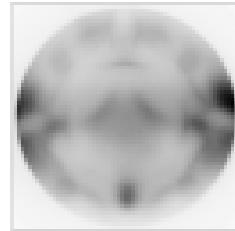


# Spin-resolved Momentum Microscopy

## Spin Resolution via W(100) Imaging Spin Filter

Reflectivity normalized

26.5eV

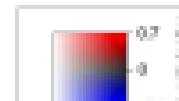


30.5eV



MA 3D: Surface Magnification  
Thursday, Sept 8, 2022

Spin-resolved Fermi Surface of Half-Metallic FePd Al<sub>0.7</sub> Monolayers

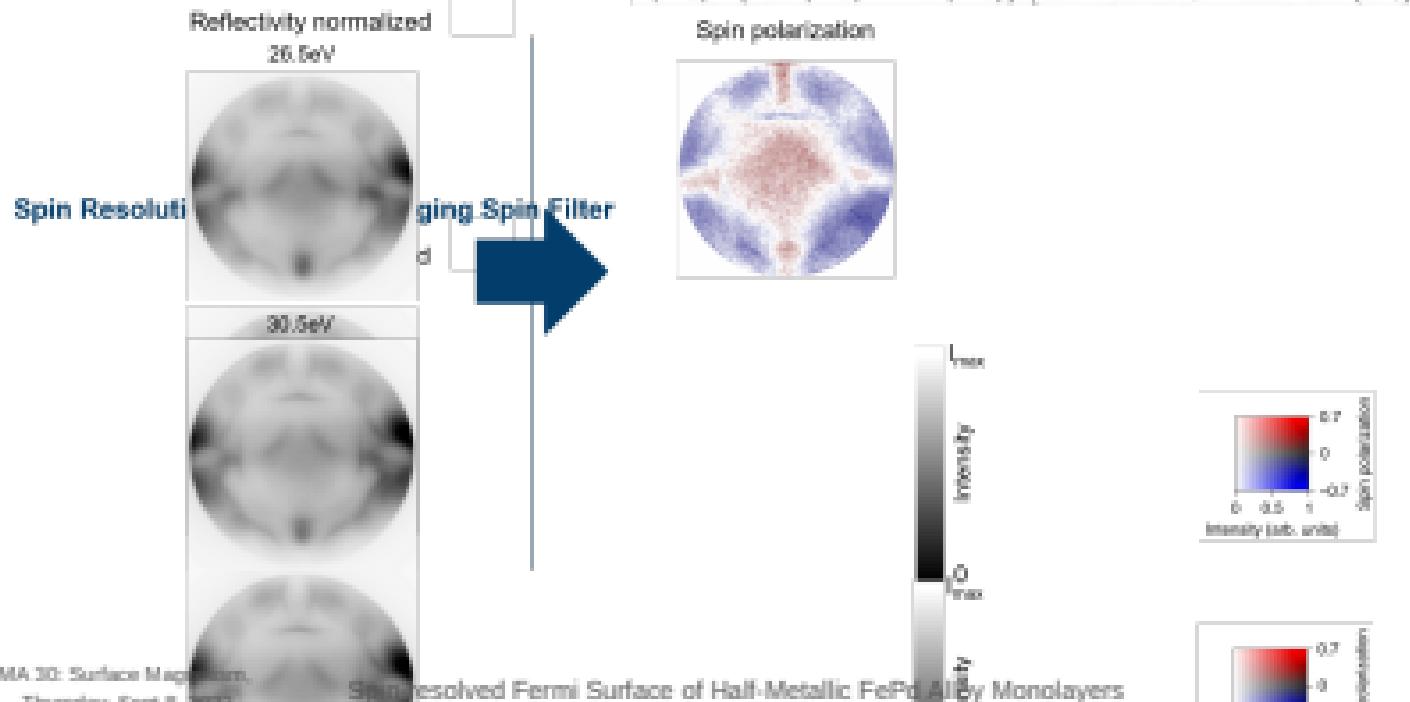




# Spin-resolved Momentum Microscopy

## Spin Resolution via W(100) Imaging Spin Filter

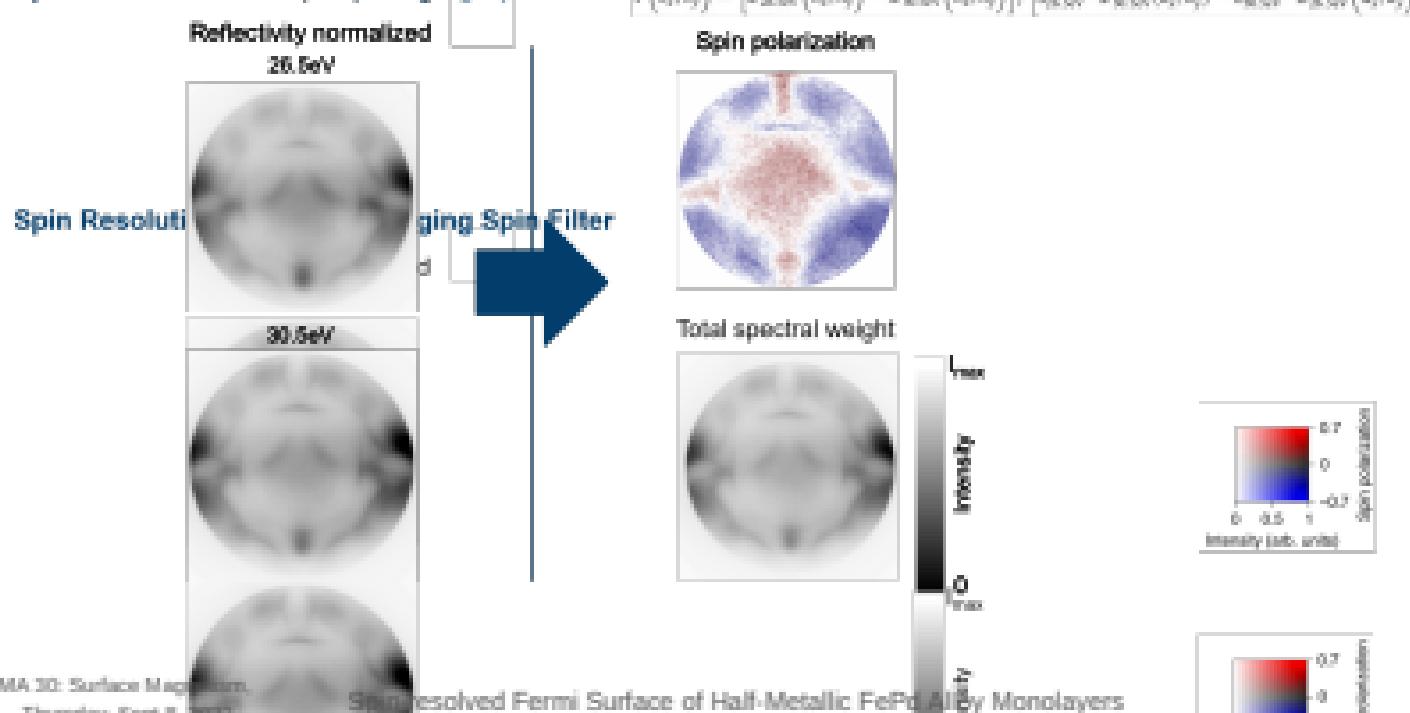
$$P(k_x, k_y) = \left[ T_{\text{MOM}}(k_x, k_y) - T_{\text{MOMV}}(k_x, k_y) \right] / \left[ S_{\text{MOMV}} \cdot T_{\text{MOM}}(k_x, k_y) - S_{\text{MOMV}} \cdot T_{\text{MOMV}}(k_x, k_y) \right]$$





# Spin-resolved Momentum Microscopy

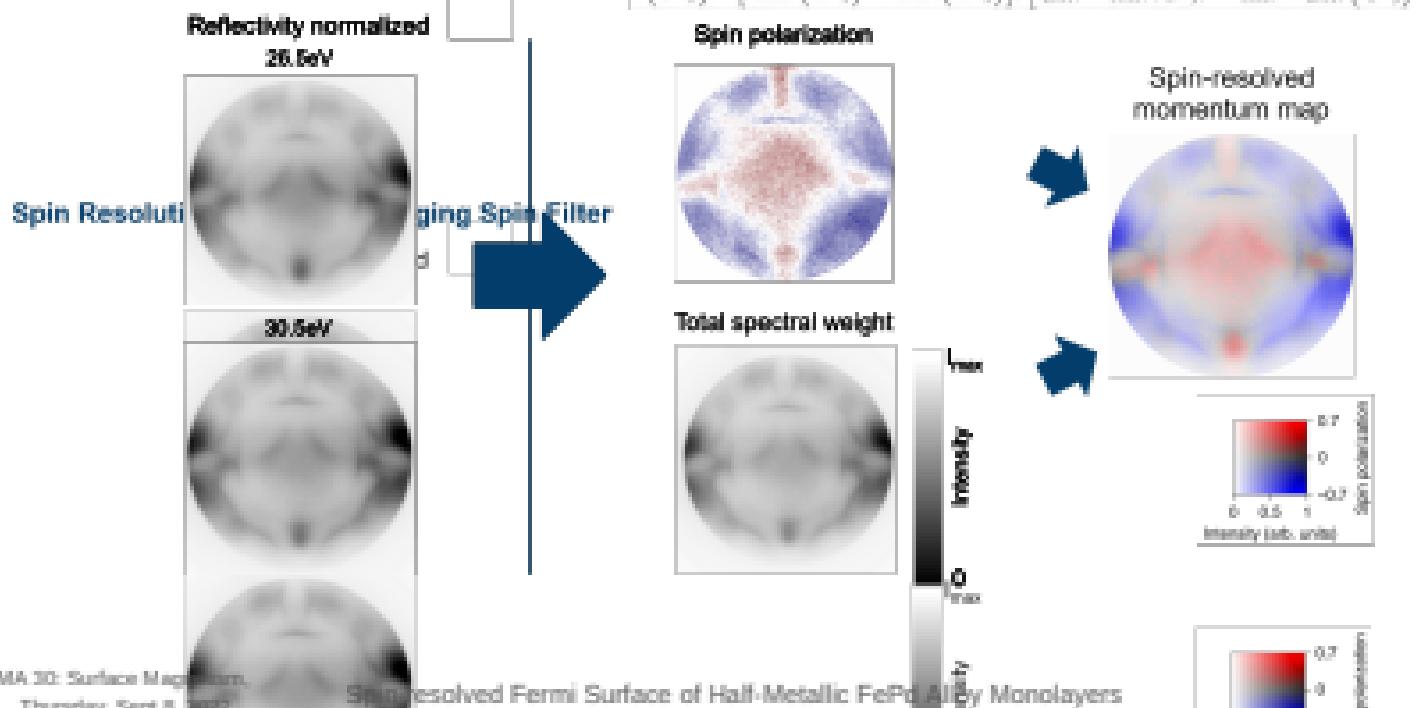
## Spin Resolution via W(100) Imaging Spin Filter





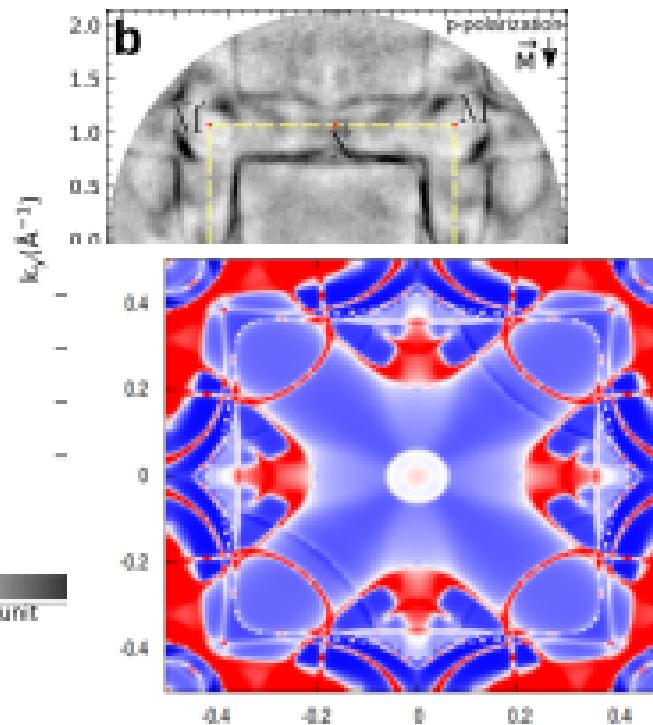
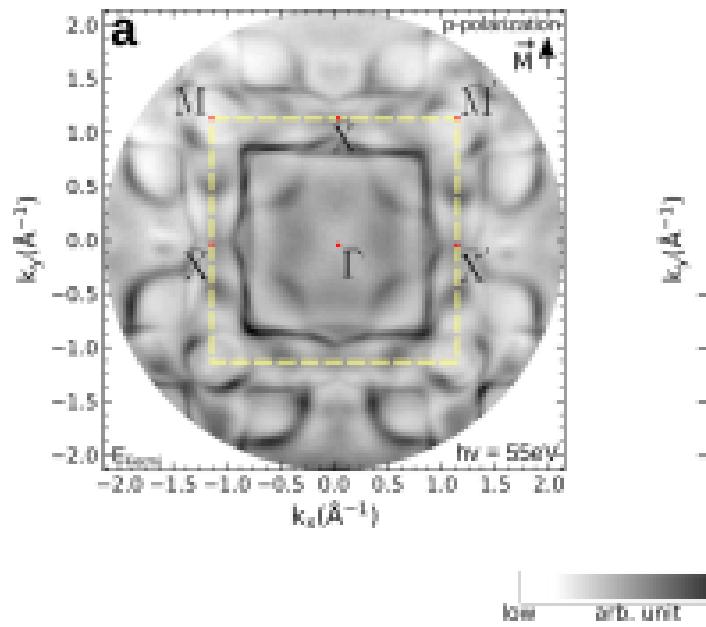
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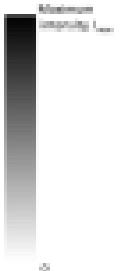
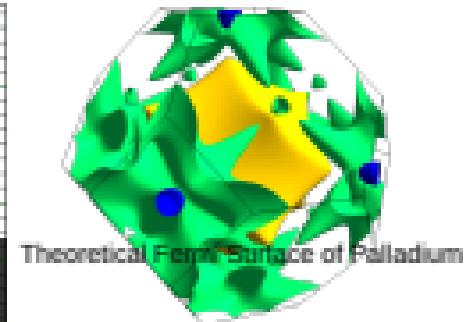
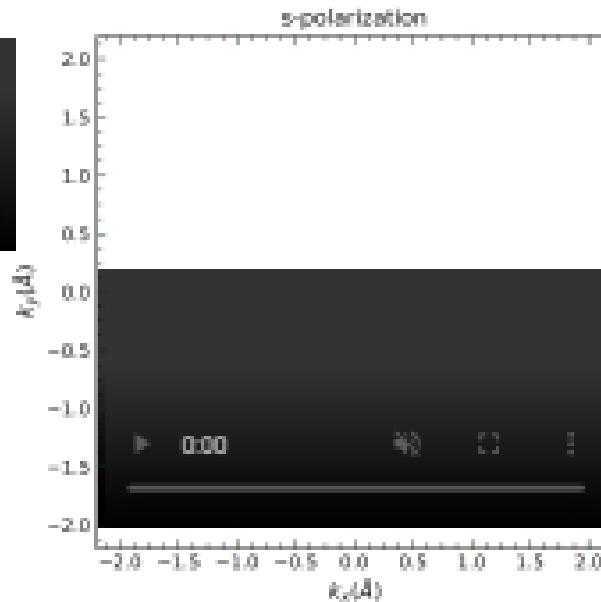
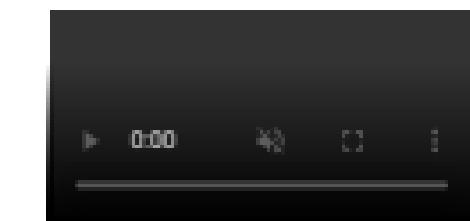


# Theoretical Calculations

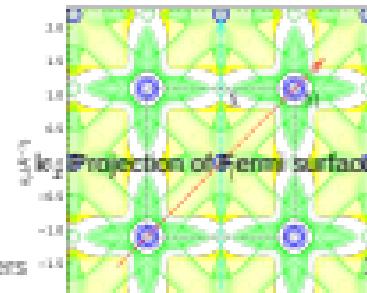




# Fermi Surface Tomography

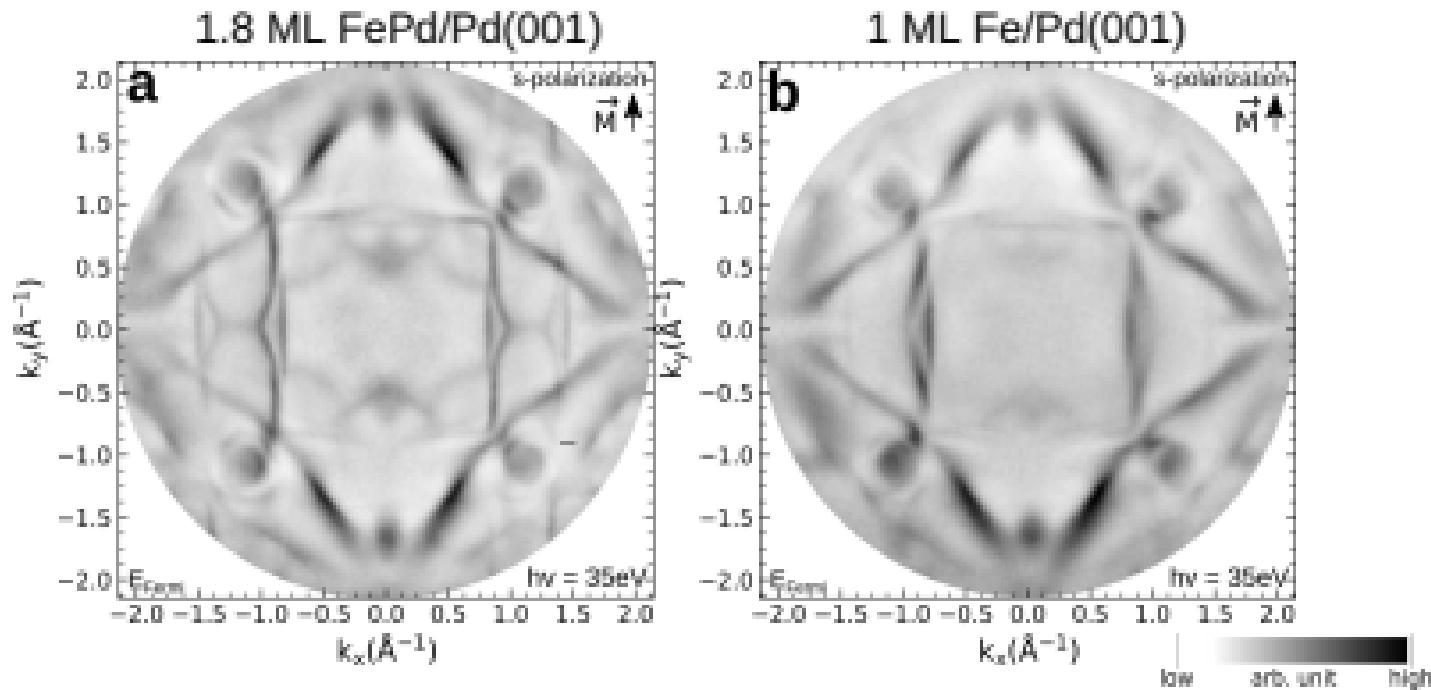


Fermi surface tomography via momentum microscopy



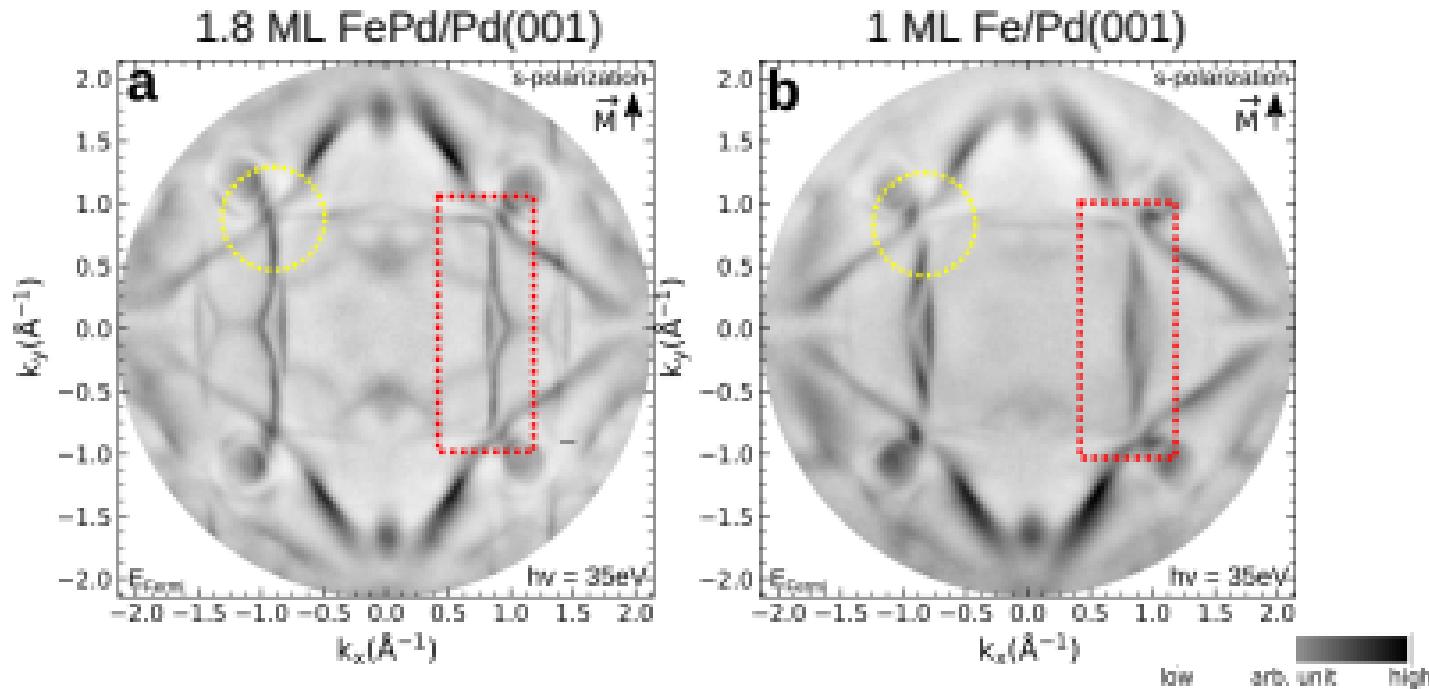


## Fermi Surface of 1.8ML FePd/Pd(001) vs 1ML Fe/Pd(001)





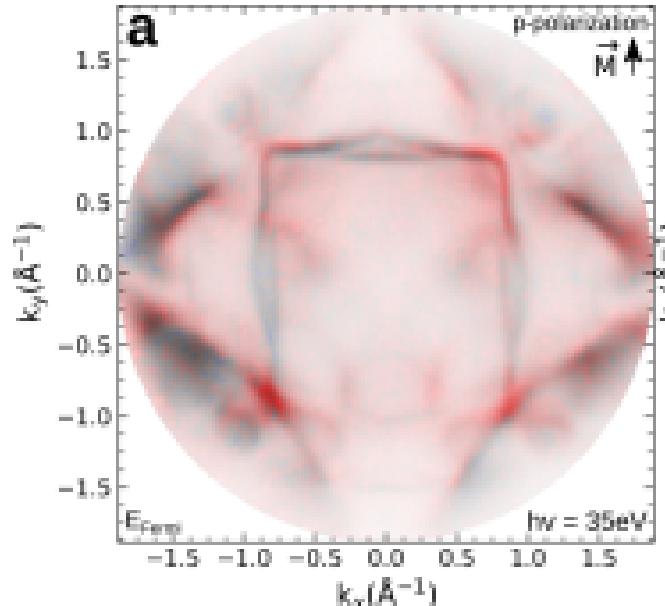
## Fermi Surface of 1.8ML FePd/Pd(001) vs 1ML Fe/Pd(001)



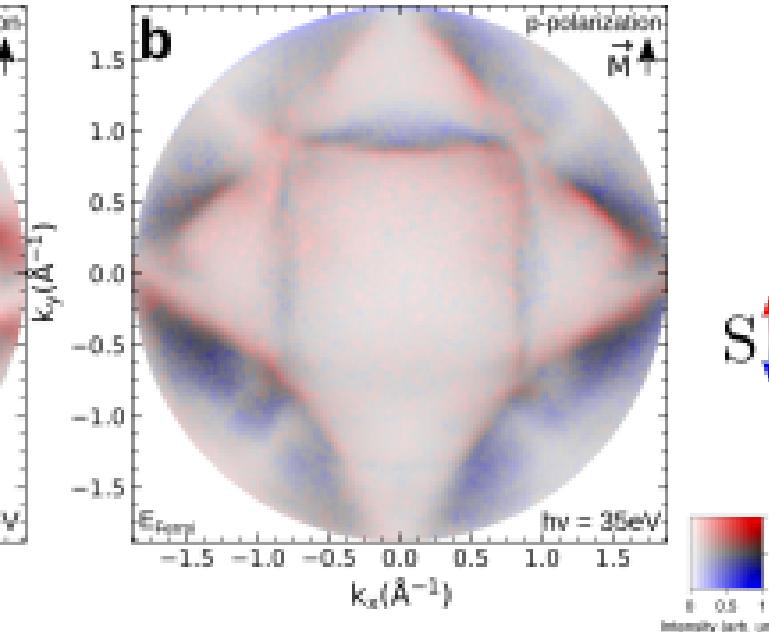


## Spin-resolved Fermi Surfaces

1.8 ML FePd/Pd(001)



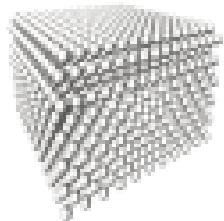
1 ML Fe/Pd(001)



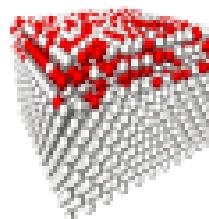


## Comparison of Fermi Surfaces

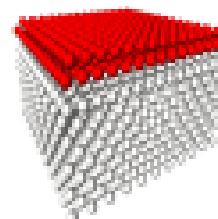
Pd(001)



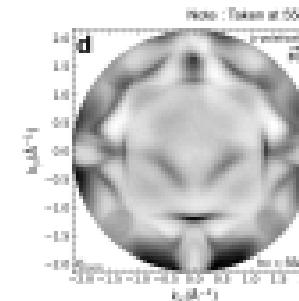
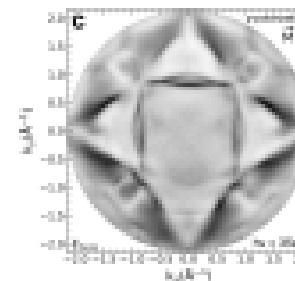
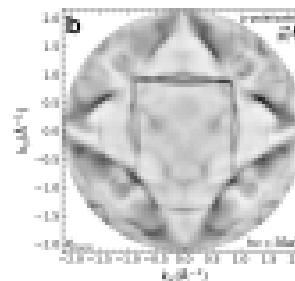
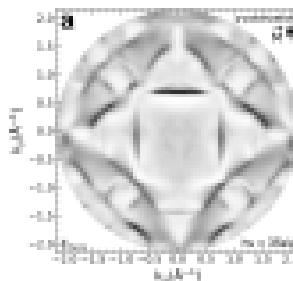
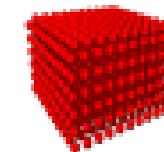
1.6ML FePd/Pd(001)



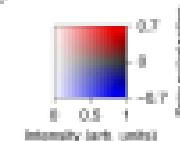
1ML Fe/Pd(001)



Fe(001), bcc



low arb. unit high

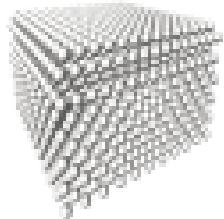


S ↑  
↓

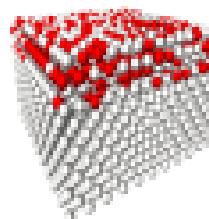


## Comparison of Fermi Surfaces

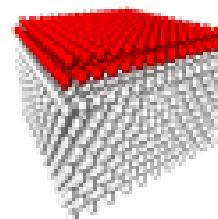
Pd(001)



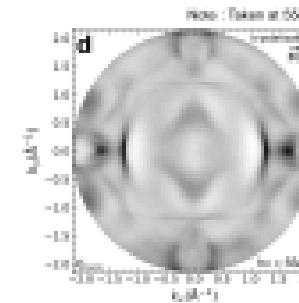
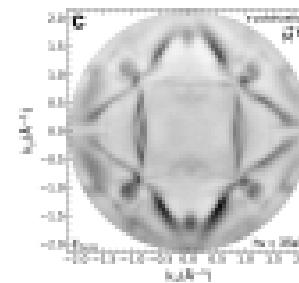
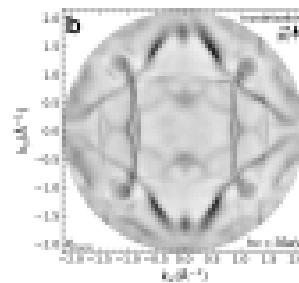
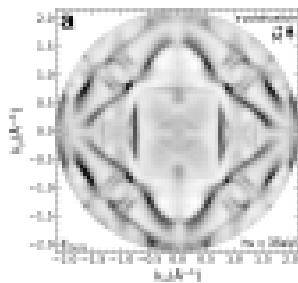
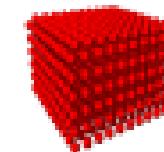
1.6ML FePd/Pd(001)



1ML Fe/Pd(001)

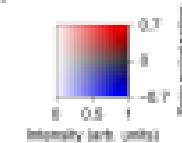


Fe(001), bcc



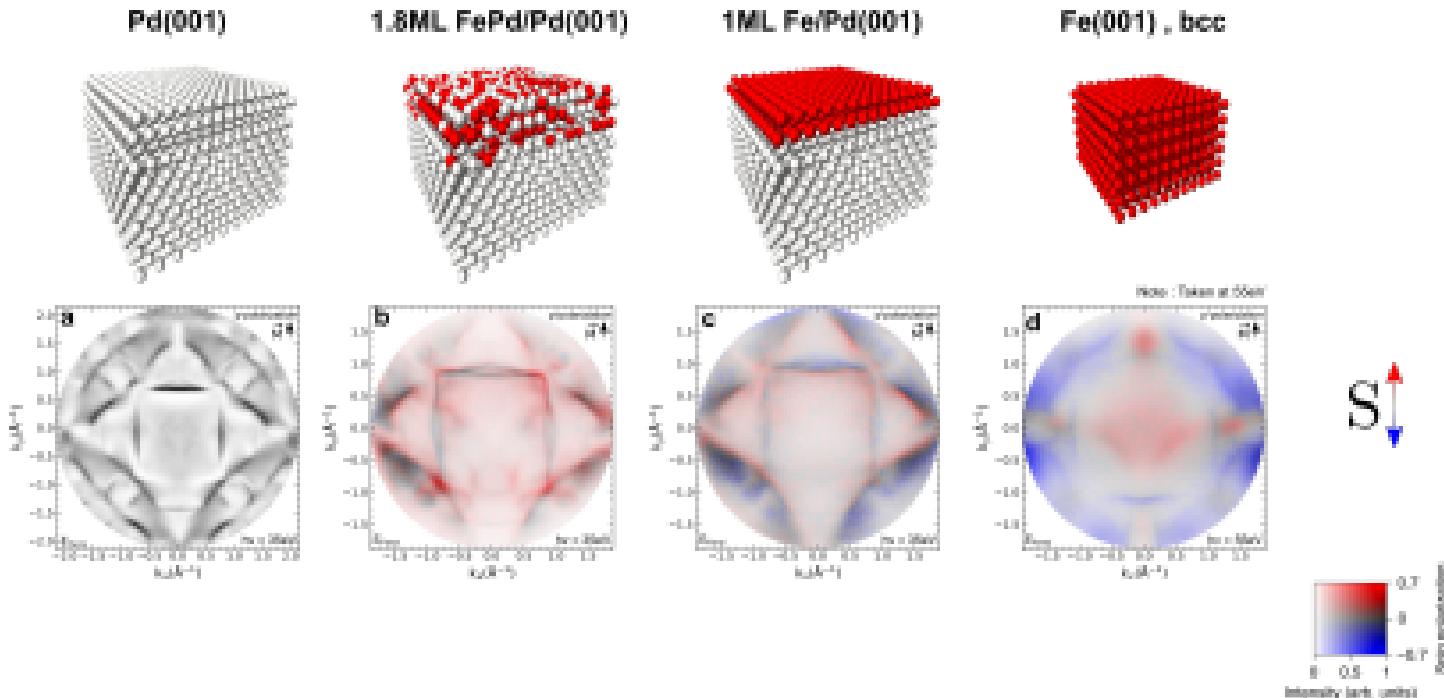
S ↗  
S ↘

low arb. unit high





## Comparison of Spin-resolved Fermi Surfaces



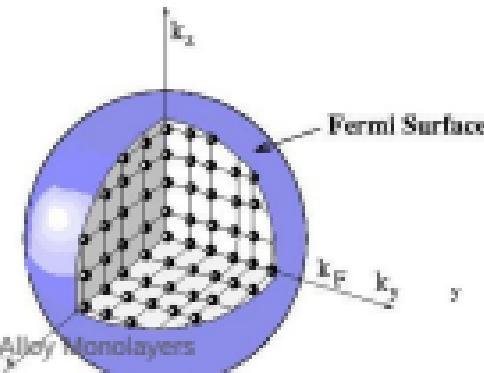


# Fermi Surface

A direct consequence of the Pauli exclusion principle

No two fermions can be in the same state.  
In their groundstate, the particles fill up all energy levels below the *Fermi energy*.

The boundary between occupied and unoccupied states





# Fermi Surface

Shape of a Fermi Surface and Periodic Potential

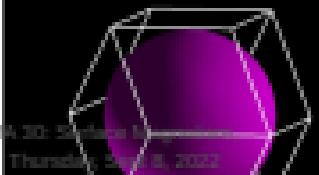


All calculations were done using the exciting code

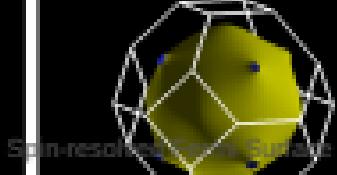
Monovalent systems in increasing periodic potential

"Noble Metals"

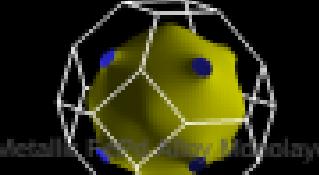
bcc Li



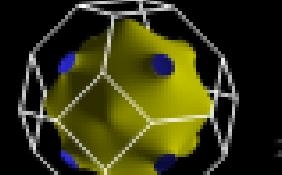
Cu



Ag



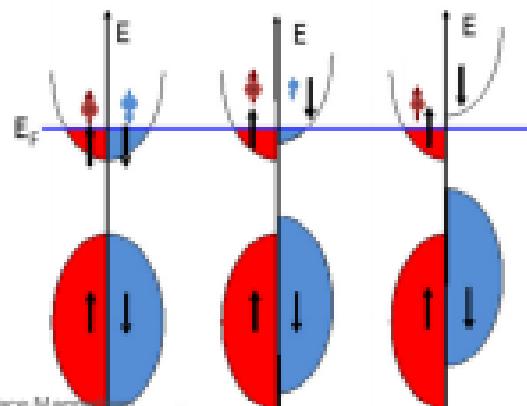
Au





# Energy Bands of Ferromagnets

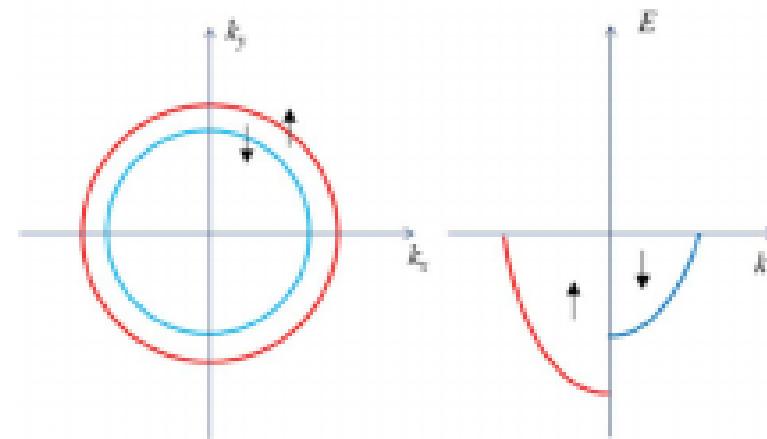
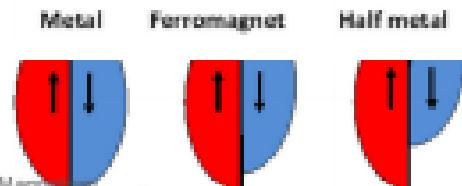
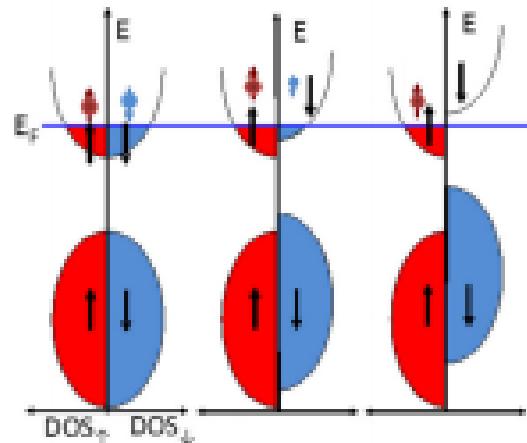
Ferromagnetism and free-electron energy band diagrams





# Energy Bands of Ferromagnets

Ferromagnetism and free-electron energy band diagrams



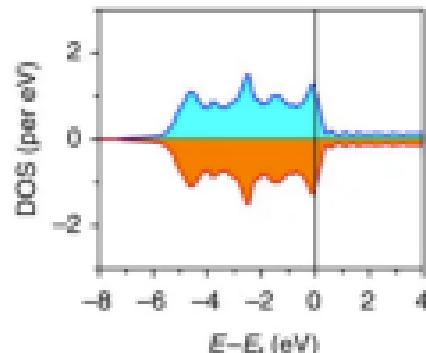
Fermi surface of a ferromagnet



# Energy Bands of Hybrid Ferromagnet

## Theoretical Calculations

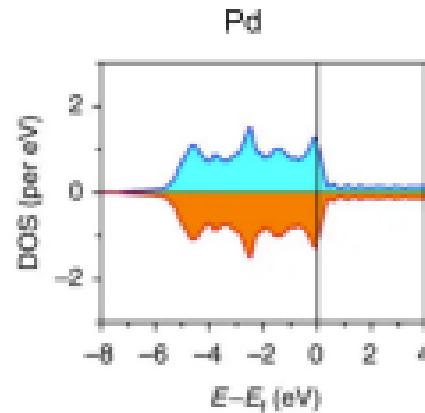
Pd



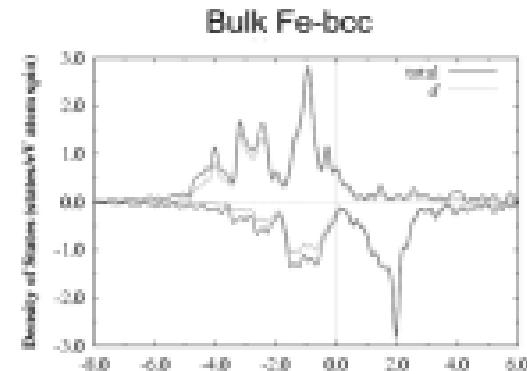


# Energy Bands of Hybrid Ferromagnet

## Theoretical Calculations



H. J. Qin, J. Kirschner, et al. Nature Communications volume 6, Article number: 6128 (2015)

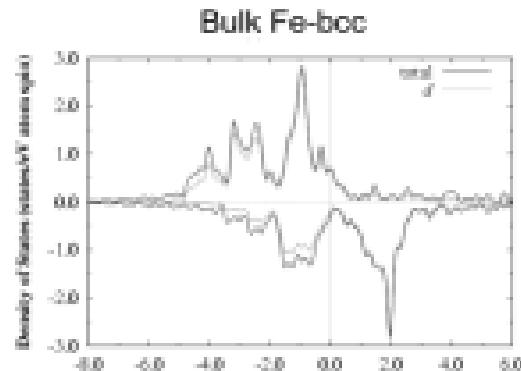
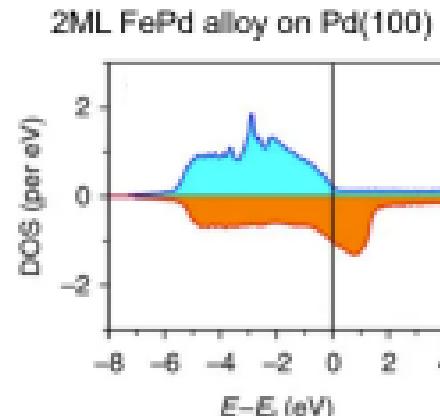
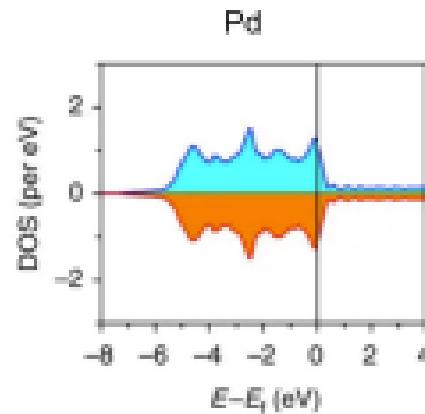


C.h. Park et al., Journal of the Korean Physical Society, Vol. 47, No. 4, (2005)

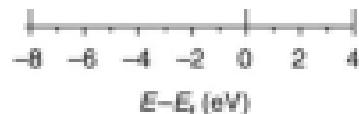


# Energy Bands of Hybrid Ferromagnet

## Theoretical Calculations



H. J. Qin, J. Kirschner, et al. Nature Communications volume 6, Article number: 6128 (2015)

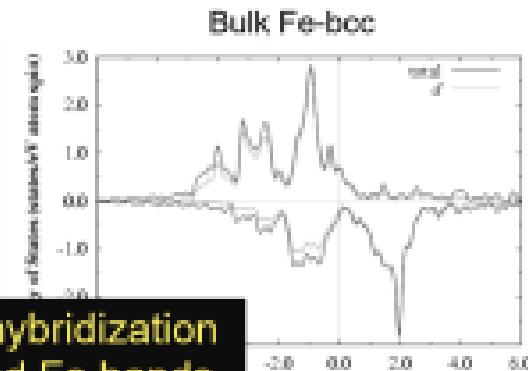
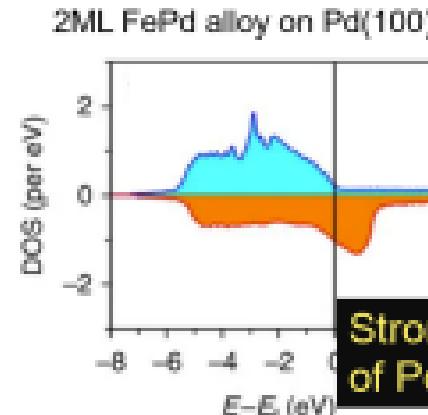
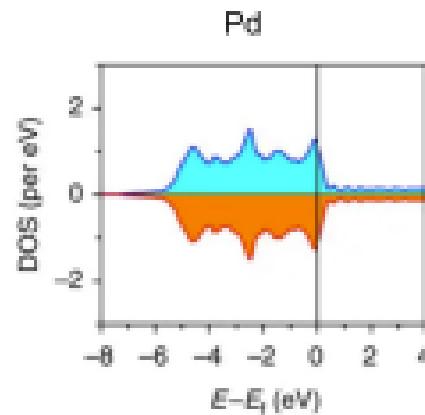


C.h. Park et al., Journal of the Korean Physical Society, Vol. 47, No. 4, (2005)

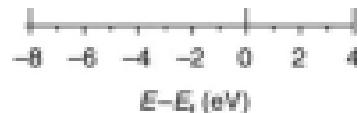


# Energy Bands of Hybrid Ferromagnet

## Theoretical Calculations



H. J. Qin, J. Kirschner, et al. Nature Communications volume 6, Article number: 6128 (2015)

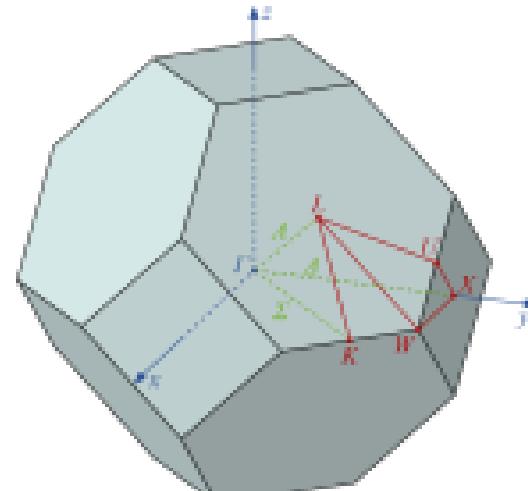
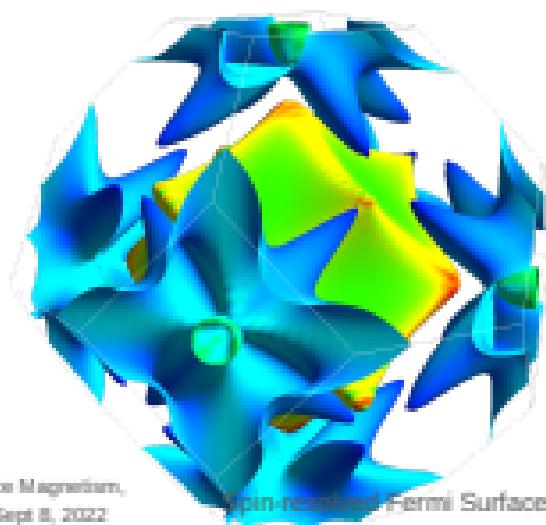


C.h. Park et al., Journal of the Korean Physical Society, Vol. 47, No. 4, (2005)



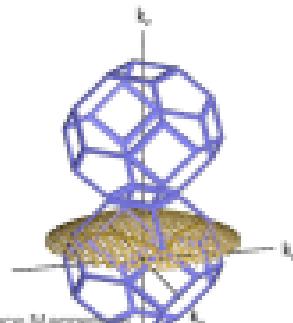
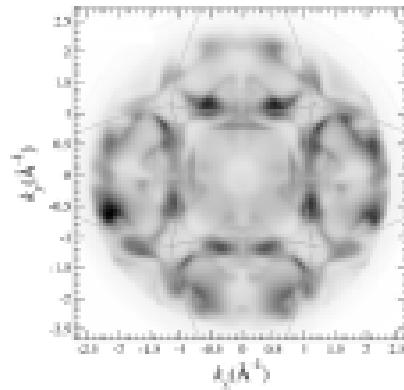
# Calculated Fermi Surface of Pd(100) (LDA+U)

exciting



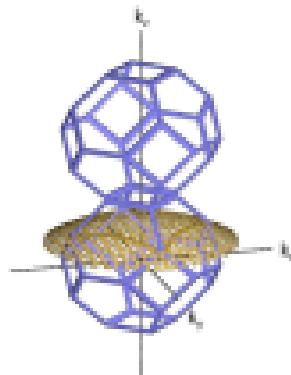
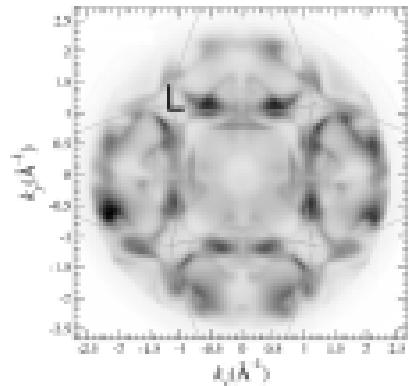


## Energy Momentum Map of Pd across High Symmetry Points

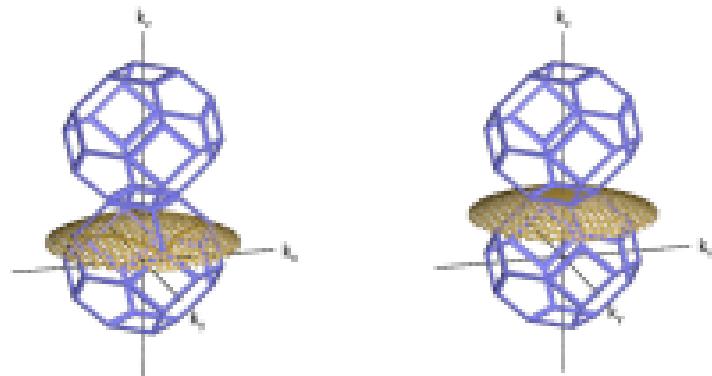
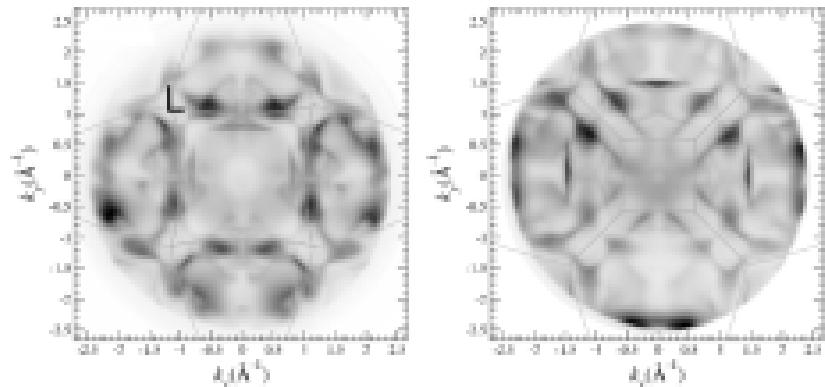




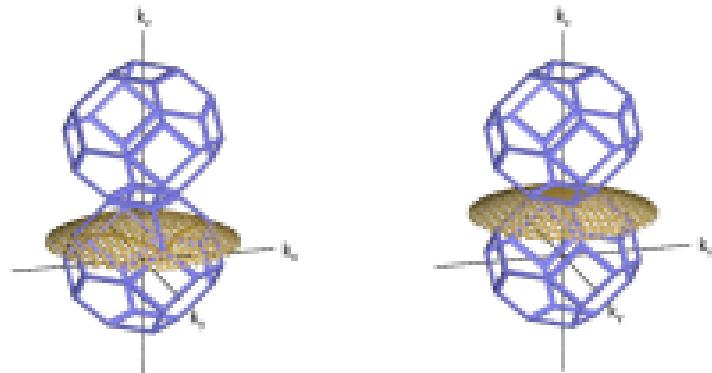
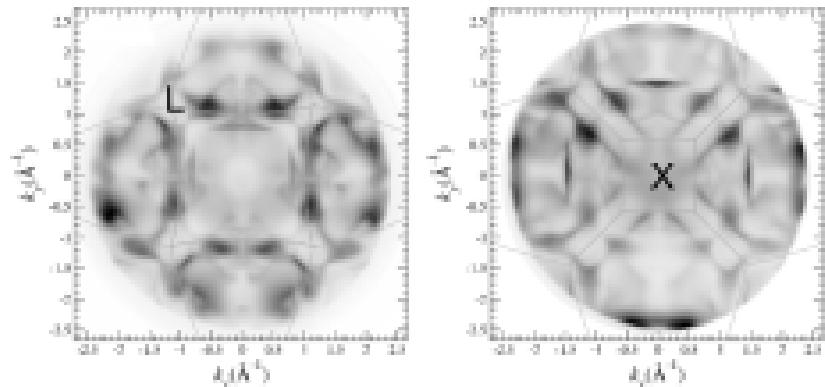
## Isosurface Momentum Map of Pd across High Symmetry Points



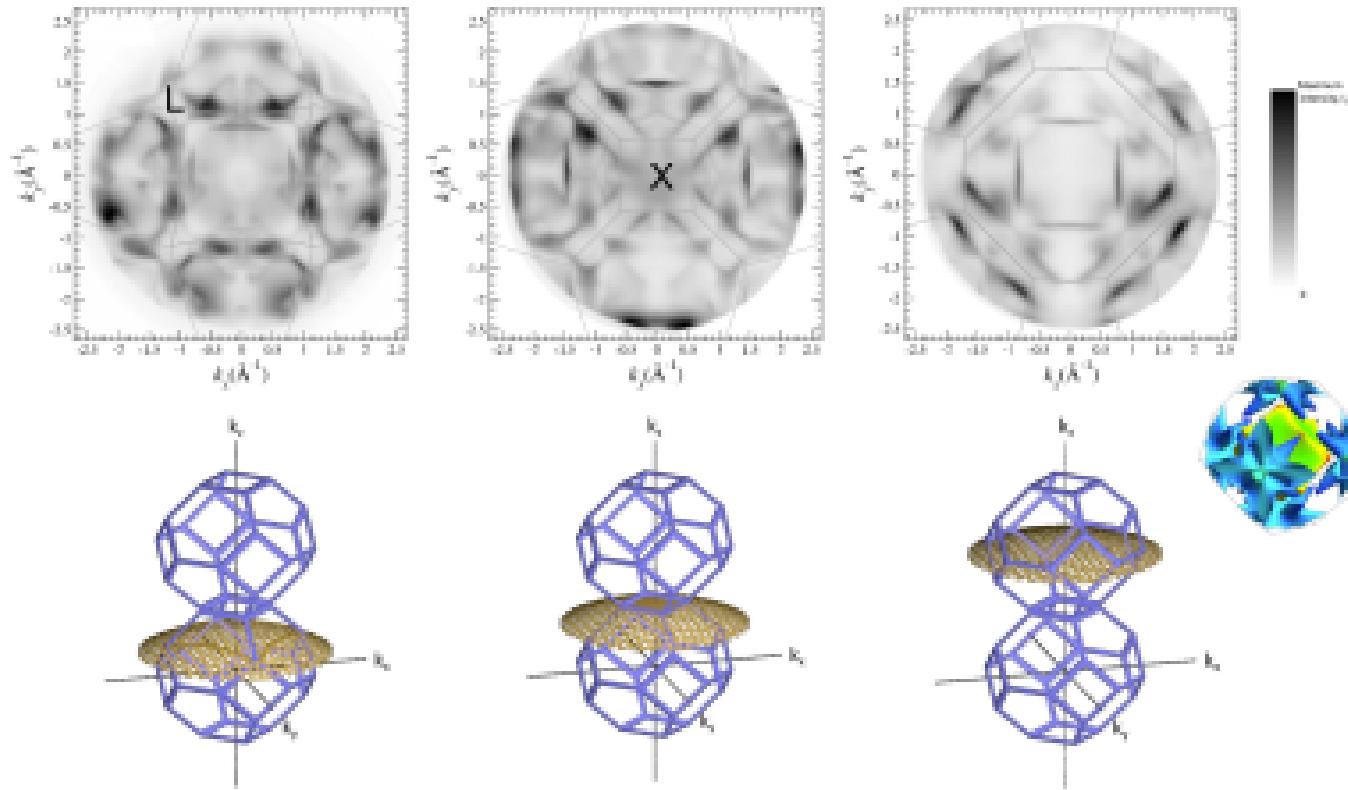
## Isoenergy Momentum Map of Pd across High Symmetry Points



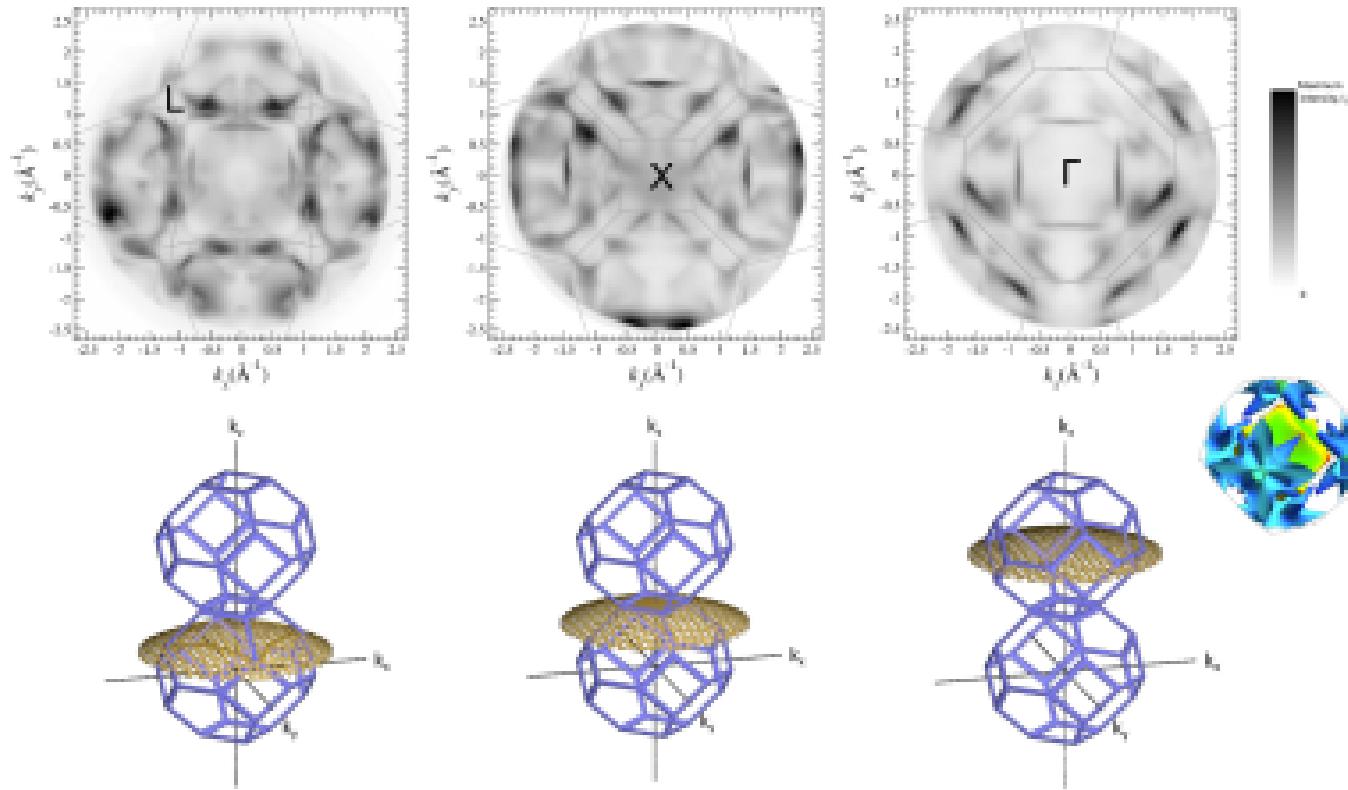
## Isoenergy Momentum Map of Pd across High Symmetry Points



# Isoenergy Momentum Map of Pd across High Symmetry Points



# Isoenergy Momentum Map of Pd across High Symmetry Points



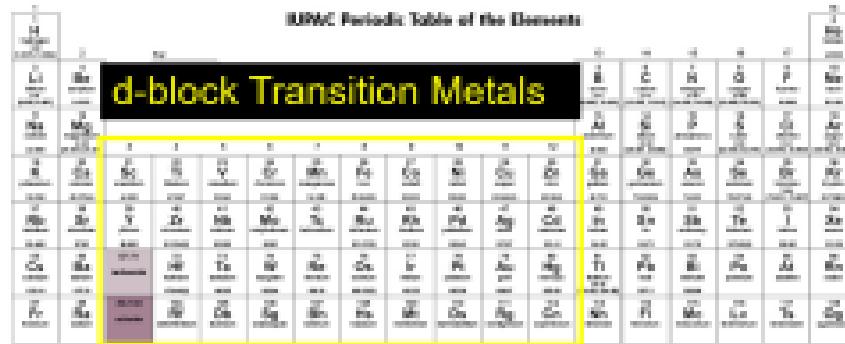


# Periodic Table of Elements

| IUPAC Periodic Table of the Elements |         |         |         |         |          |         |          |         |         |           |          |         |            |         |          |         |         |
|--------------------------------------|---------|---------|---------|---------|----------|---------|----------|---------|---------|-----------|----------|---------|------------|---------|----------|---------|---------|
|                                      |         |         |         |         |          |         |          |         |         |           |          |         |            |         |          |         |         |
| H                                    | He      | Li      | Be      | B       | C        | N       | O        | F       | Ne      | Na        | Mg       | Al      | Si         | P       | S        | Cl      | Ar      |
| Hydrogen                             | Helium  | Lithium | Boron   | Carbon  | Nitrogen | Oxygen  | Fluorine | Neon    | Sodium  | Magnesium | Aluminum | Silicon | Phosphorus | Sulfur  | Chlorine | Argon   |         |
| 1                                    | 2       | 3       | 4       | 5       | 6        | 7       | 8        | 9       | 10      | 11        | 12       | 13      | 14         | 15      | 16       | 17      | 18      |
| 1s                                   | 2s      | 2p      | 3s      | 3p      | 3d       | 4s      | 4p       | 4d      | 5s      | 5p        | 5d       | 6s      | 6p         | 6d      | 7s       | 7p      | 7d      |
| 1s2                                  | 2s2     | 2p2     | 3s2     | 3p2     | 3d2      | 4s2     | 4p2      | 4d2     | 5s2     | 5p2       | 5d2      | 6s2     | 6p2        | 6d2     | 7s2      | 7p2     | 7d2     |
| 1s2 2s2                              | 2s2 2p2 | 2p2 3s2 | 3s2 3p2 | 3p2 3d2 | 3d2 4s2  | 4s2 4p2 | 4p2 4d2  | 4d2 5s2 | 5s2 5p2 | 5p2 5d2   | 5d2 6s2  | 6s2 6p2 | 6p2 6d2    | 6d2 7s2 | 7s2 7p2  | 7p2 7d2 | 7d2 8s2 |



# Periodic Table of Elements



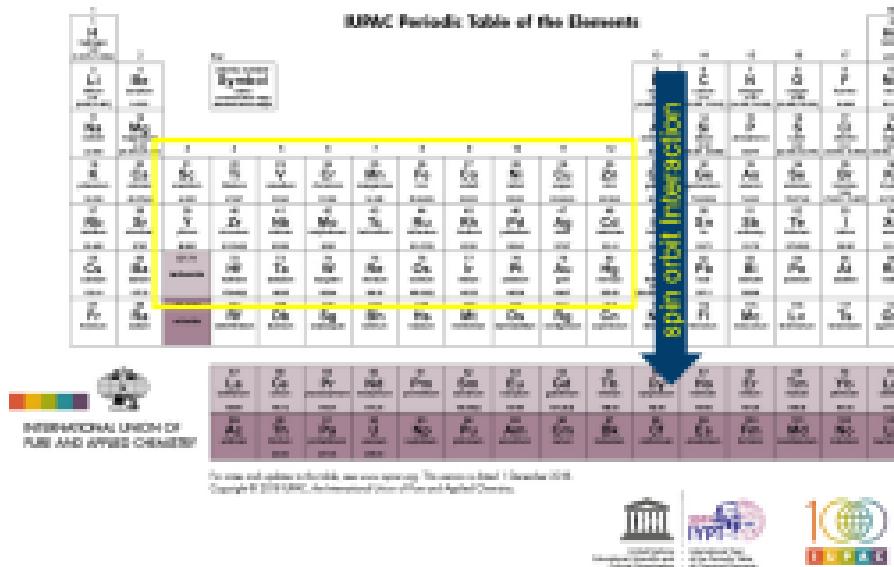
INTERNATIONAL UNION  
OF  
PURE AND APPLIED CHEMISTRY

This use and abuse of this table was recently discussed in *Elementa: Earth & Planetary Science*.  
Source: © 2019 IUPAC. International Union of Pure and Applied Chemistry.



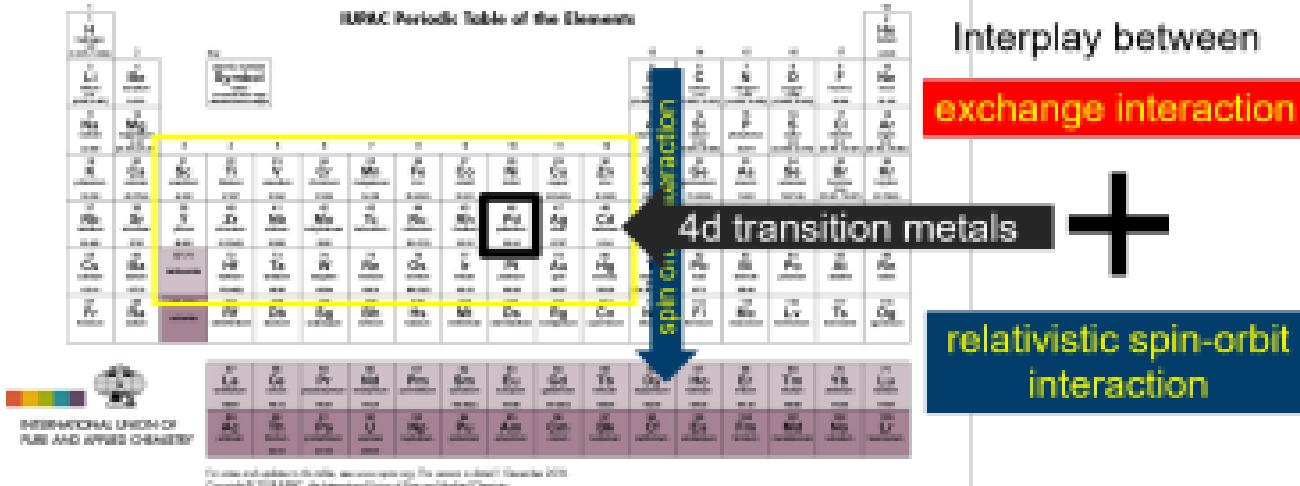


# Periodic Table of Elements



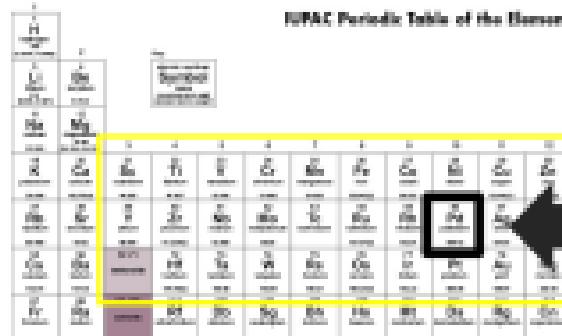


# Periodic Table of Elements





# Periodic Table of Elements



INTERNATIONAL UNION  
PURE AND APPLIED CHEMISTRY

|    |    |    |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| Mg | Al | Si | P | S | Cl | Ar | K  | Ca | Sc | Ti | V  | Cr | Mn | Fe | Co | Ni | Cu | Zn |
| Li | Be | B  | N | O | F  | Ne | Rb | Na | Ta | Hf | Ta | Ru | Rh | Pd | Pt | Ag | Ca |    |

Source of data in the table: [www.iupac.org](http://www.iupac.org). Last update: 10/10/2010.  
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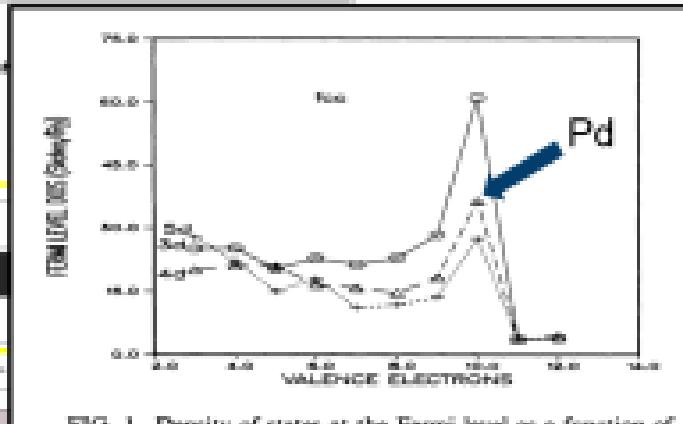
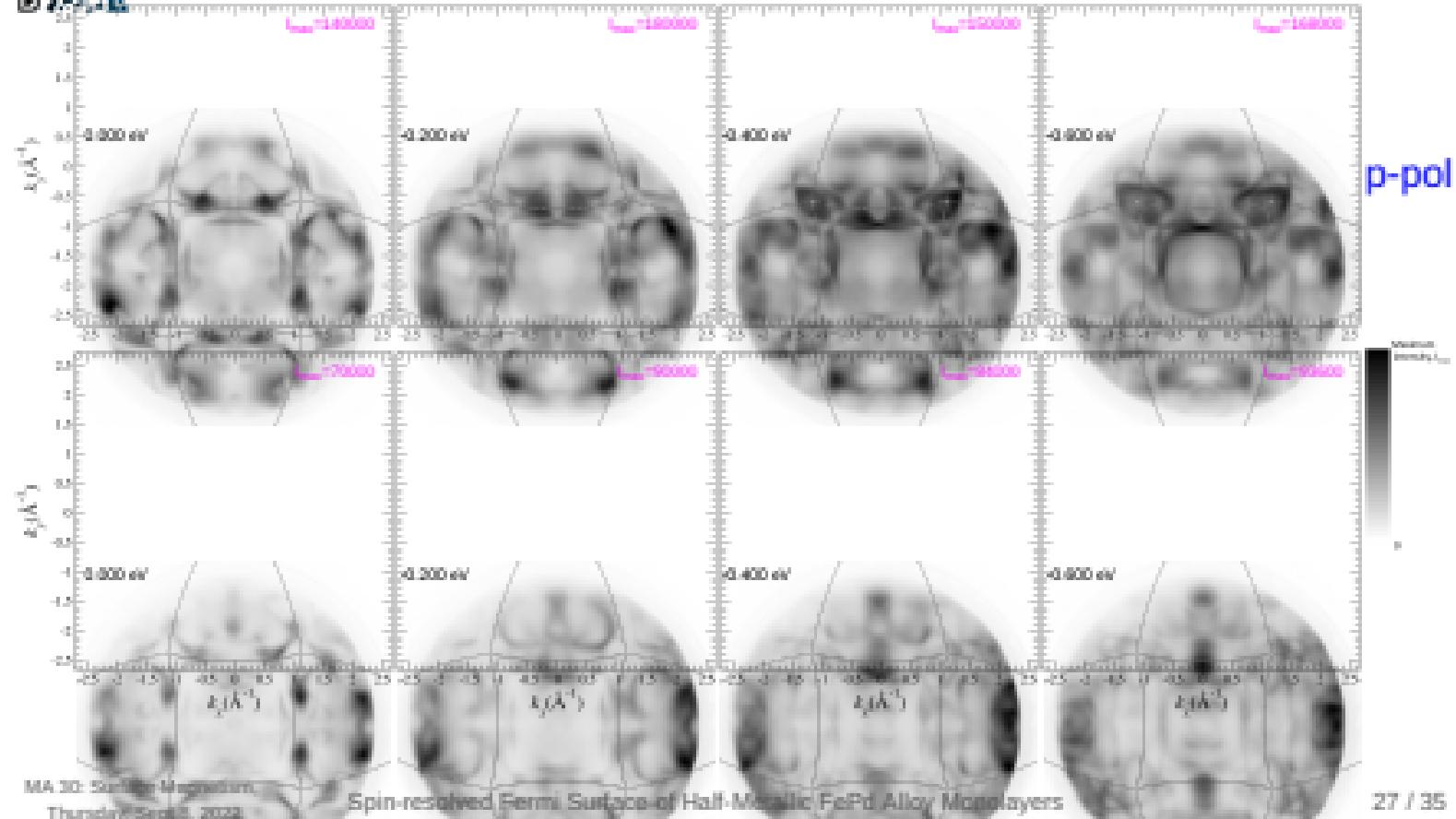


FIG. 1. Density of states at the Fermi level as a function of valence electrons for the fcc metals.

Sigalas, M., Papaconstantopoulos, D. A., & Bacalis, N. C. (1992). *Physical Review B*, *45*(11), 5777–5783

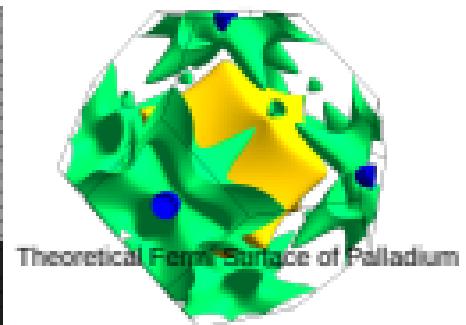
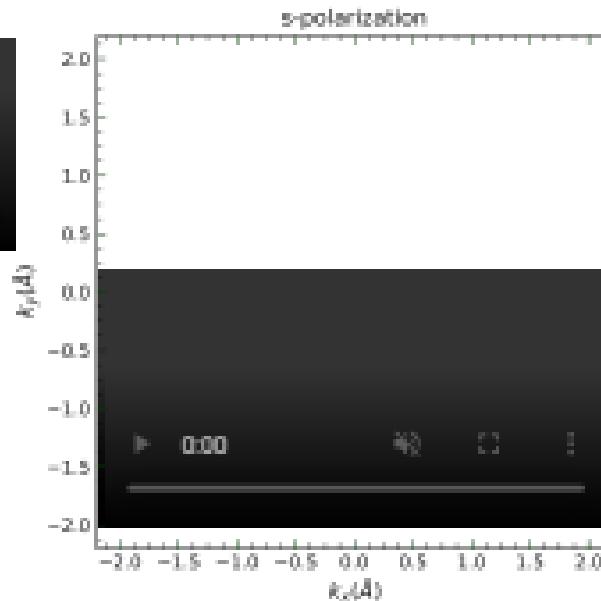
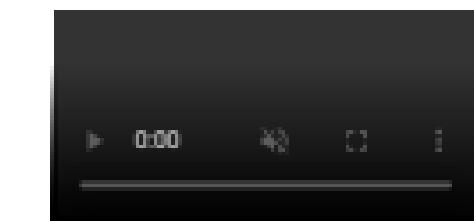


# Isocenergy Momentum Map across L-point @ $h\nu=55\text{eV}$

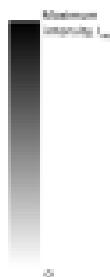




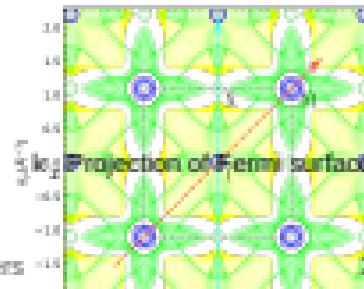
# Fermi Surface Tomography of Pd(100)



Theoretical Fermi Surface of Palladium



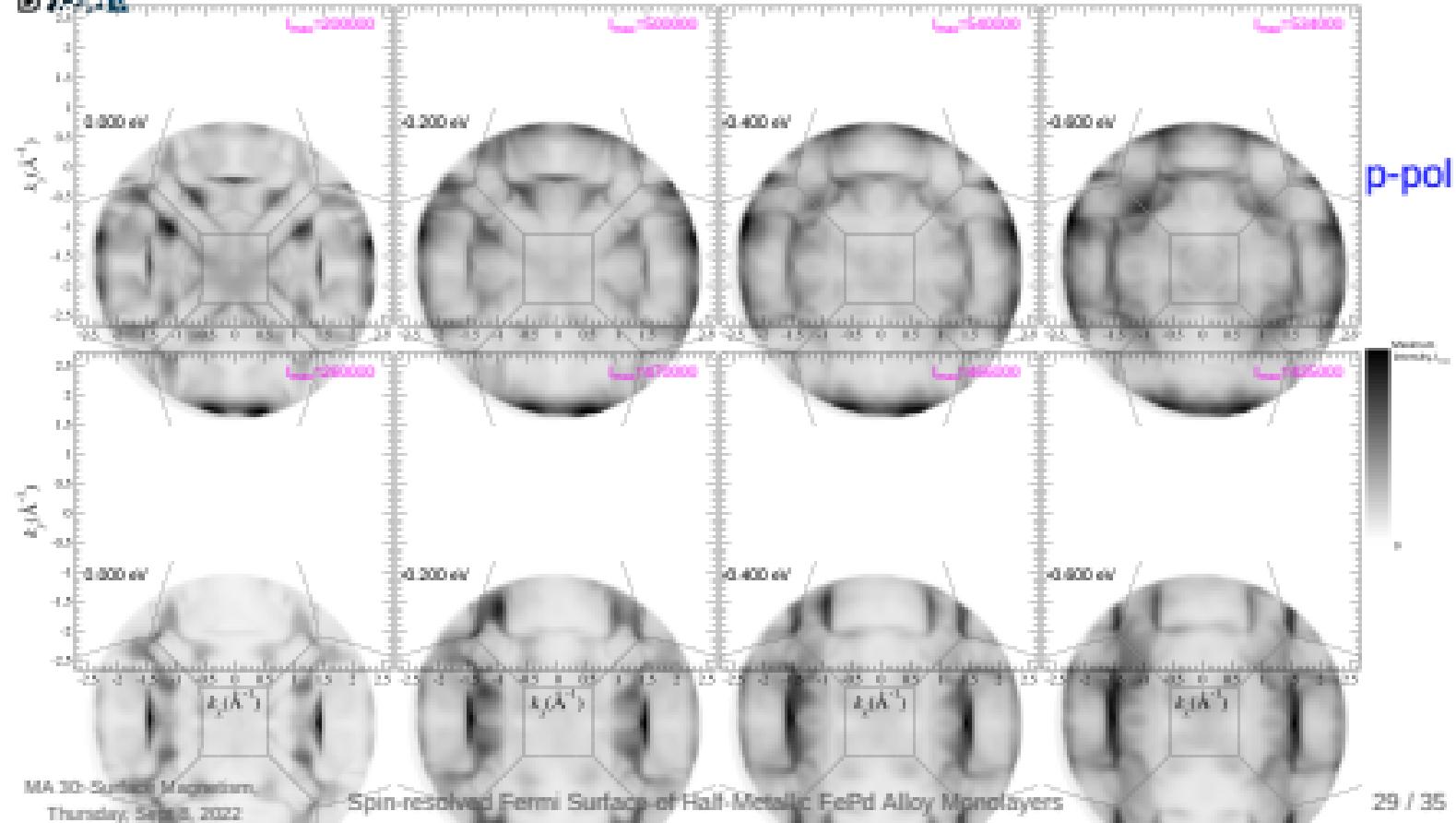
Fermi surface tomography via momentum microscopy



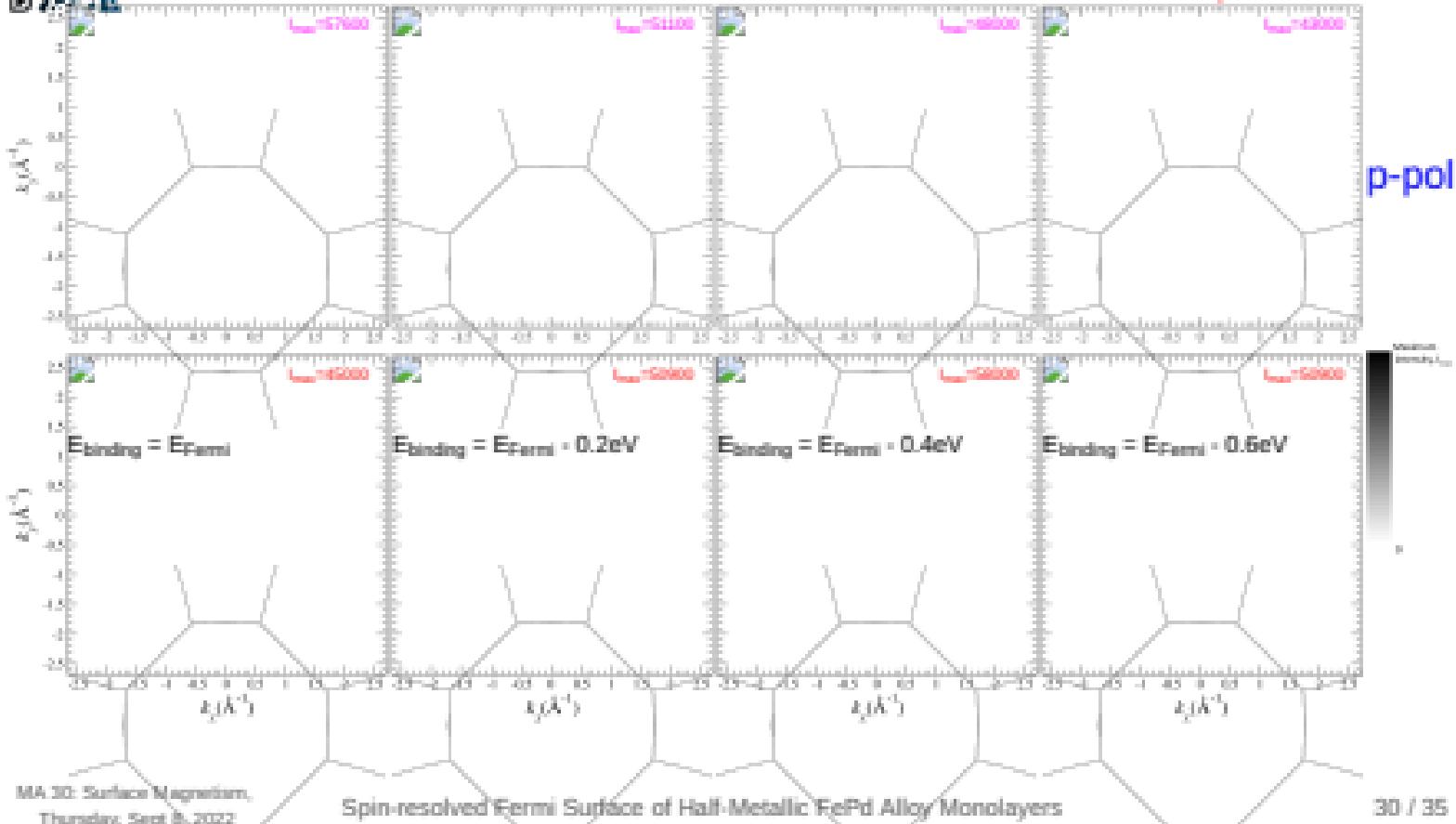
Projection of Fermi surface



# Isocenergy Momentum Map across X-point @ $h\nu=75\text{eV}$



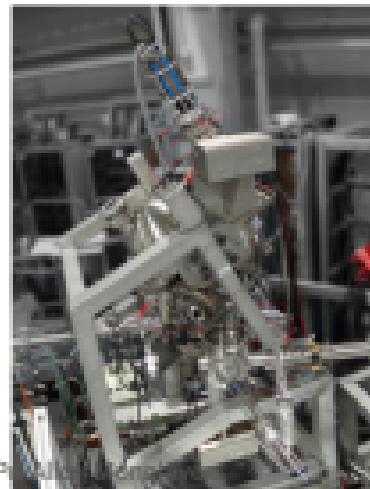
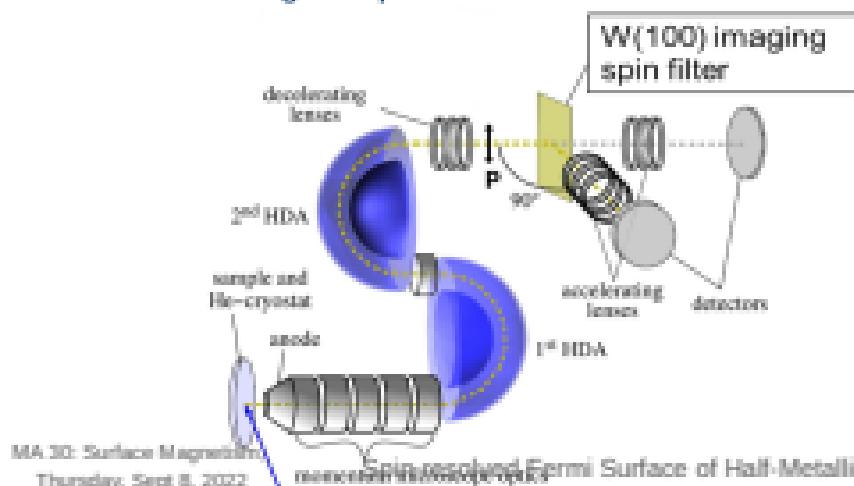
# Isocenergy Momentum Map across $\Gamma$ -point @ $h\nu=155\text{eV}$





# The Momentum Microscope

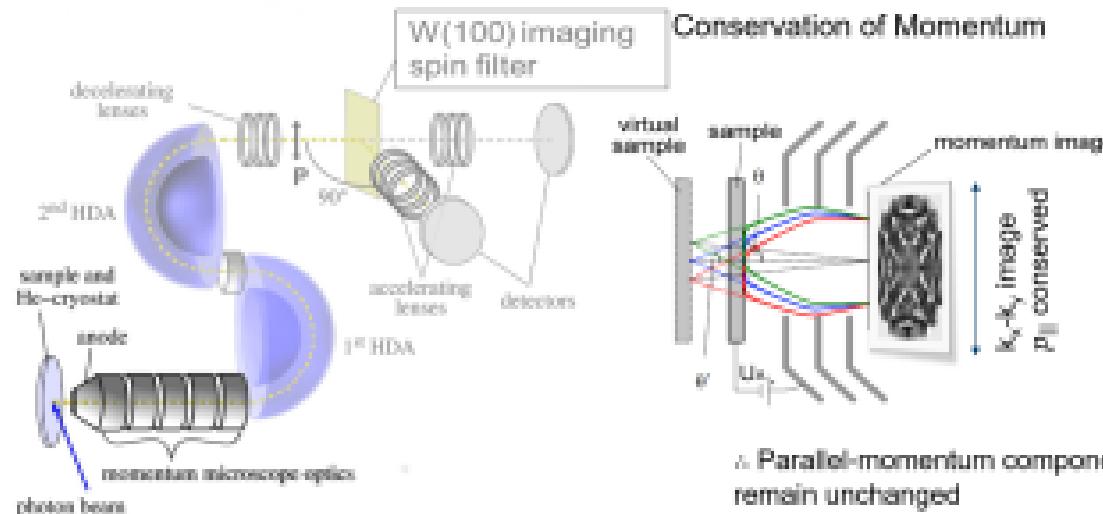
## Direct Probing of k-space





# The Momentum Microscope

## Direct Probing of k-space



MA 3D: Surface Magnetism  
Thursday, Sept 8, 2022

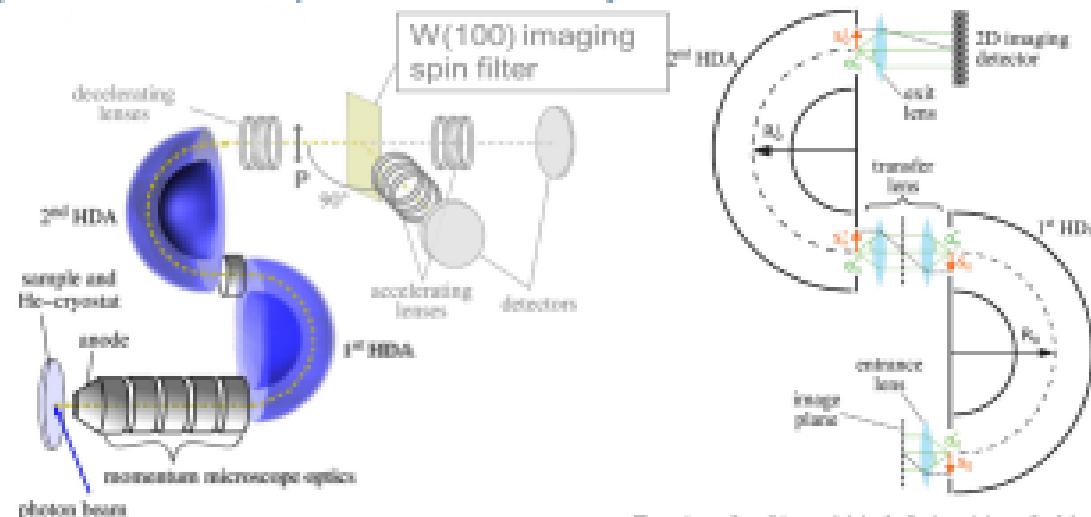
momentum-resolved Fermi Surface of Half-Metallic FeP





# The Momentum Microscope

## Energy Resolution via Hemispherical Deflection Analyzers



Tusche, C.; Krasyuk, A. & Kirschner, J.  
Ultramicroscopy , Vol. 150 , pp. 520-529 , 2015

Tusche, C.; Chen, Y.J. & Schneider, G. M.  
& Kirschner, J. Ultramicroscopy , Volume  
206, November 2019, 112815

Y



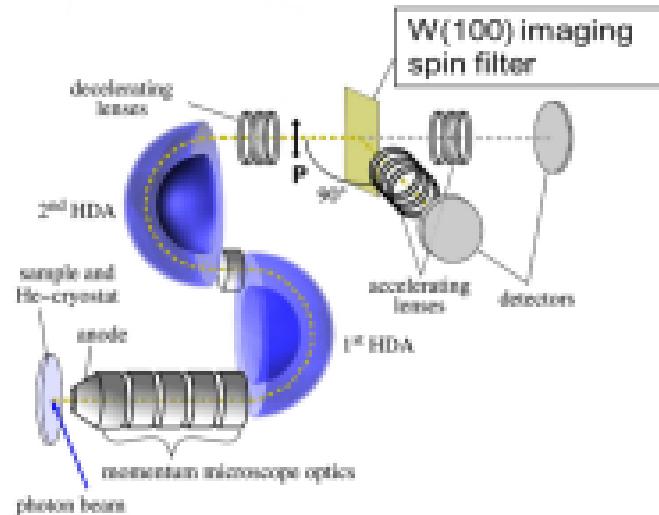
MA 3D: Surface Magnetism  
Thursday, Sept 8, 2022



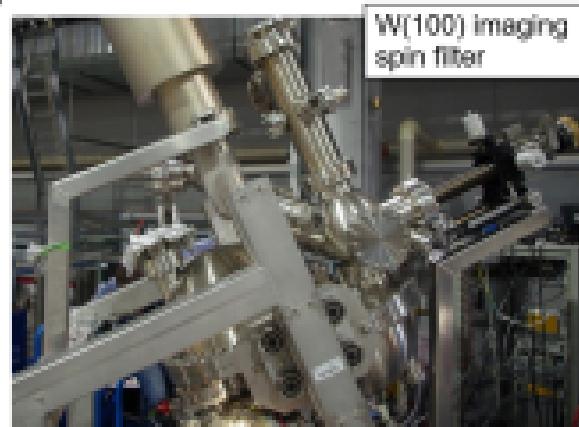


# The Momentum Microscope

Spin Resolution via W(100) Imaging Spin Filter



Tusche, C.; Krasyuk, A. & Kirschner, J.  
Ultramicroscopy , Vol. 150 , pp. 520-529 , 2015

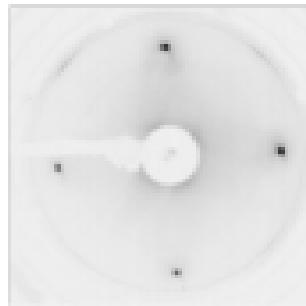


MA 3D: Surface Magnetism  
momentum resolved Fermi Surface of Half-Metallic FeP  
Thursday, Sept 8, 2022





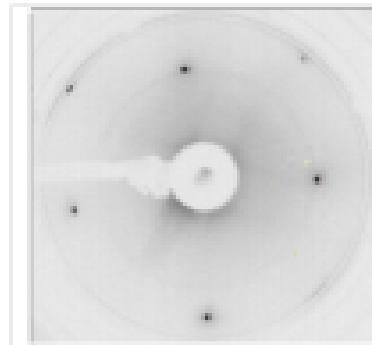
## Supplementary



LEED Pd(100) at 56eV

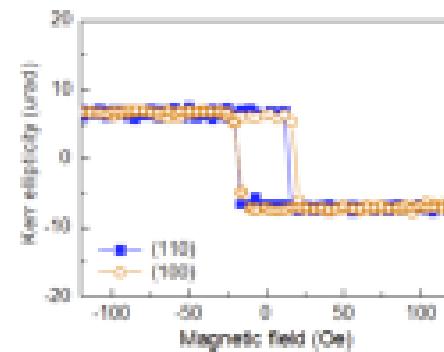
MA 3D: Surface Magnetism.

Thursday, Sept 8, 2022:



LEED 1.8ML FePd/Pd(100)  
at 70eV

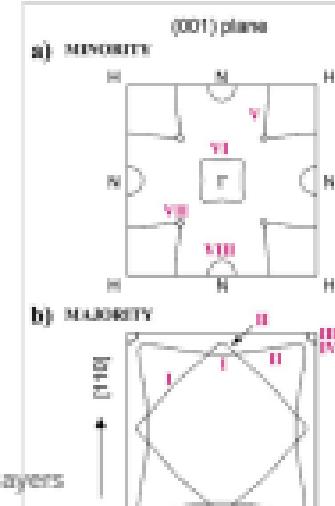
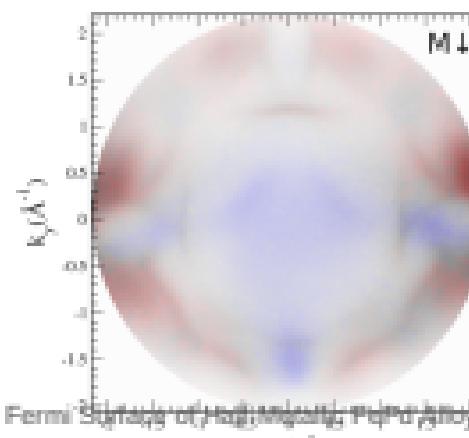
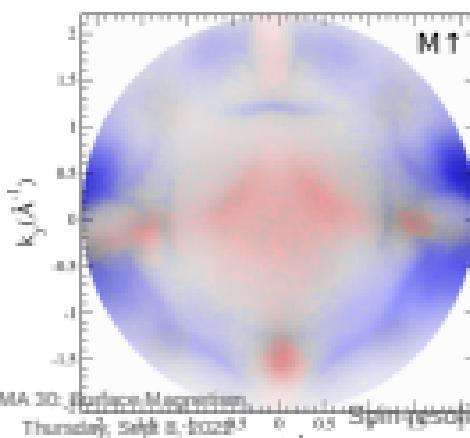
Spin-resolved Photoemission of Half-Metallic FePd Alloy M



MOKE of 2ML FePd/Pd(100).  
Courtesy of Dr. Y.J. Chen



## Supplementary





# Supplementary