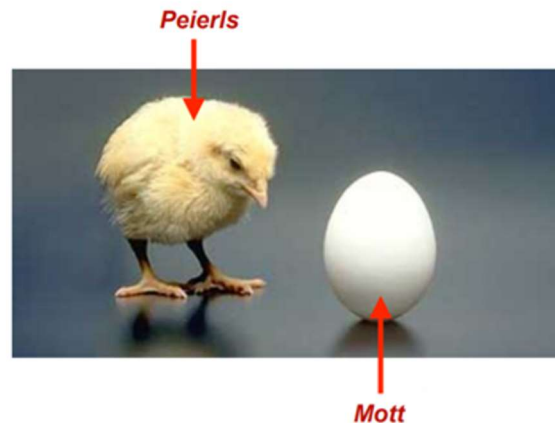


# Electronic structure of the metal-to-insulator transition in $\text{VO}_2$ : the chicken-and-egg dilemma of condensed matter

Emma David, Daisuke Shiga, Amitayush Jha-Thakur, Maximilian Thees, Pedro Henrique Rezende Gonçalves, Alexandre Antezak, Xianglin Cheng, Tatsuhiko Kanda, Taehyun Kim, Emmanouil Frantzeskakis, Franck Fortuna, Hiroshi Kumigashira, Andres Santander-Syro



# A nice research team = nice physics



Andres Santander



Franck Fortuna



Emmanouil Frantzeskakis



Pedro Rezende



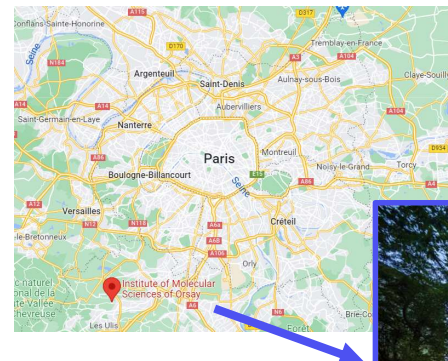
Amitayush Jha Thakur



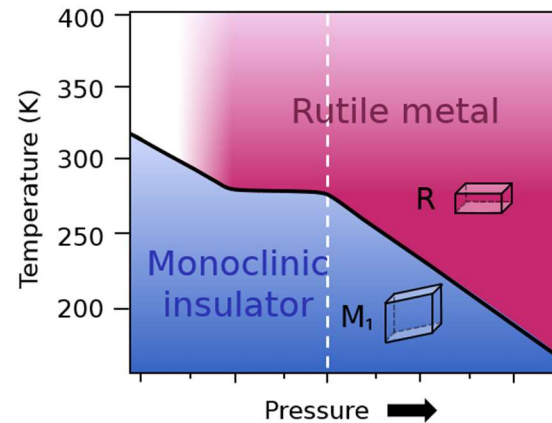
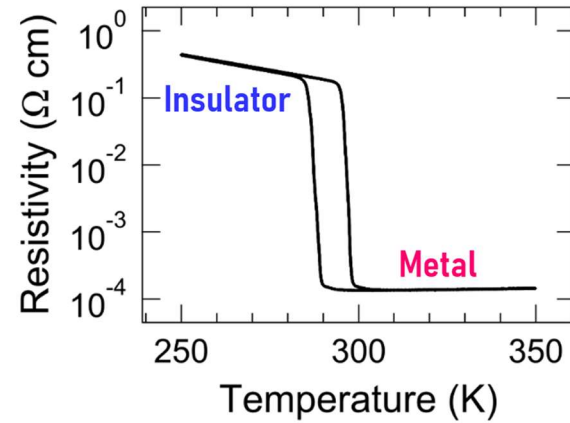
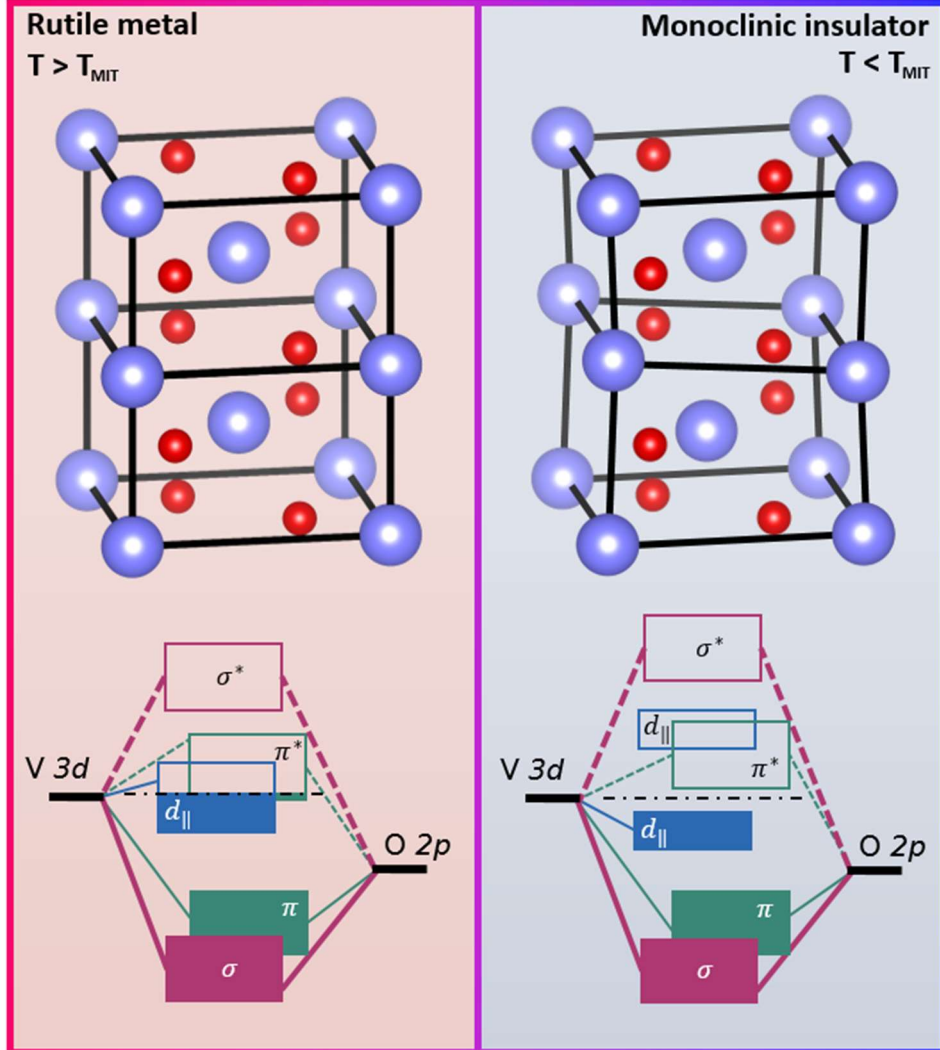
Emma David



Alexandre Antezak



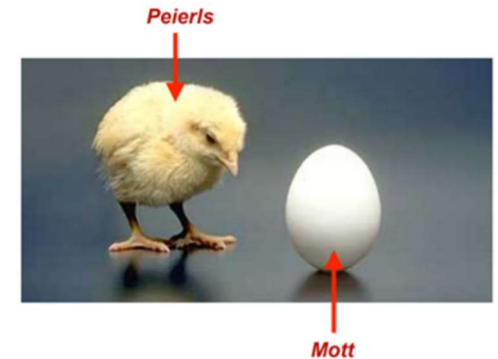
# Introducing: $V O_2$



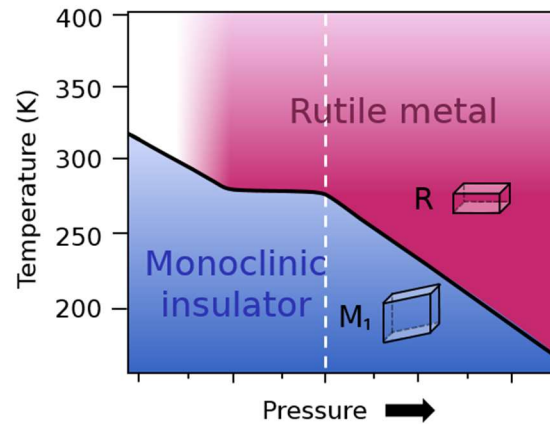
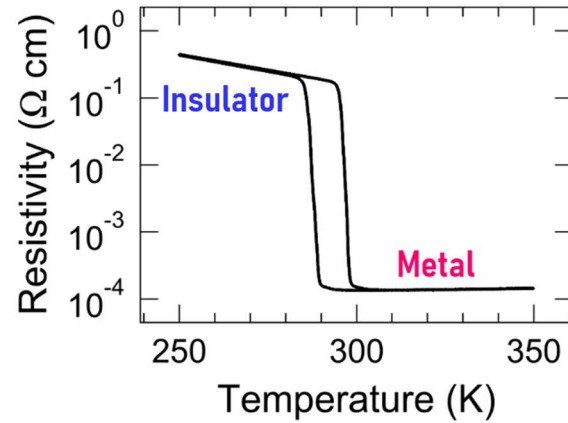
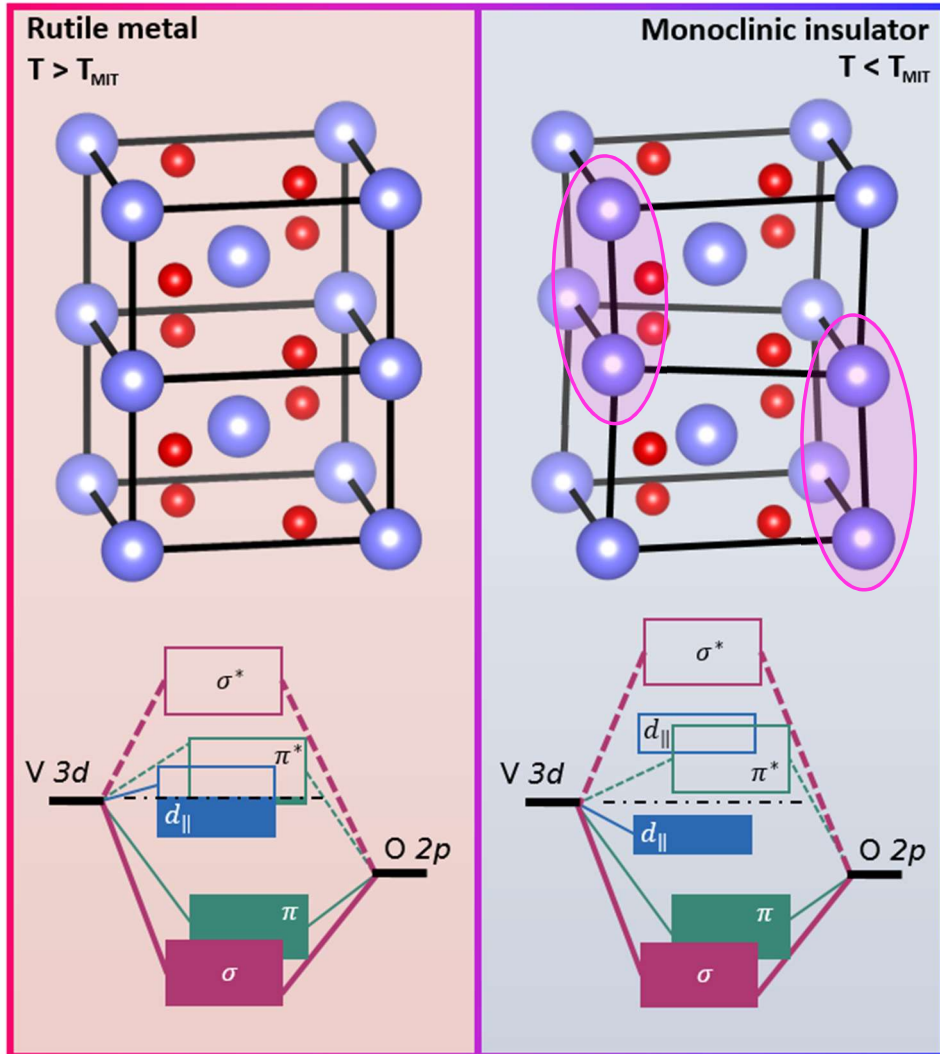
## According to theory: correlation-assisted Peierls transition

«  $VO_2$  is **not a conventional Mott insulator**, [...] the formation of dynamical V-V singlet pairs due to **strong Coulomb correlations** is **necessary** to trigger the opening of a **Peierls gap** »

S. Biermann *et al.*, PRL (2005)



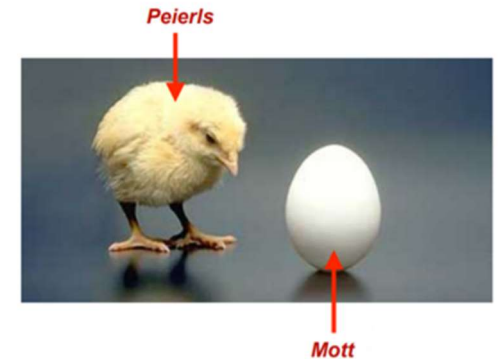
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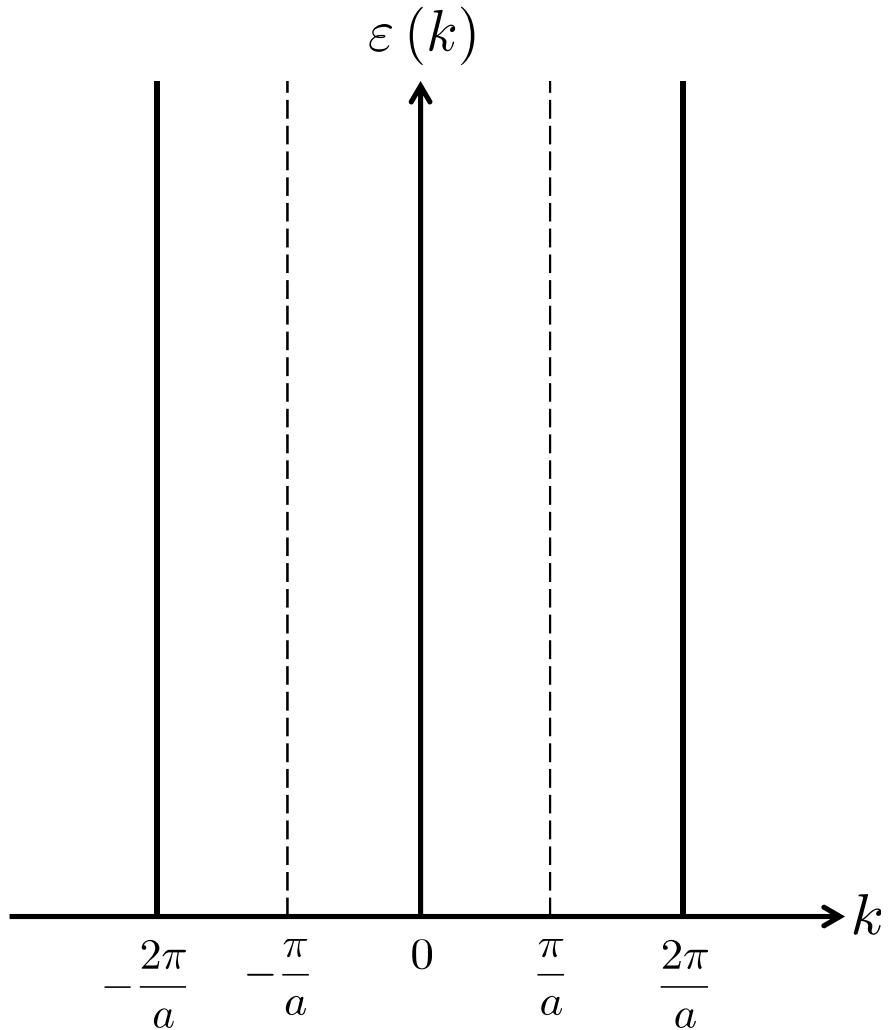
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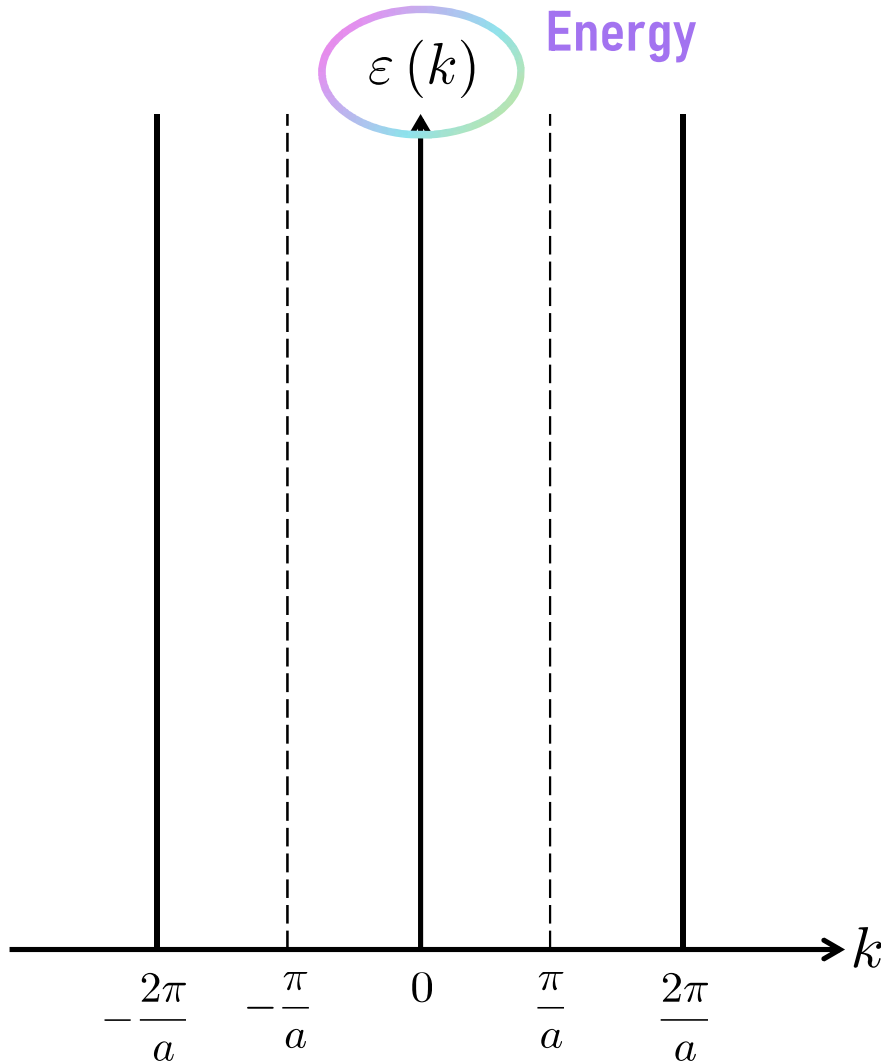
S. Biermann *et al.*, PRL (2005)



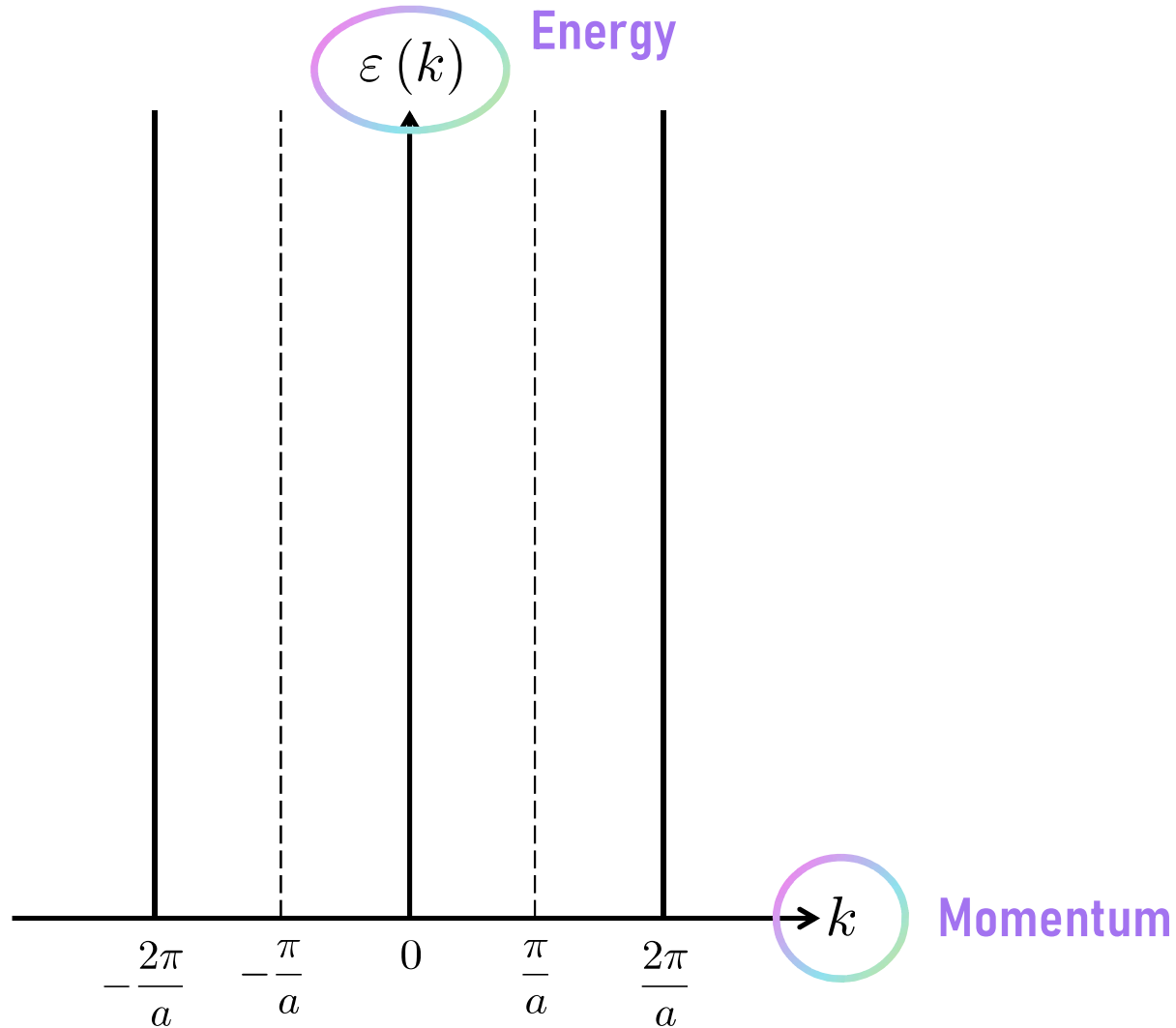
# Metals, insulators and energy bands 101



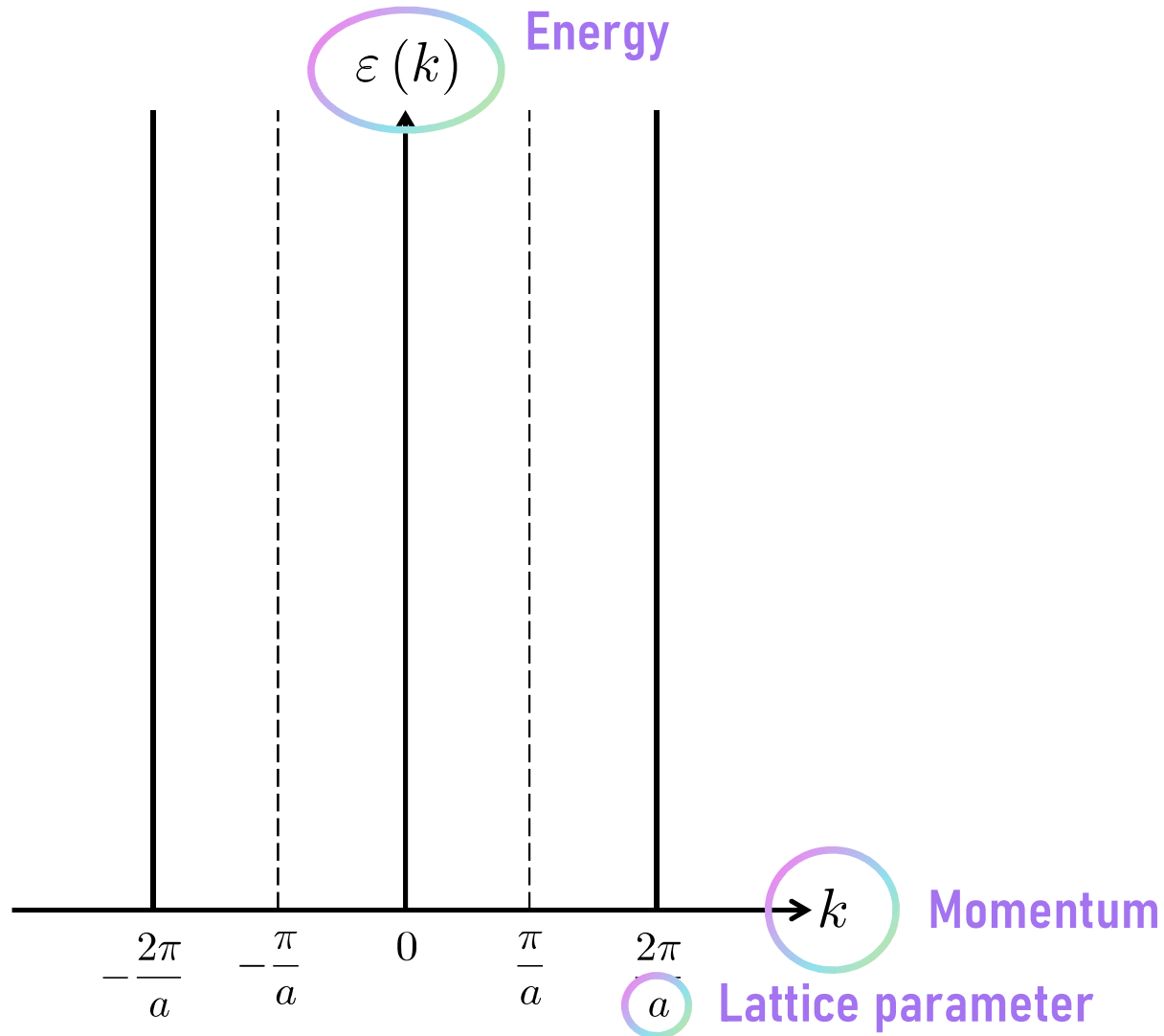
# Metals, insulators and energy bands 101



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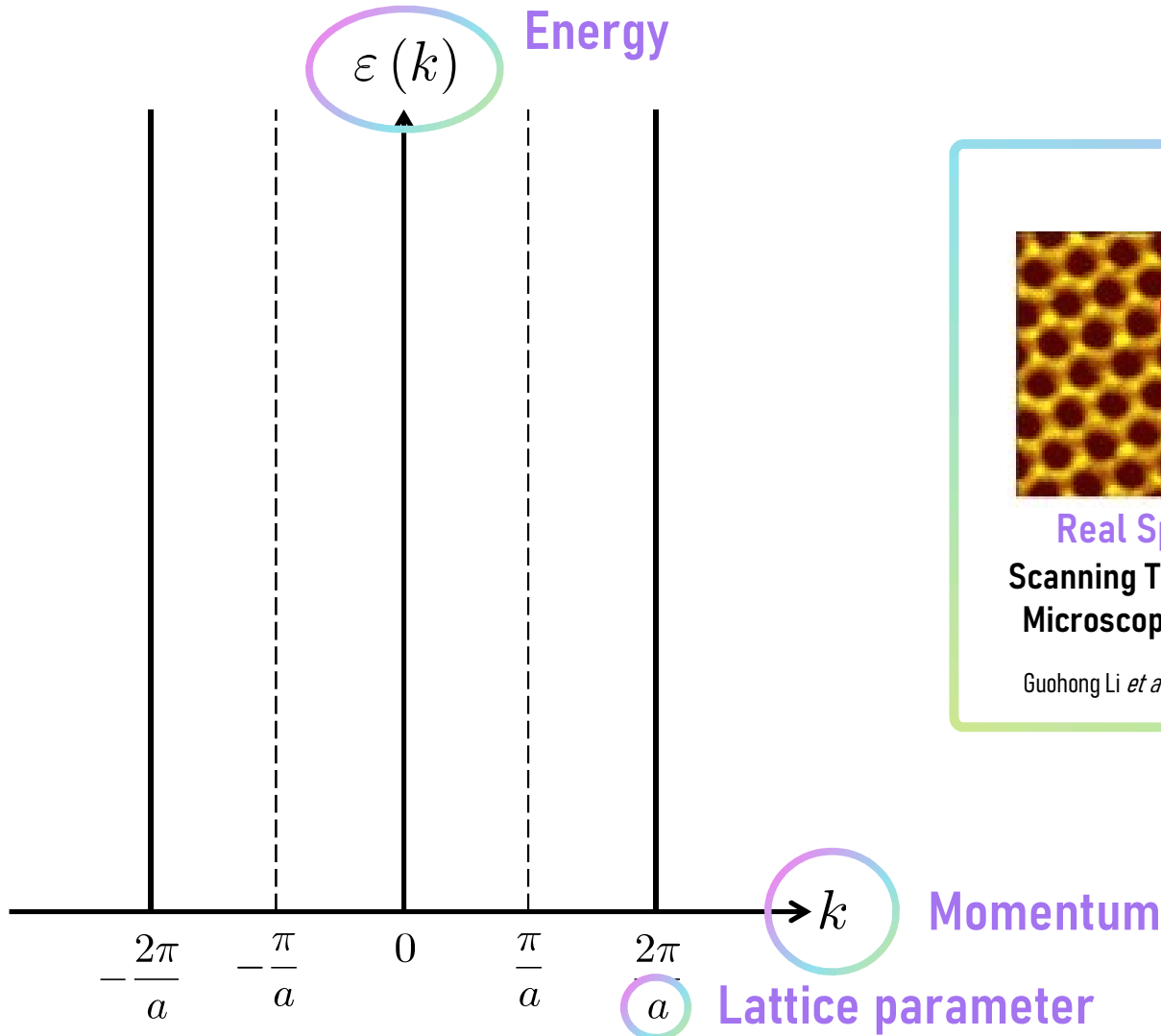


# Metals, insulators and energy bands 101





# Metals, insulators and energy bands 101



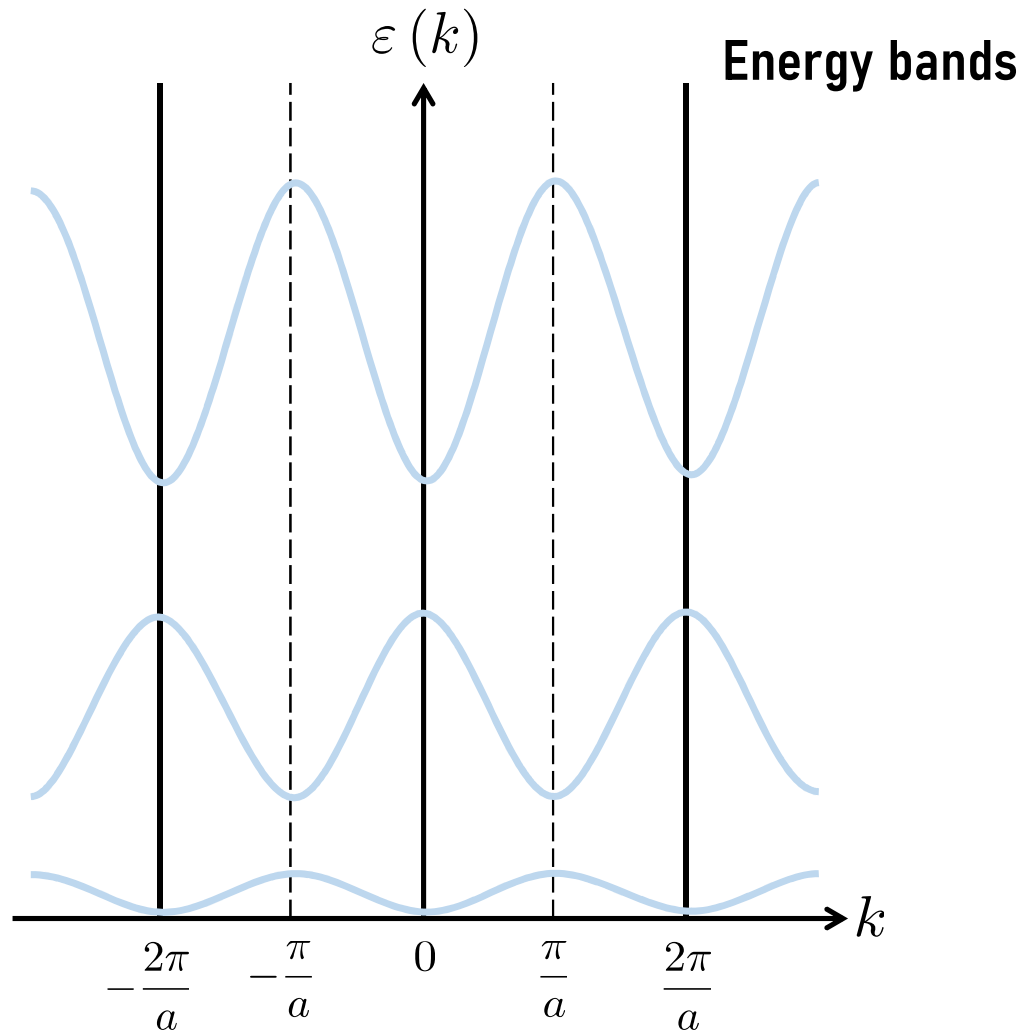
### Real vs. Reciprocal Space

Real Space  
Scanning Tunneling Microscopy (STM)  
Guohong Li *et al.*, PRL (2009)

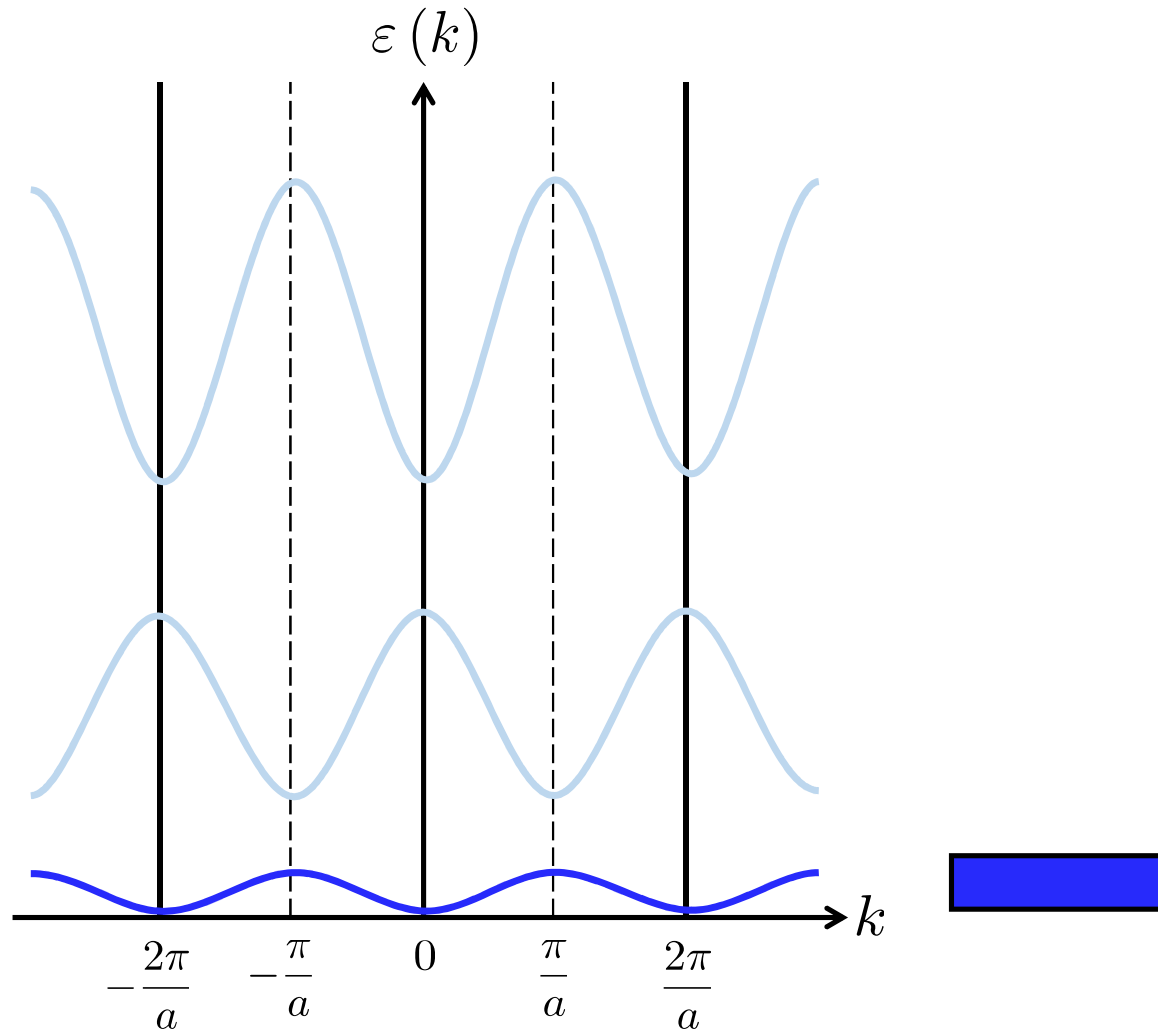
Fourier transform

Reciprocal Space  
Electron diffraction  
Wei Zhao *et al.*, Science Advances (2017)

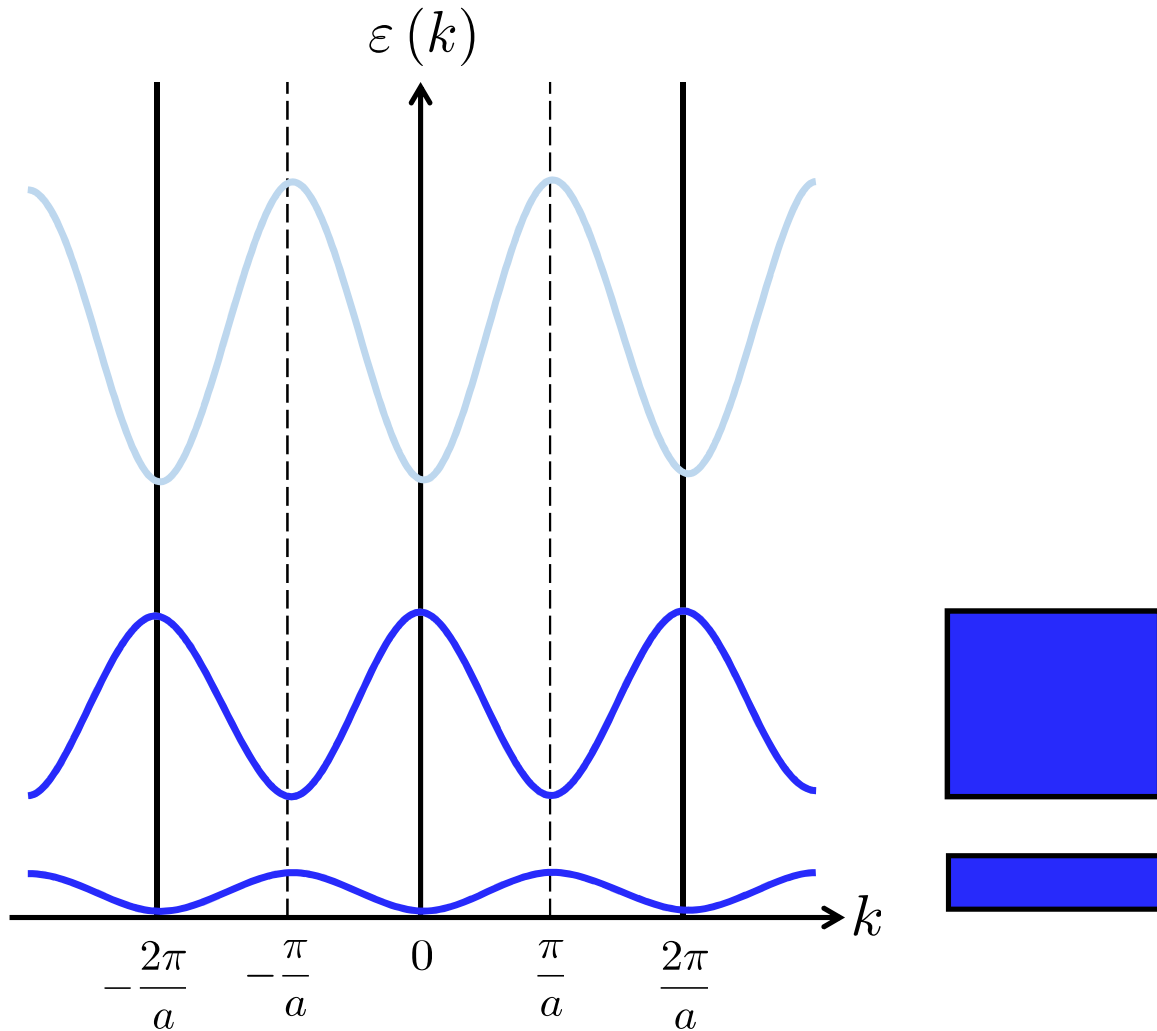
# Metals, insulators and energy bands 101



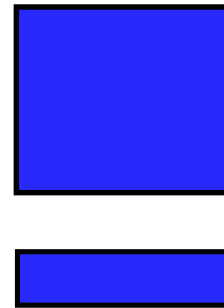
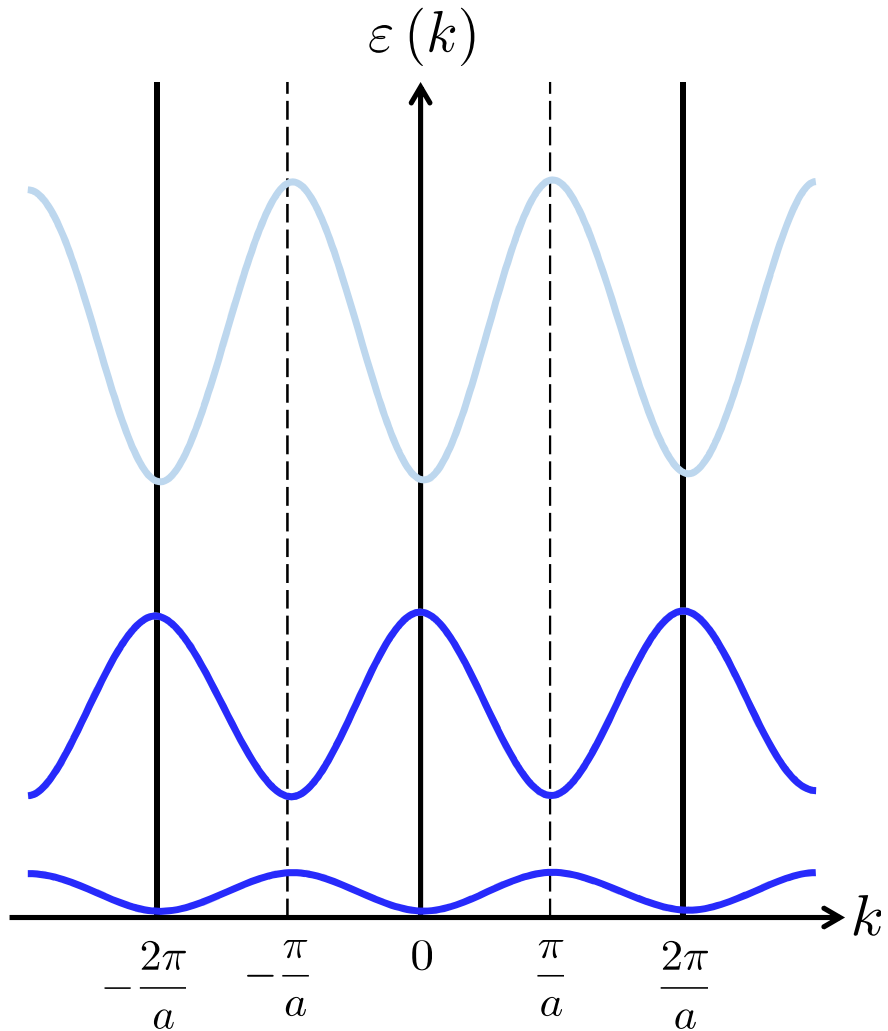
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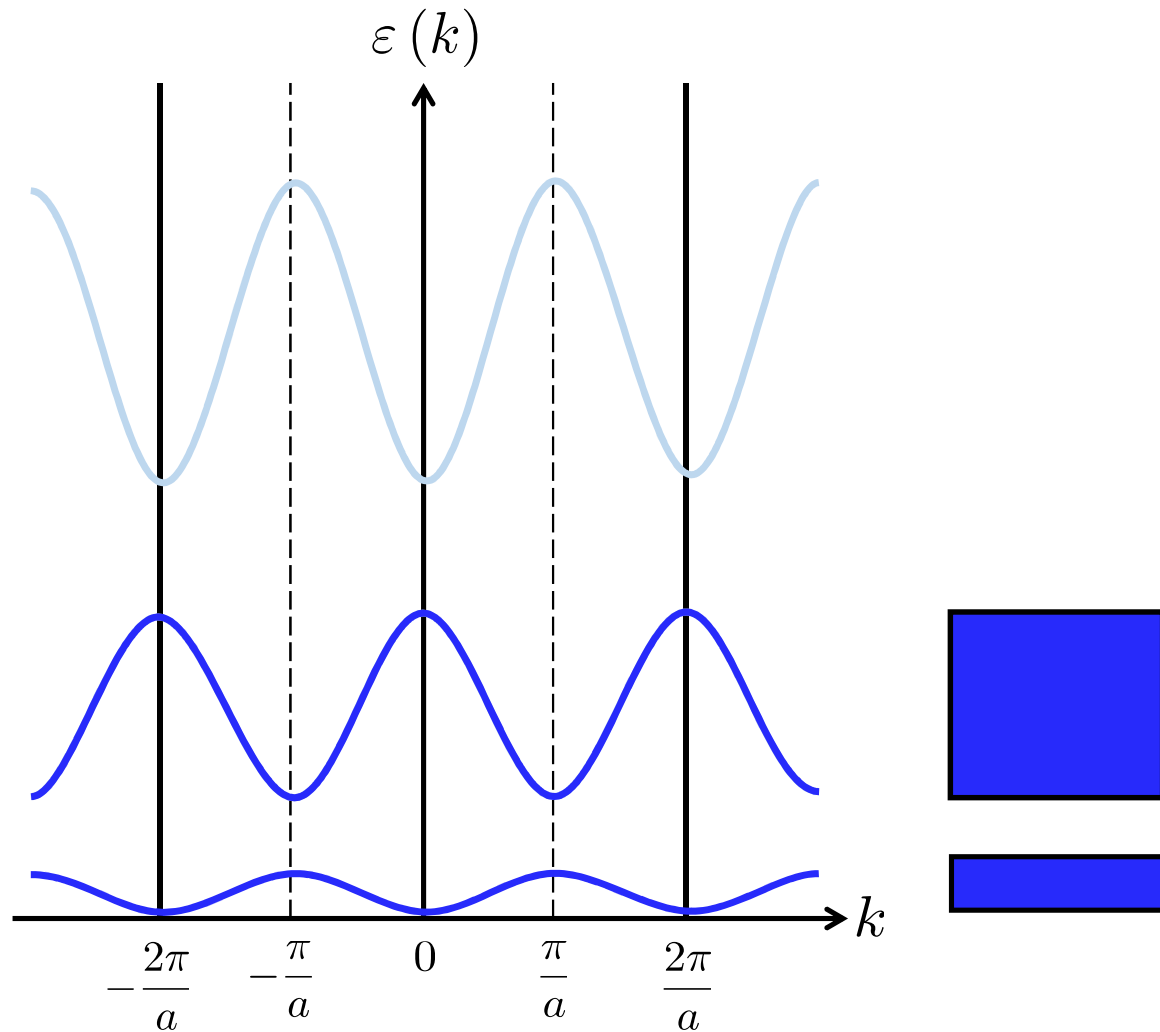
# Metals, insulators and energy bands 101



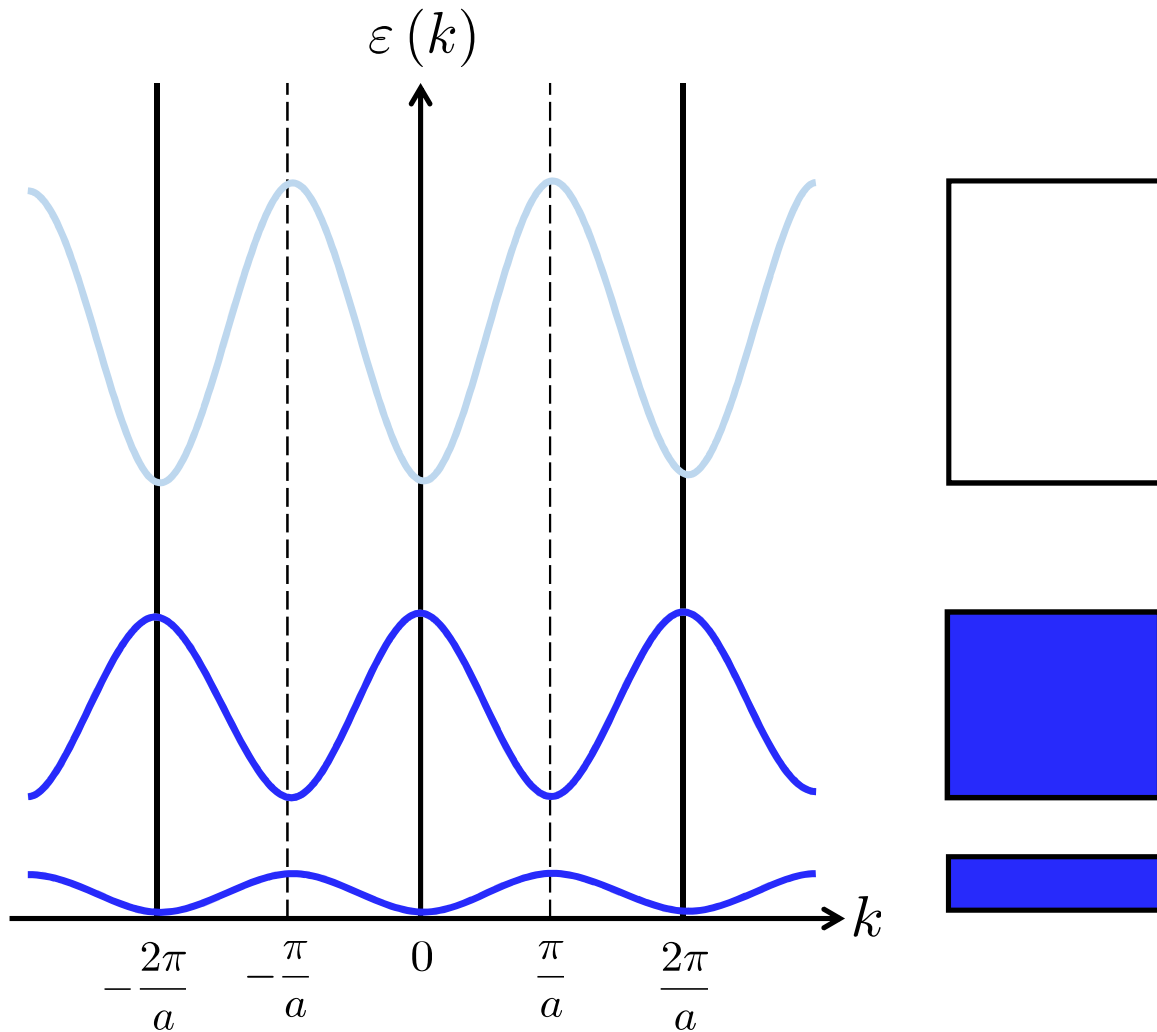
Last band fully filled

**Insulator**

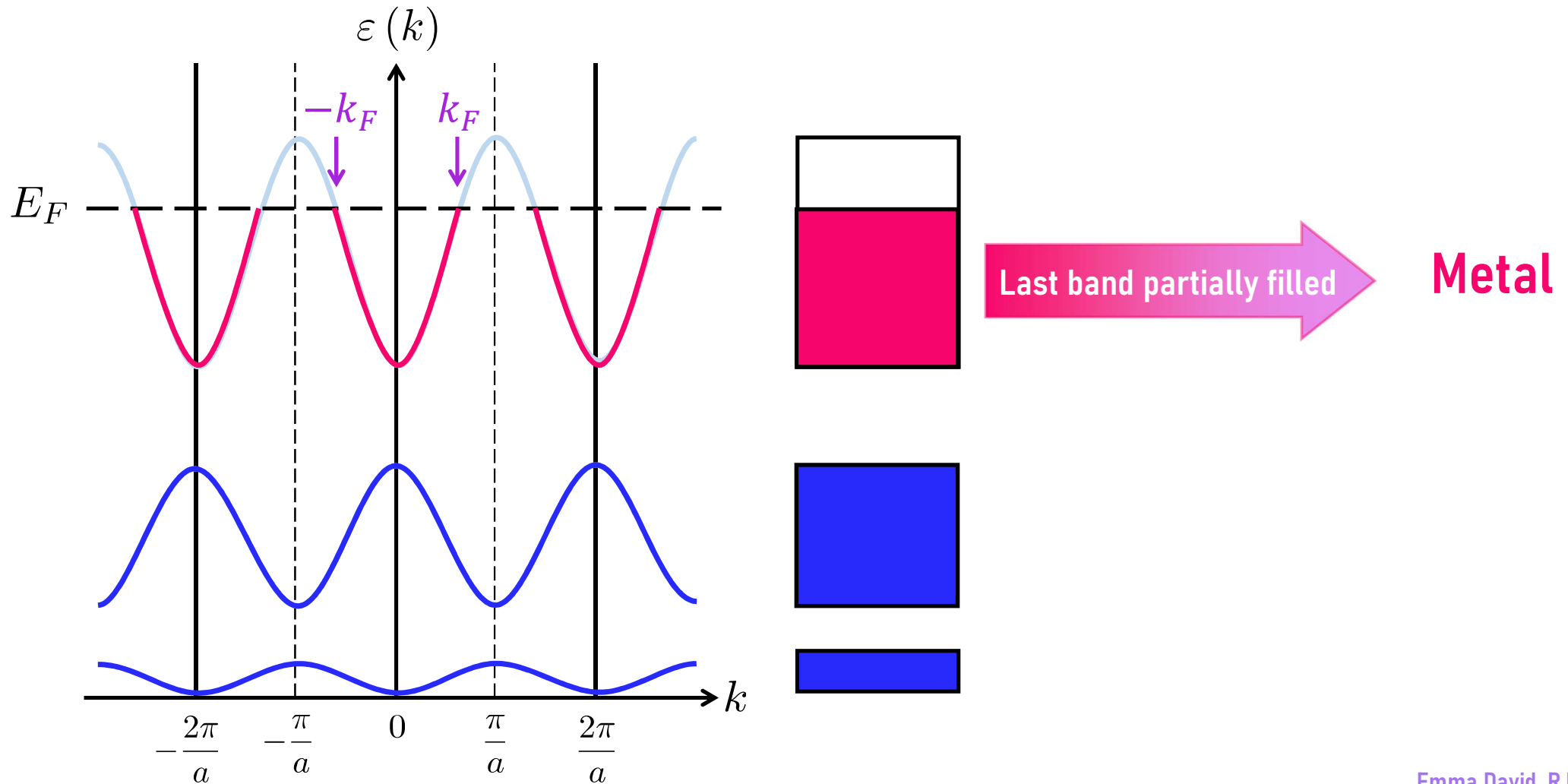
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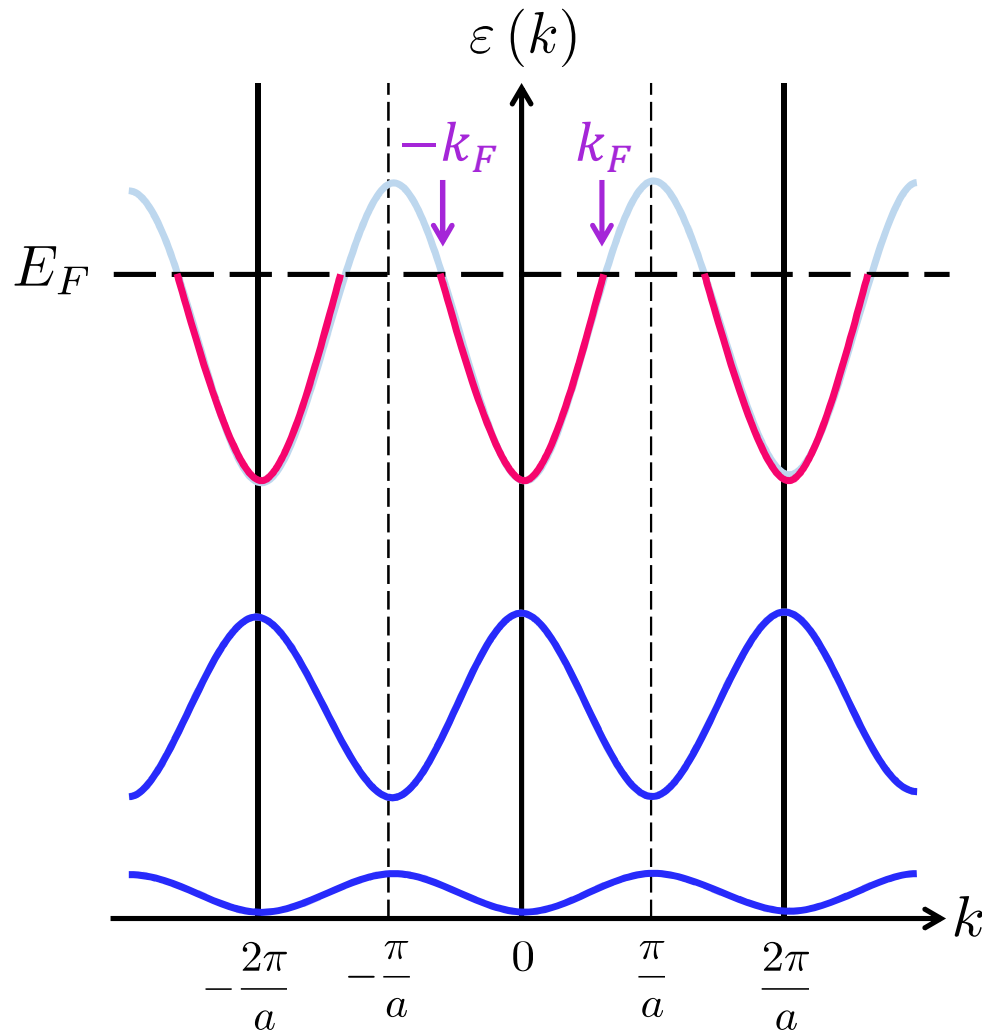


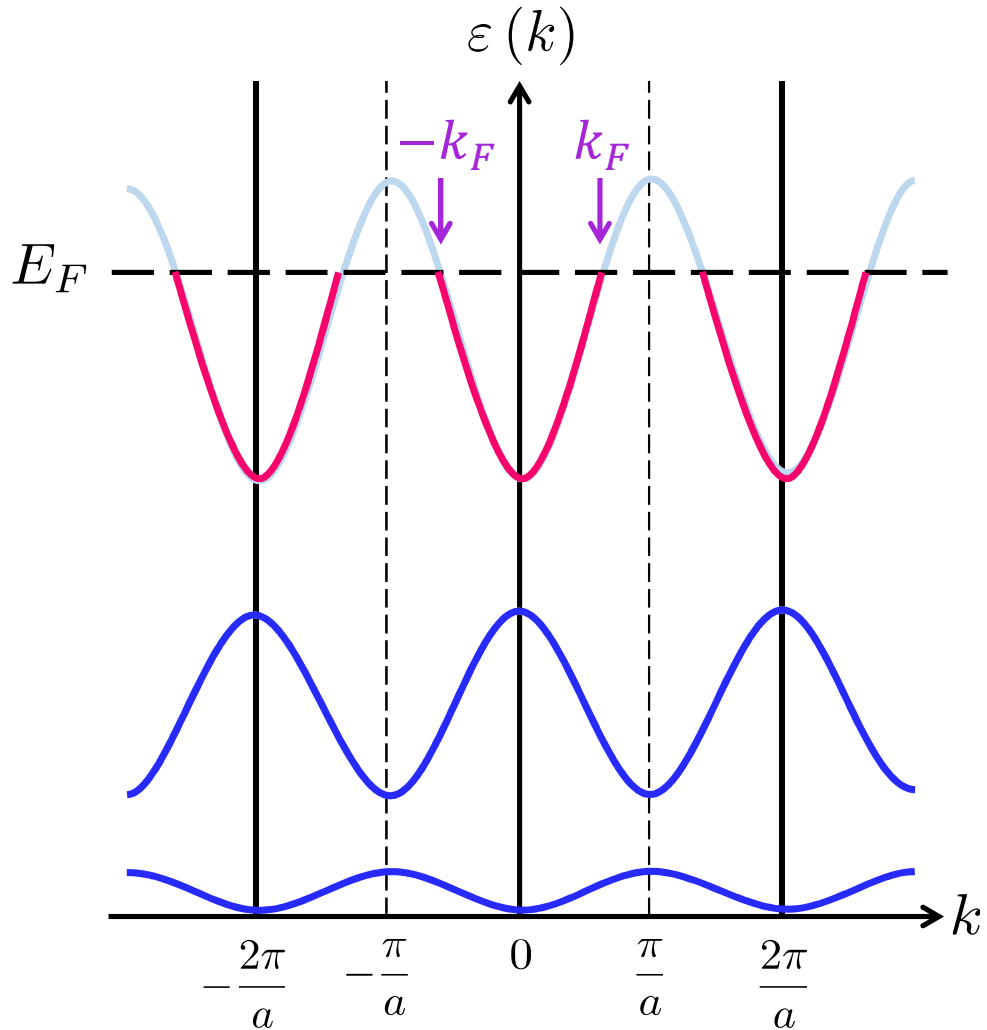
# Metals, insulators and energy bands 101



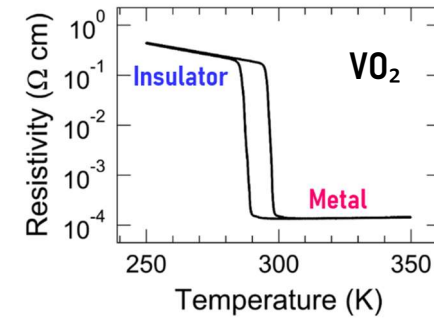


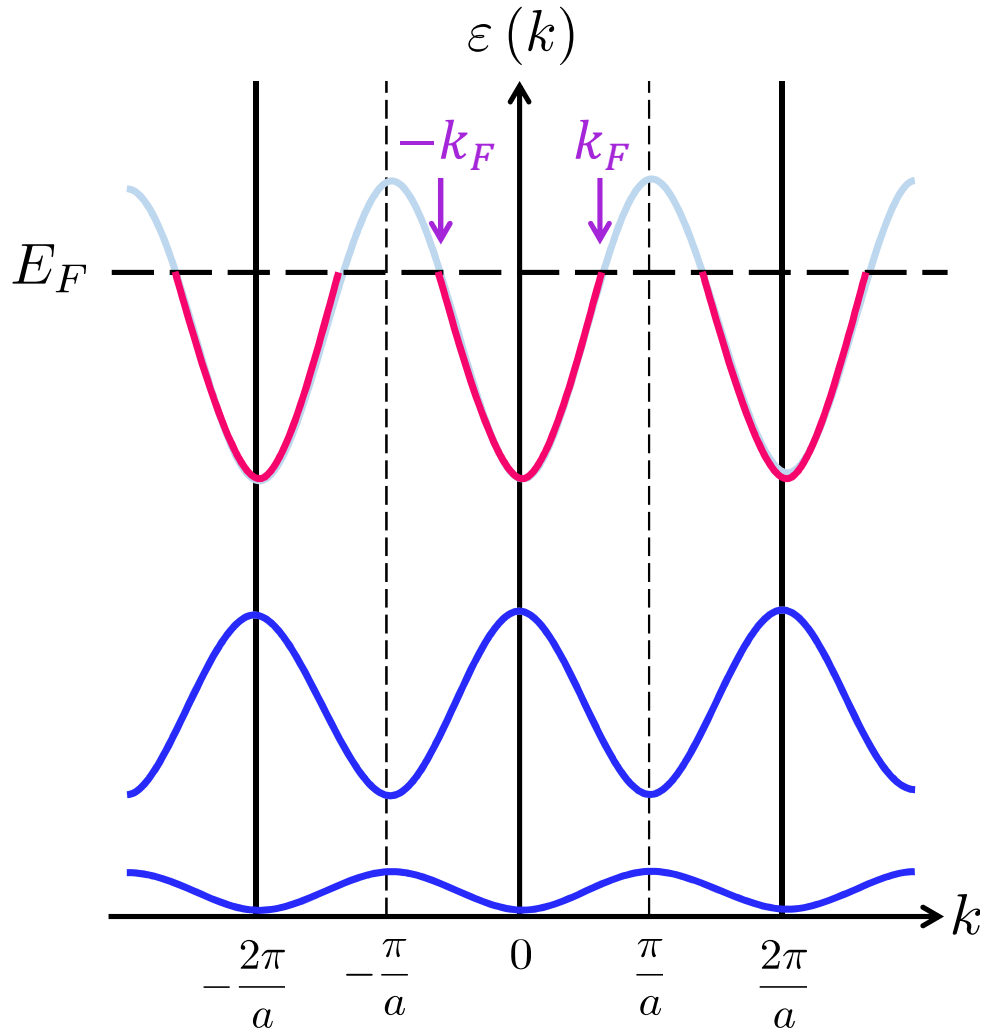
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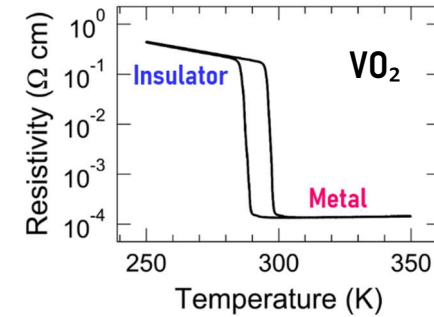


What went wrong?

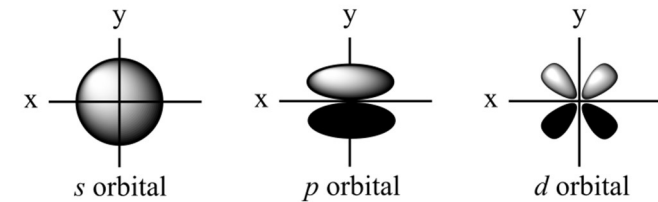




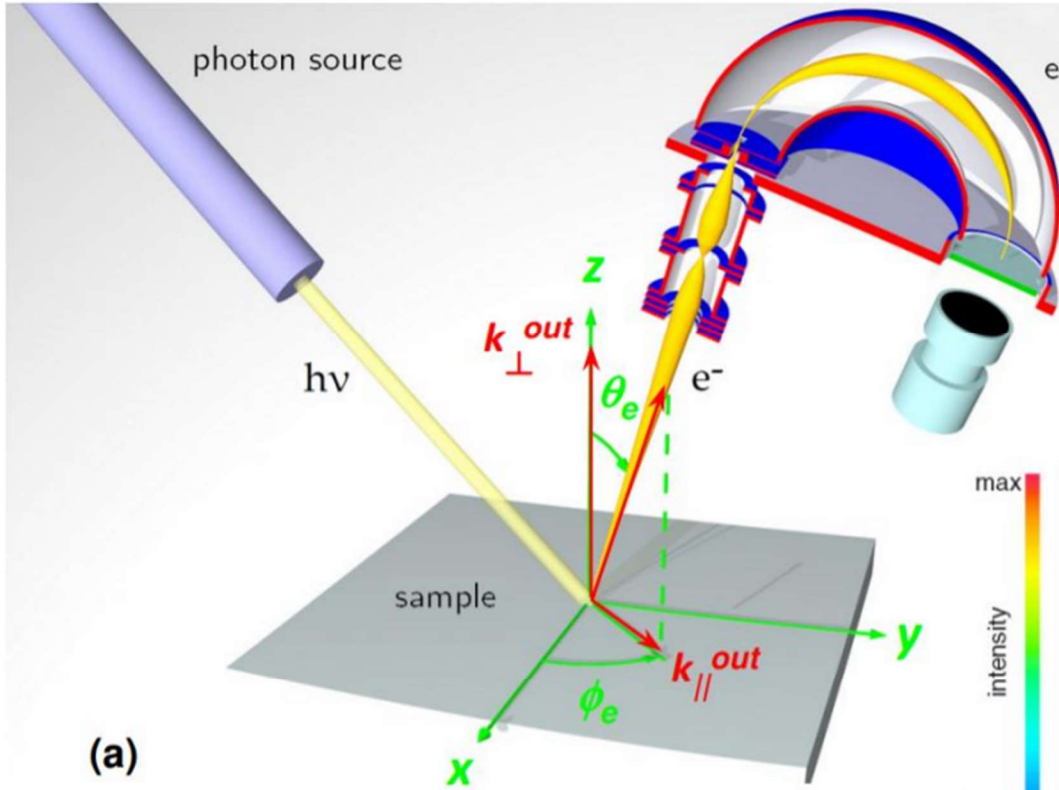
## What went wrong?



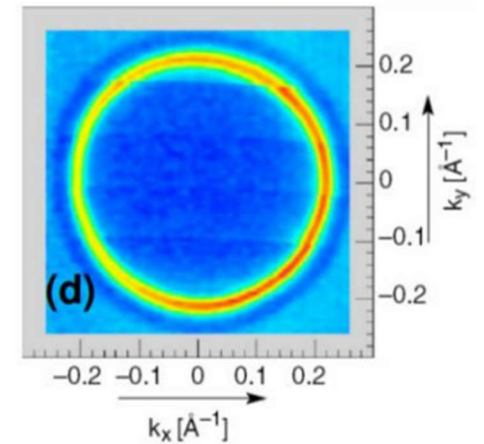
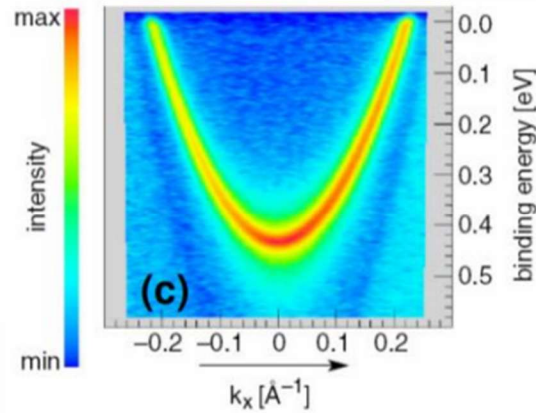
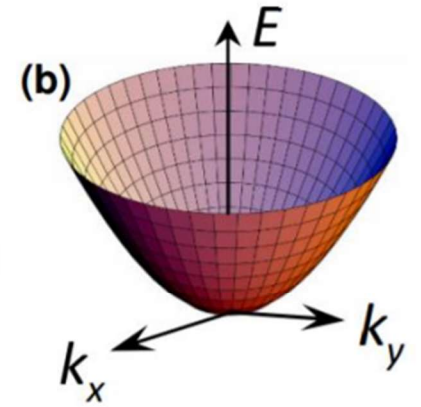
→ **Correlations:** This band picture forgets about electron-electron interactions



# Angle Resolved Photoemission Spectroscopy



Simple example:  
Cu(111) surface-state

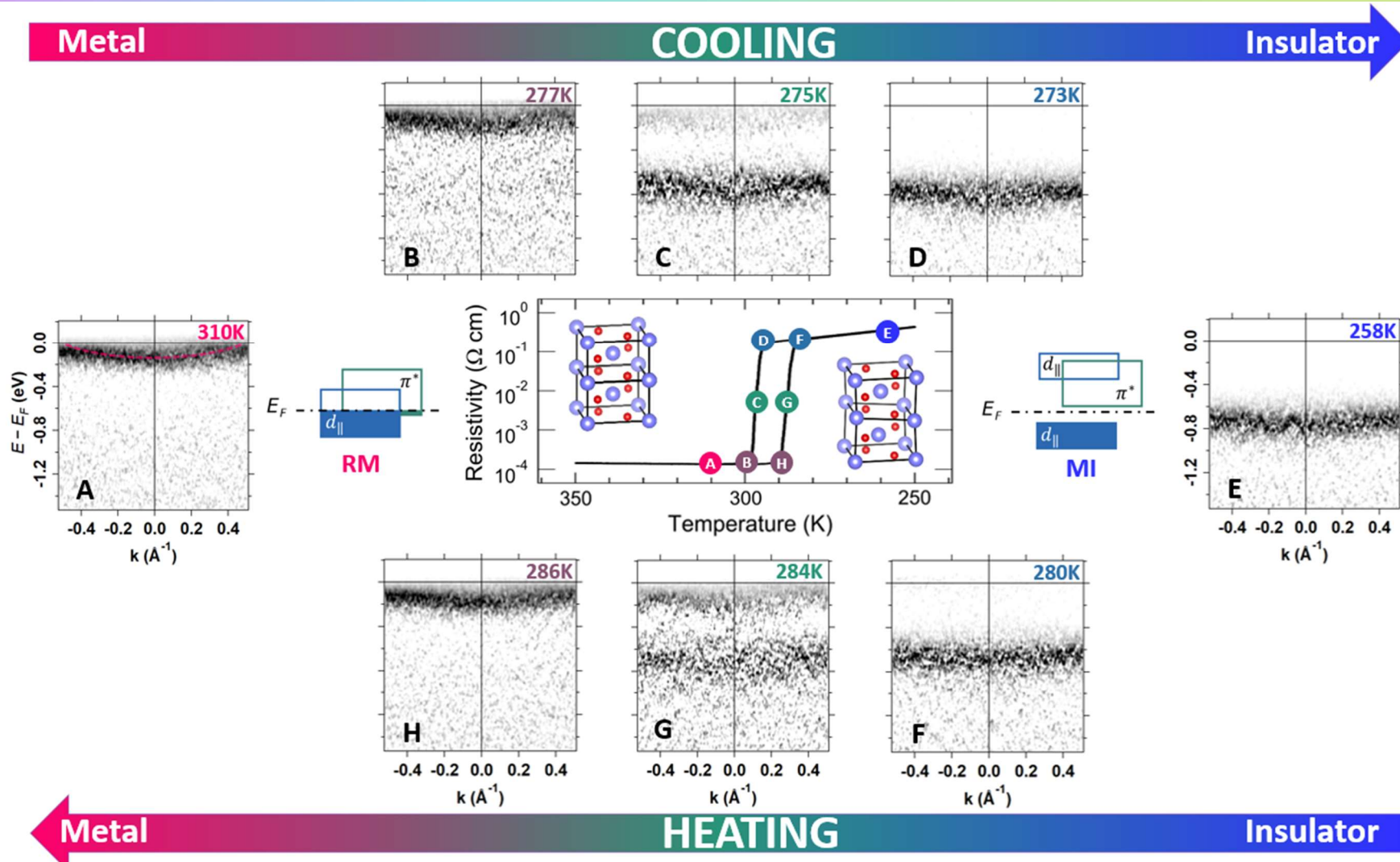


## ARPES

Friedrich Reinert and Stefan Hüfner,  
*New Journal of Physics* (2005)

# Temperature-dependent electronic structure

6



**Metal**

**HEATING**

**Insulator**

## ARPES: to be or not to be?

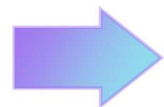
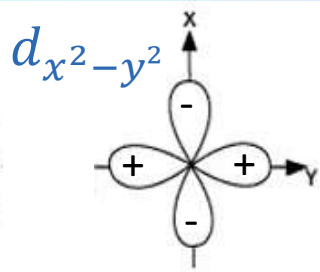
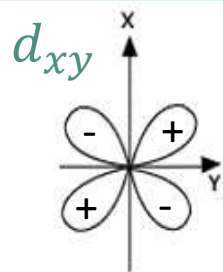
ARPES intensity:  $I(E, h\nu) \propto |M_{fi}|^2 A(\vec{k}, E) f(E, T)$

Matrix element

$$|M_{fi}|^2 \propto | \langle \Phi_f | \hat{H}_{int} | \Phi_i \rangle |^2$$

0 if product is  
**ODD**

≠0 if product is  
**EVEN**



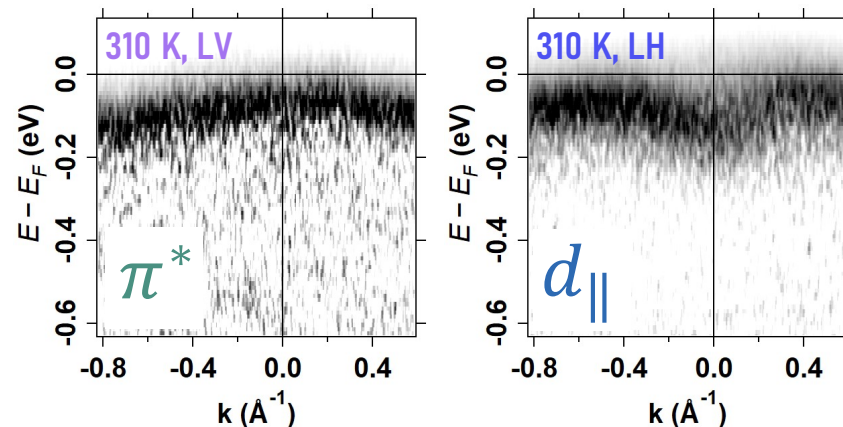
→  $d_{||}$  band (comes from  $d_{xy}$ )

LV	LH
0	≠0

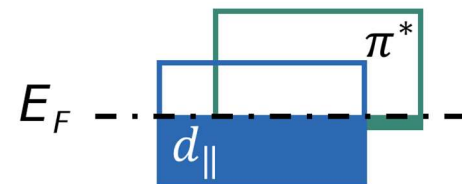
→  $\pi^*$  band (comes from  $d_{x^2-y^2}$ )

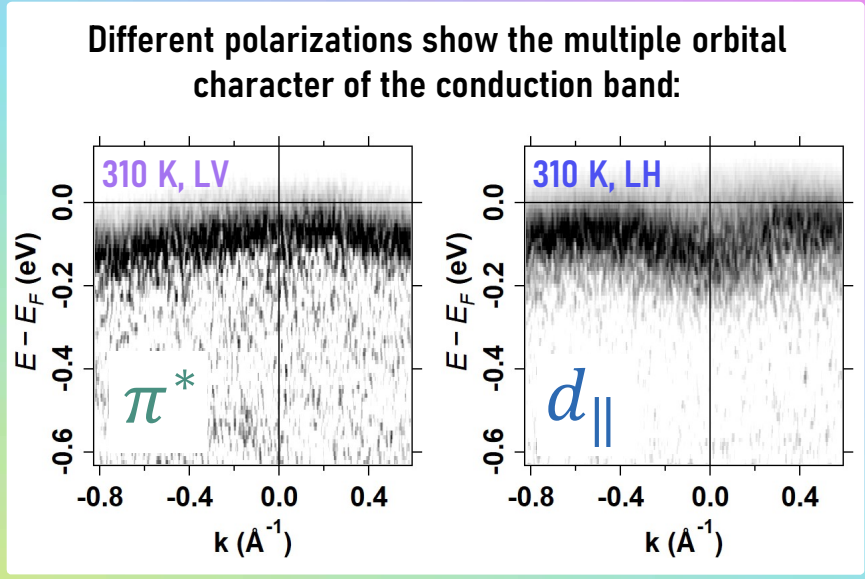
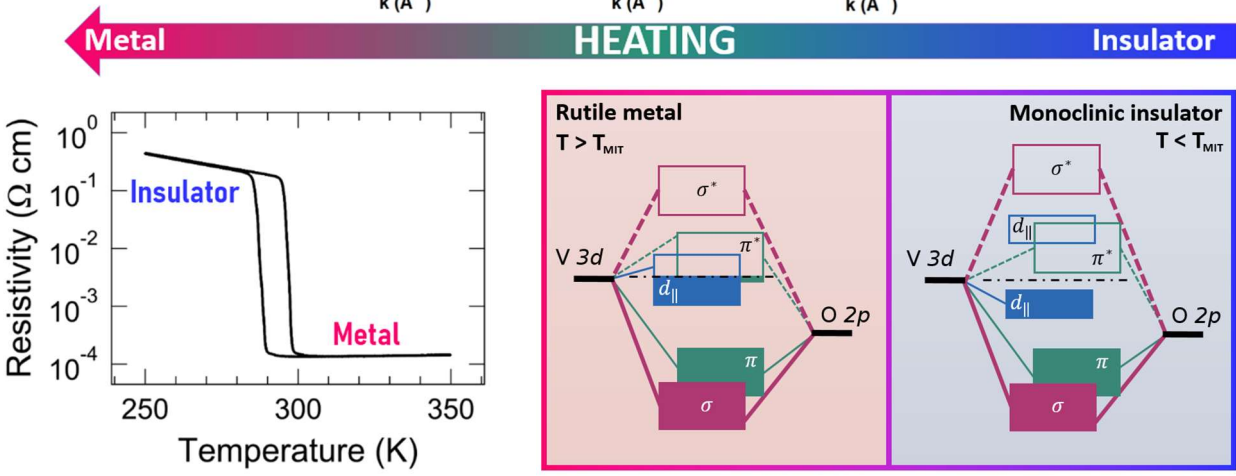
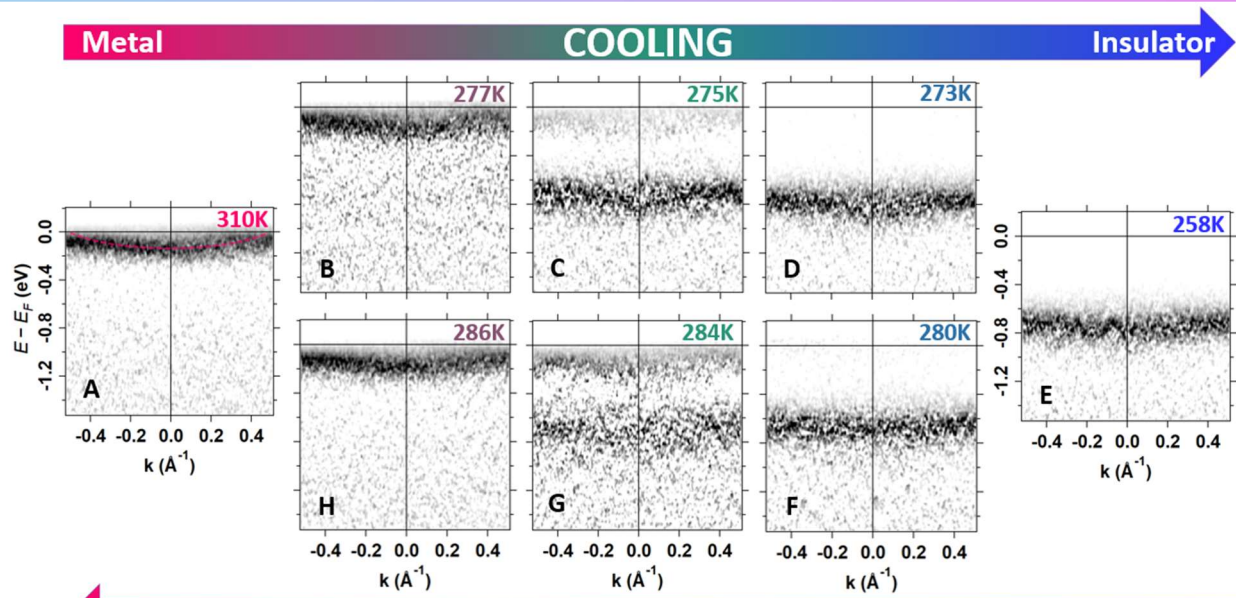
LV	LH
≠0	0

## Metallic phase in different polarizations



Theoretical band structure at the Fermi level:





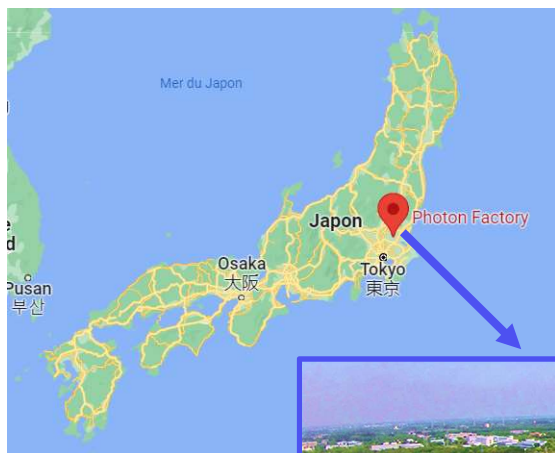
→ In the metallic state, we find that the  $d_{||}$  and  $\pi^*$  orbitals coexist in the conduction band

→ The temperature-dependent data shows different states between the metallic and insulating phases, as well as a gradual transfer of spectral weight between those states during the transition, in accordance with the electronic hysteresis

A wide-angle landscape photograph of a mountain valley. In the foreground, a river flows through a rocky, grassy valley. The middle ground shows rolling hills with sparse vegetation and scattered rocks. In the background, majestic mountain ranges with significant snow cover rise against a bright blue sky filled with fluffy white clouds. The overall scene is bright and clear, suggesting a sunny day.

**Thank you for your attention!**





大学共同利用機関法人 高エネルギー加速器研究機構 物質構造科学研究所  
放射光実験施設  
Photon Factory

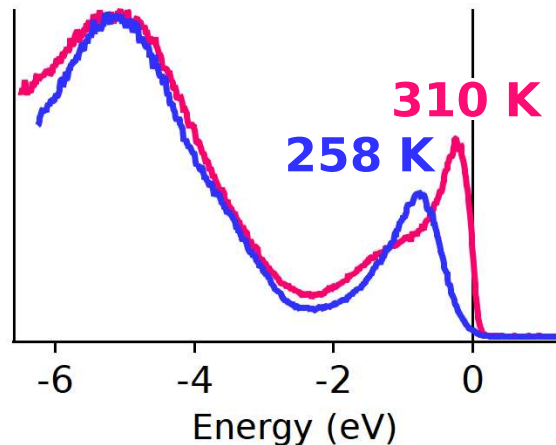
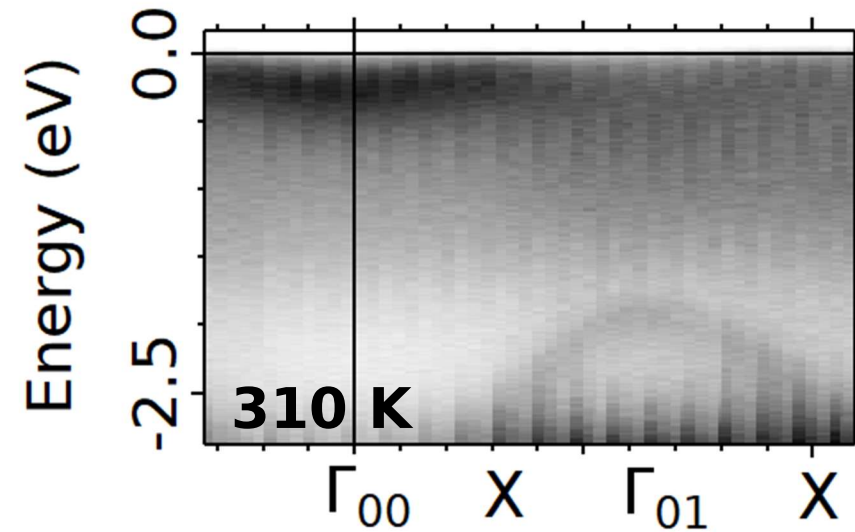
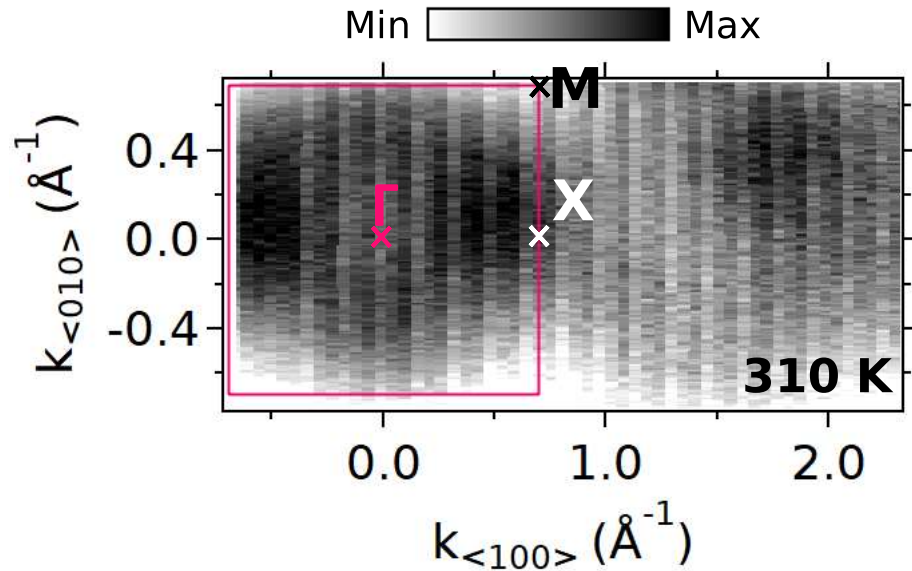


BL-2A/B

- We worked with **thin films** of (001) oriented 10 nm thick  $\text{VO}_2$  deposited on a  $\text{Nb:TiO}_2$  substrate
- Samples were made by **PLD** (Pulsed Laser Deposition) by Hiroshi Kumigashira's group

# Electronic structure in the metallic phase

26



- Two electron-like pockets around  $\Gamma$ , the flower-like shape matches with calculations
- Matrix elements play a great role
- The electronic structure is in accordance with published data