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Metal – Insulator Transition of Na_xWO_3 Studied by High-Resolution ARPES

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Collaborators :

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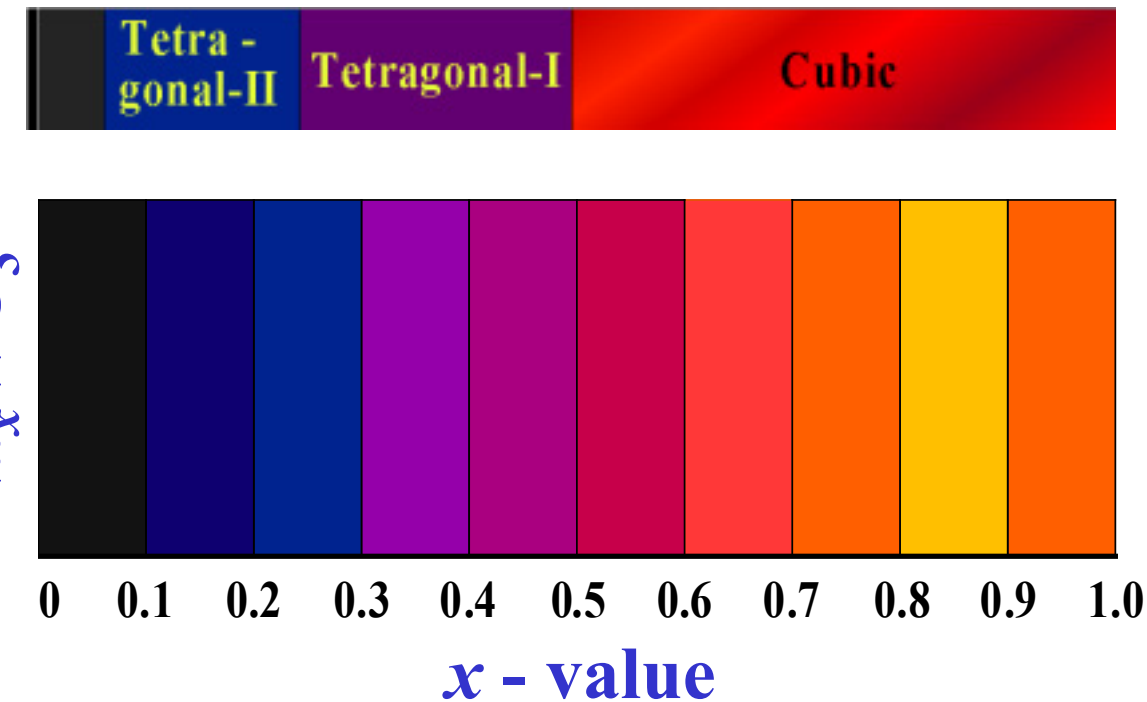
Introduction

Sodium Tungsten Bronze: Old compound, 1823
Interesting structural & physical properties

Monoclinic
Orthorhombic

Color & Crystal structure

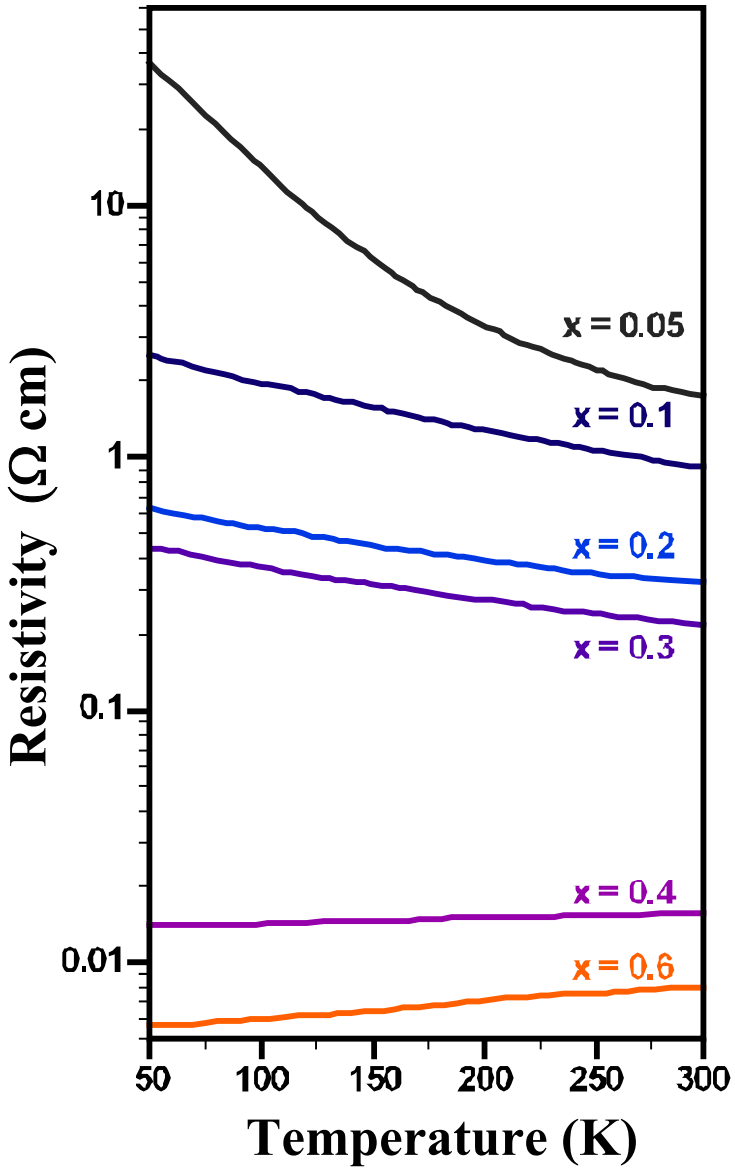


WO_3 as parent compound
Na : electropositive element

Oxidation states of W
Changes from +6 to +5
By addition of Na

⇒Mixed Valence Compound

Resistivity of Na_xWO_3



Metal-to-Insulator transition

at $x \sim 0.3$

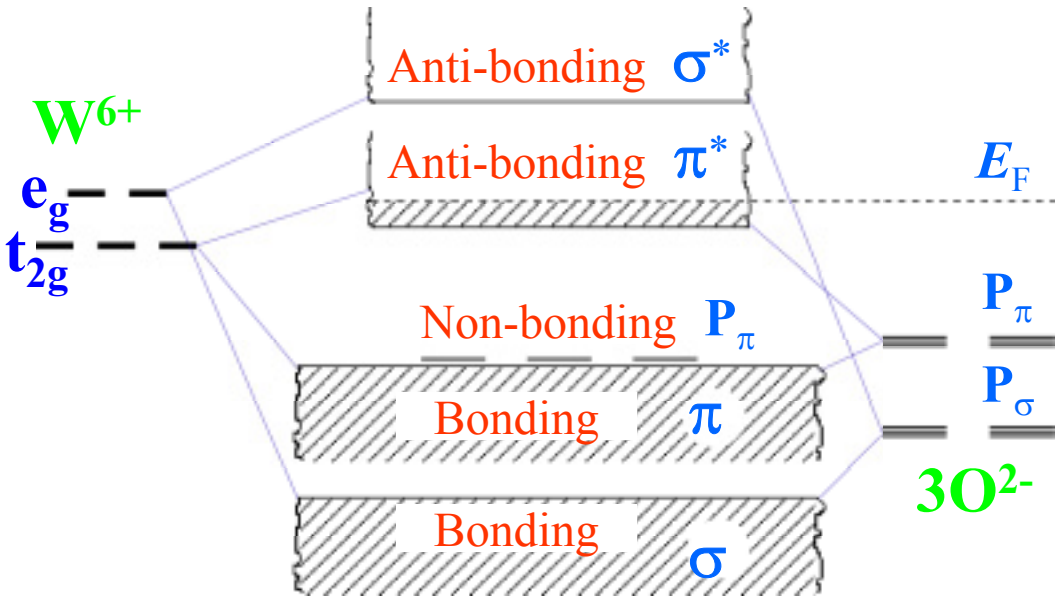
 # Data from Poly-crystalline samples

Crystal structure of Na_xWO_3

WO_6 octahedron

Cubic crystal Structure

Rigid Band Model



- Band model from molecular orbital theory and symmetry of the crystal structure
- Na reduces W^{+6} to a lower oxidation state
- $NaWO_3$ is similar to ReO_3, hence Na has no role in VB & CB except donating an Electron to W 5*d* CB

Sample Preparation

Single crystal Na_xWO_3 → $x = 0.58$, $x = 0.7$, $x = 0.8$ } Metallic

Metallic sample : Molten salt electrolysis method

Na_2WO_4 + 40 mol % WO_3

Cubic structure : a=3.7845 + 0.0820 *x* A°

XRD & SEM show samples are single phase with proper *x* value.

ARPES Experiment

Tohoku Univ. (He-Lamp, SES-200)

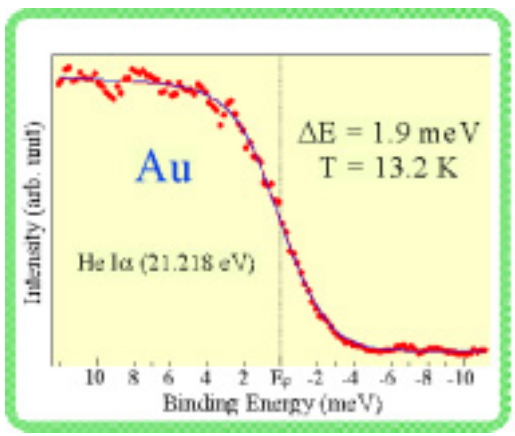
Photon energy : He Iα (21.218 eV)

Energy resolution : 5 ~ 11 meV

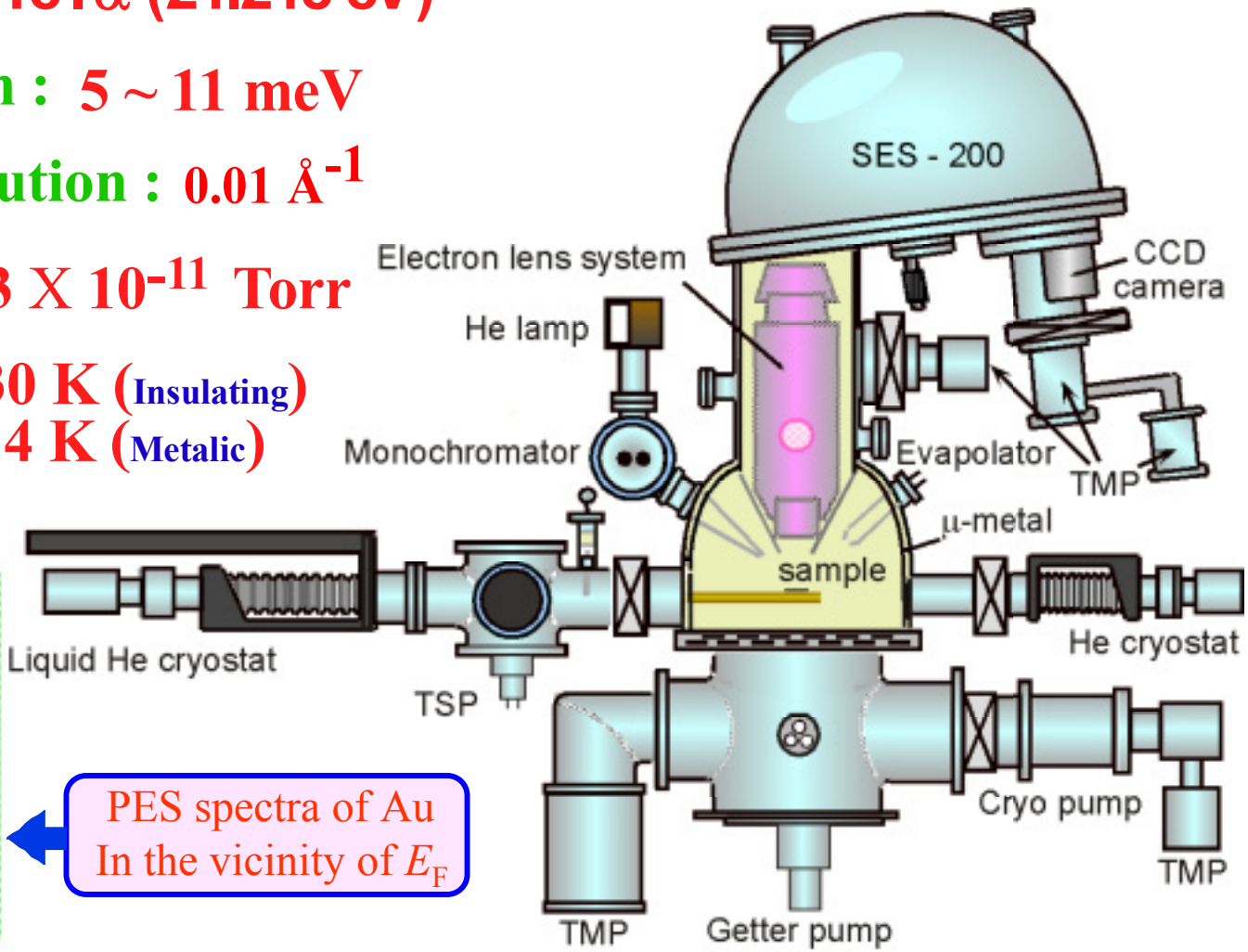
Momentum resolution : 0.01 Å^{-1}

Base pressure : 3 X 10^{-11} Torr

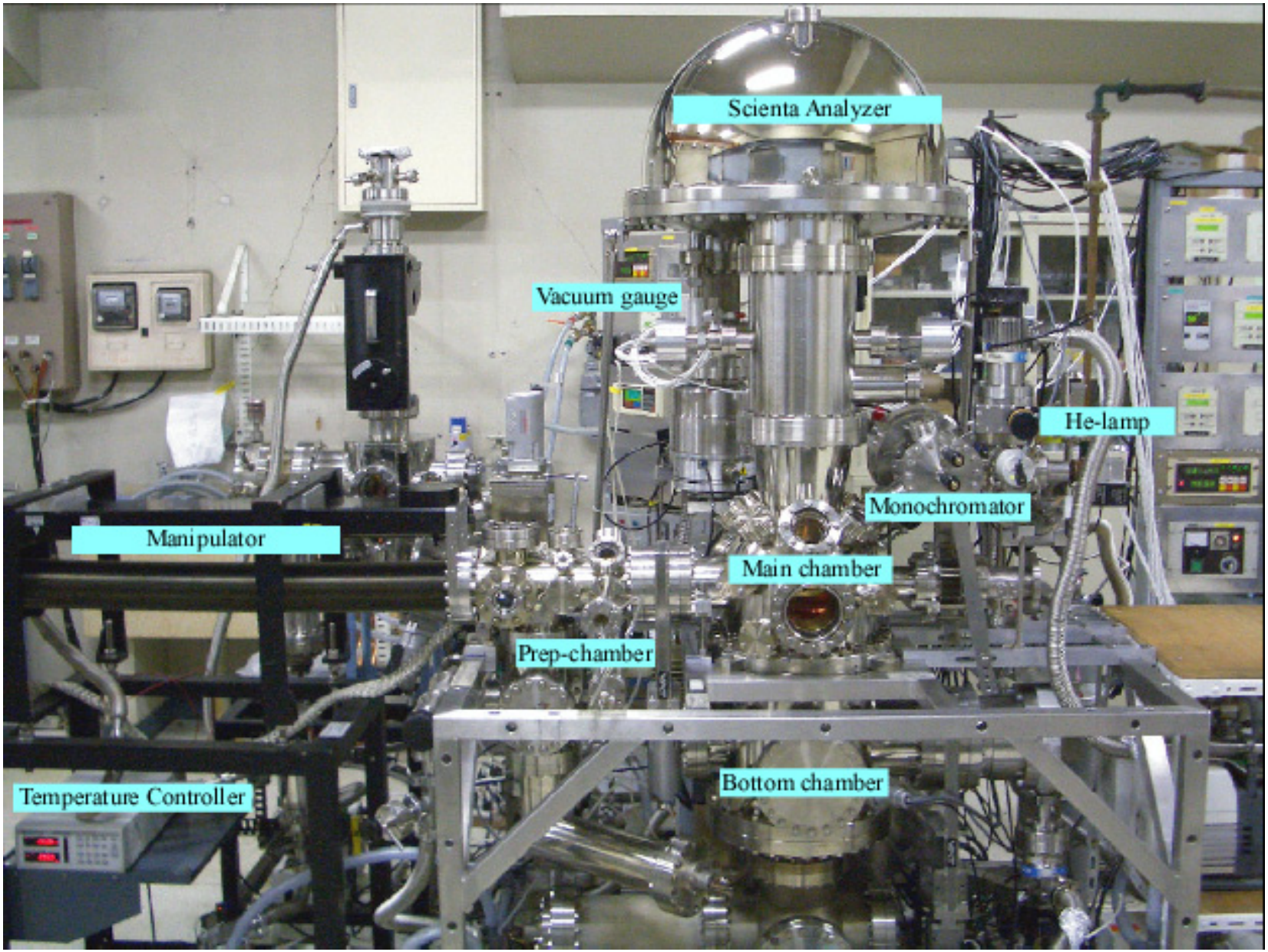
Temperature : 130 K (Insulating)
14 K (Metalic)



PES spectra of Au
In the vicinity of E_F

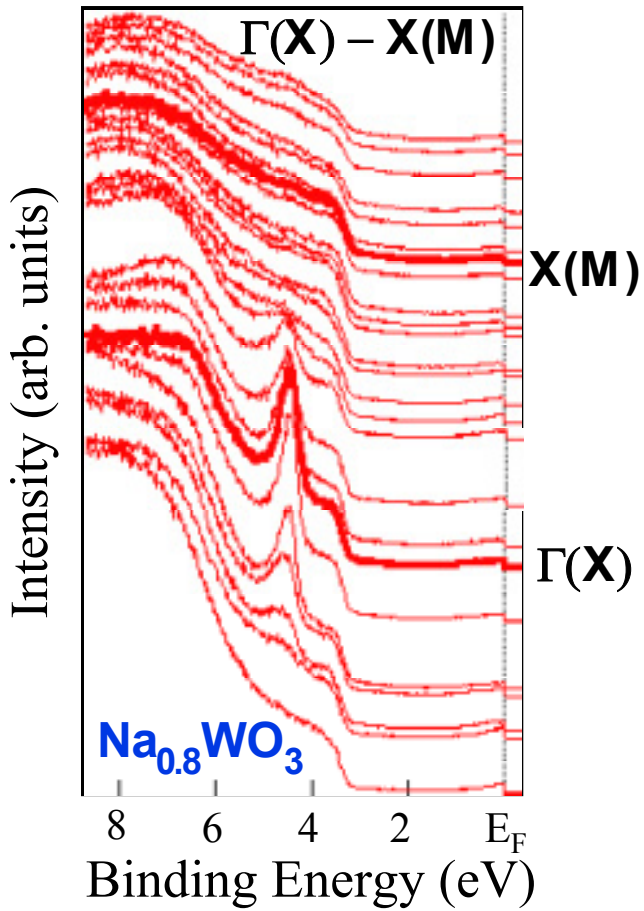


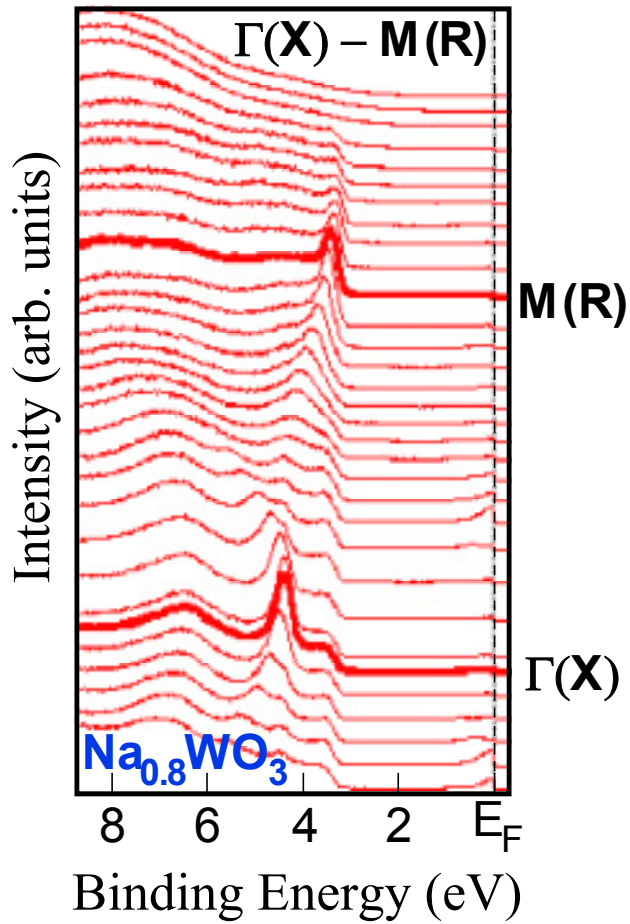
High-Resolution Electron Spectrometer



Metallic Na_xWO_3

Valence band ARPES spectra of metallic Na_xWO_3



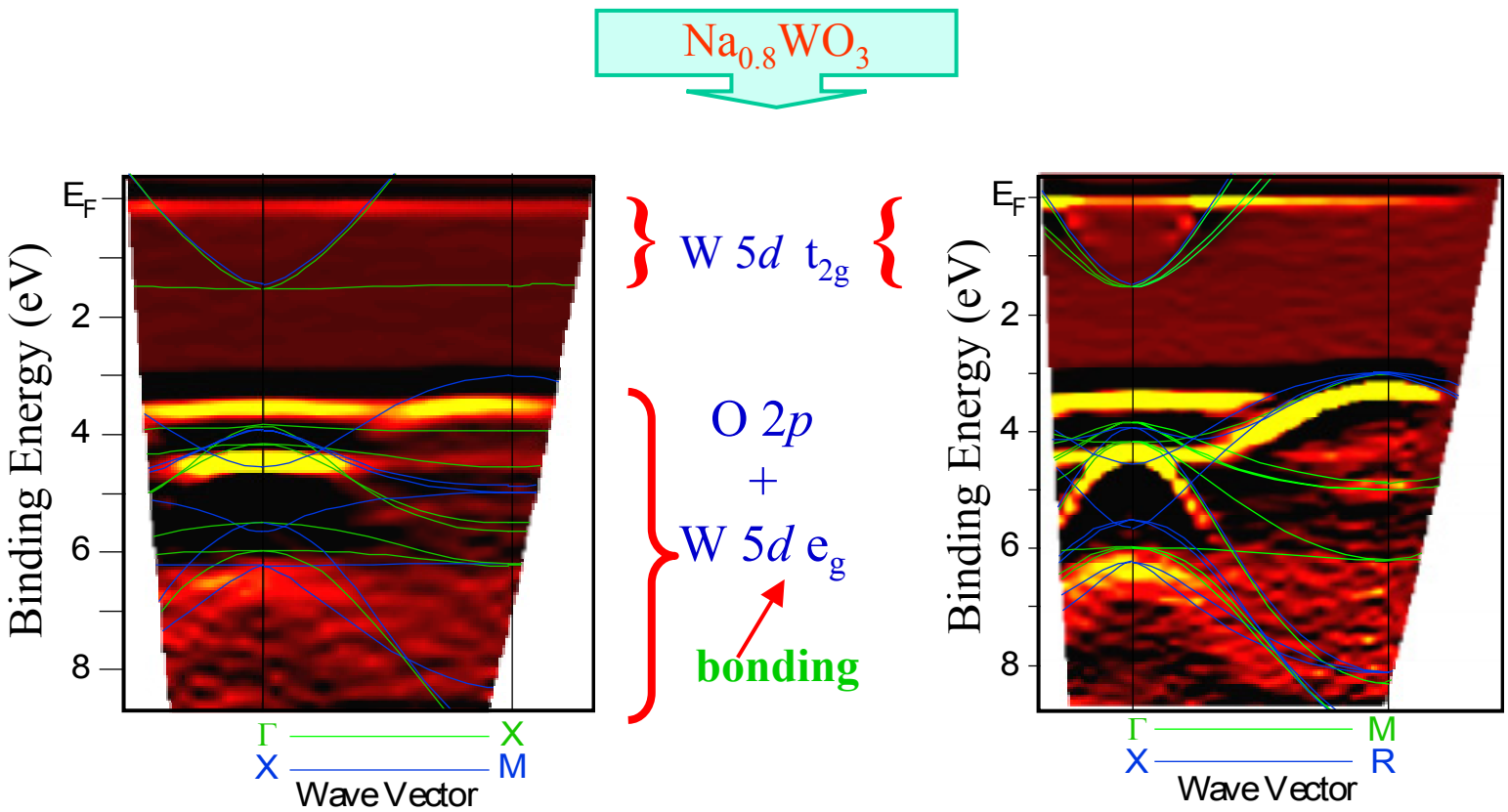


Top of valence band upto 3.0 eV

Bottom of Conduction band upto 1.0 eV

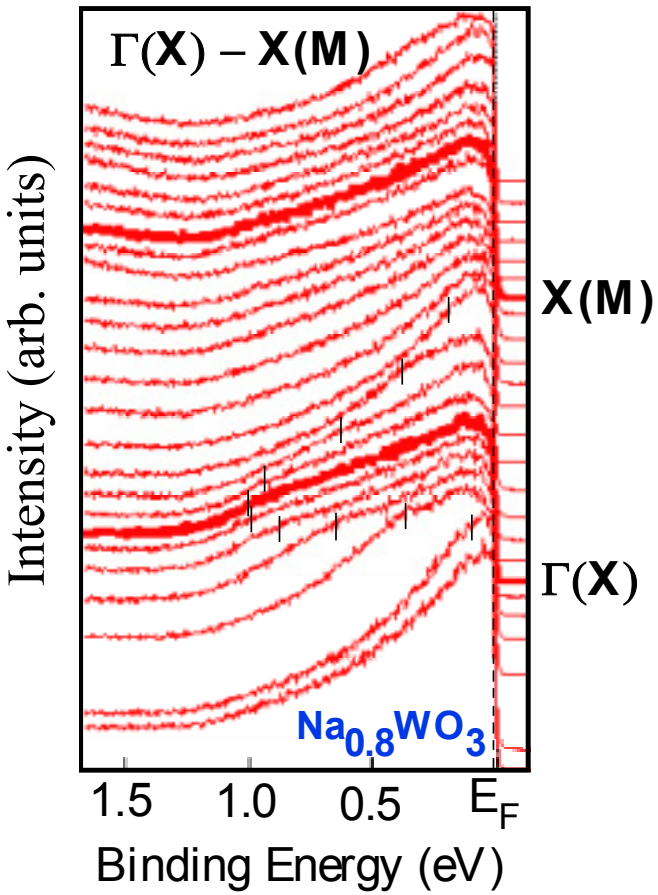
2.0 eV band gap between 3.0 ~ 1.0 eV BE

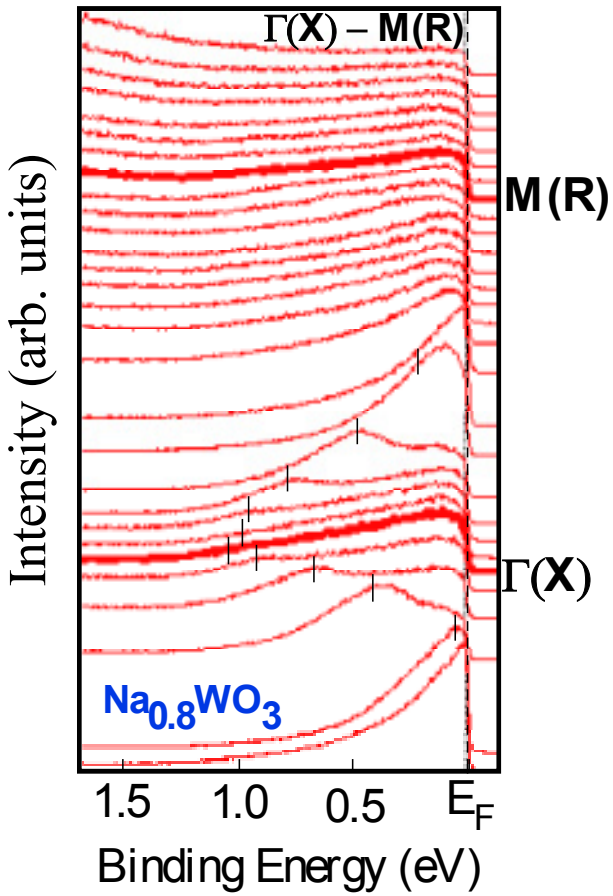
Valence band structure of metallic Na_xWO_3



 # FLAPW Band structure calculation of $NaWO_3$

ARPES spectra near-E_F of metallic Na_xWO_3



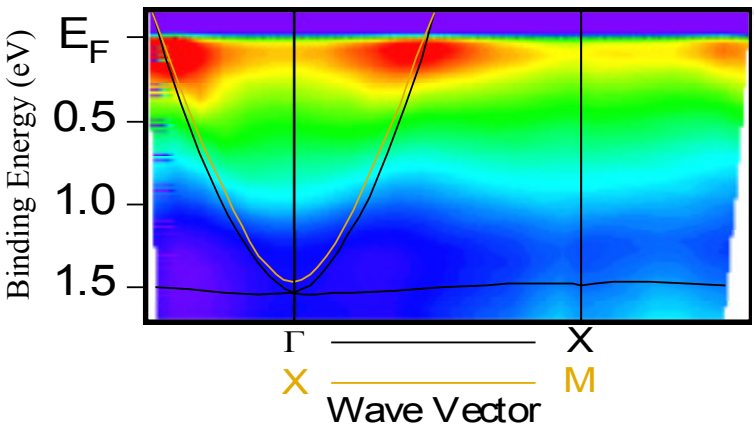


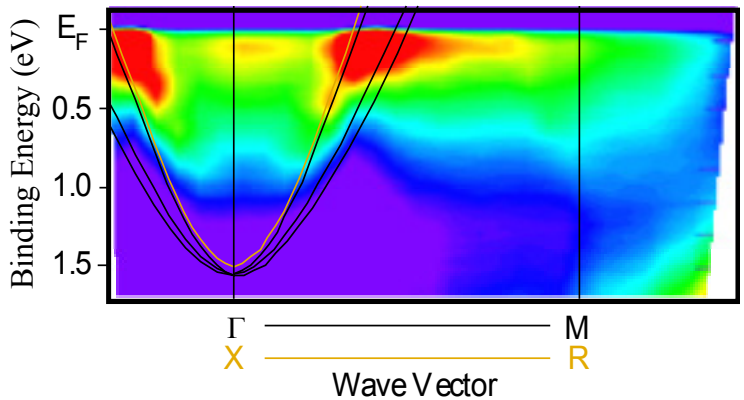
Near E_F region : W 5d t_{2g}

Na 3*s* electrons → W 5d t_{2g}

Near-E_F band structure of metallic Na_xWO_3

$Na_{0.8}WO_3$





Electron-like pocket At Γ(X) point

No surface Reconstruction

Summary

- Band structure of Na_xWO_3 is studied by high-resolution ARPES
- FLAPW band calculation agrees well with the experimental band structure
- Electron-like pocket at Γ(X) point agrees with the FLAPW band calculation


THANK YOU