Transparent Conductive Oxides

high transmission in the visible range (>80%)
low resistivity (10^{-3} Ω cm)
mechanical and corrosion resistance

(PV solar cells - Transparent electronics - Light emitting devices)

Tin – doped Indium oxide Sn : InO (ITO)

Aluminum – doped Zinc oxide Al : ZnO (AZO)

Al-doping induced states in the valence band of ZnO

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HAXPES in Al : ZnO

- large probing depth (surface contamination and Al migration)
- increased sensitivity to s-states

Samples @ Universidad de Malaga

- sputter – deposited films with 0 / 0.1 / 0.7 / 2.0 % Al : Zn ratio
- TEM / XRD / optical / Ω characterization

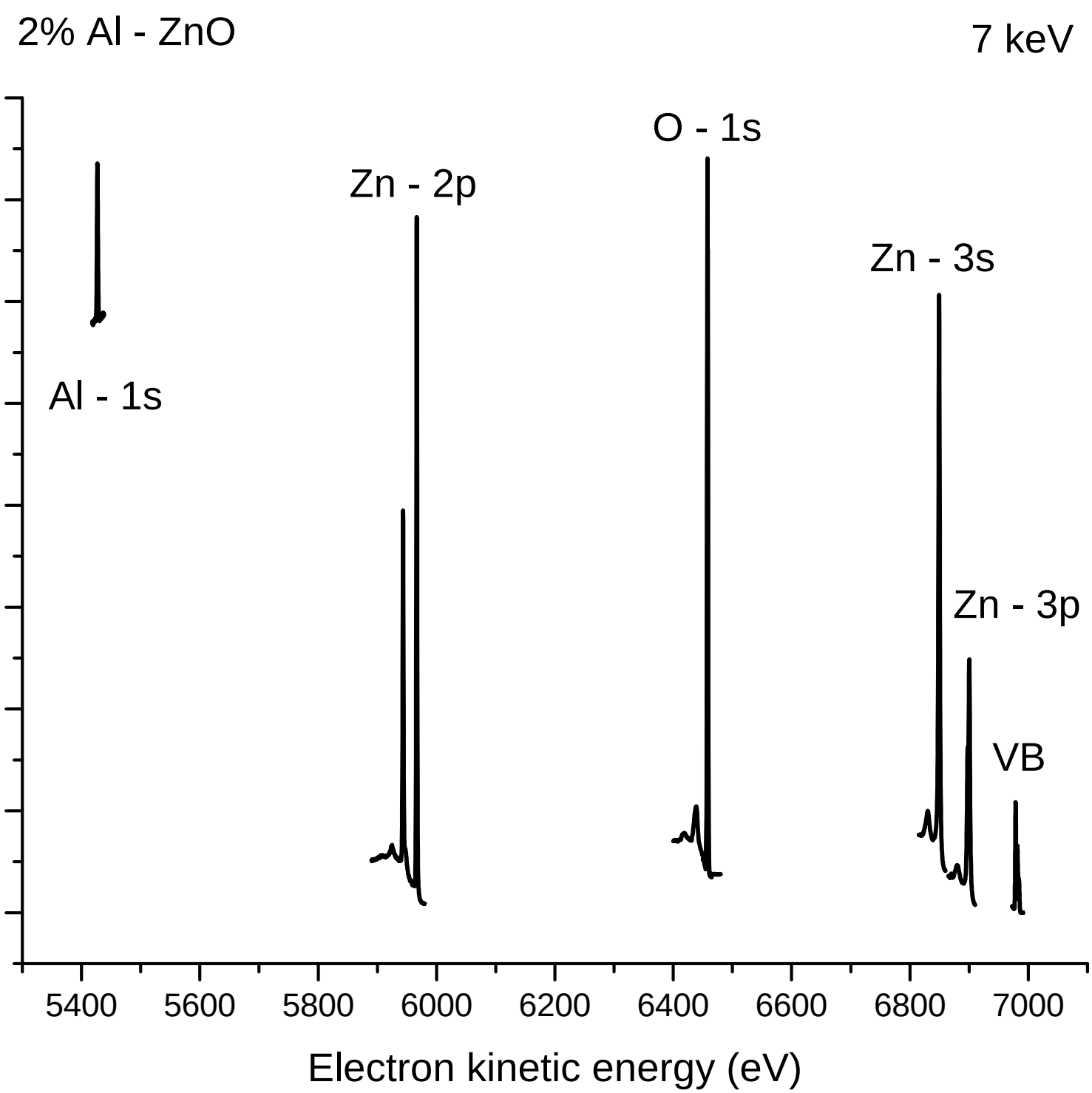
(3.2 eV optical bandgap, 80% transmission, 1- 2 mΩcm)

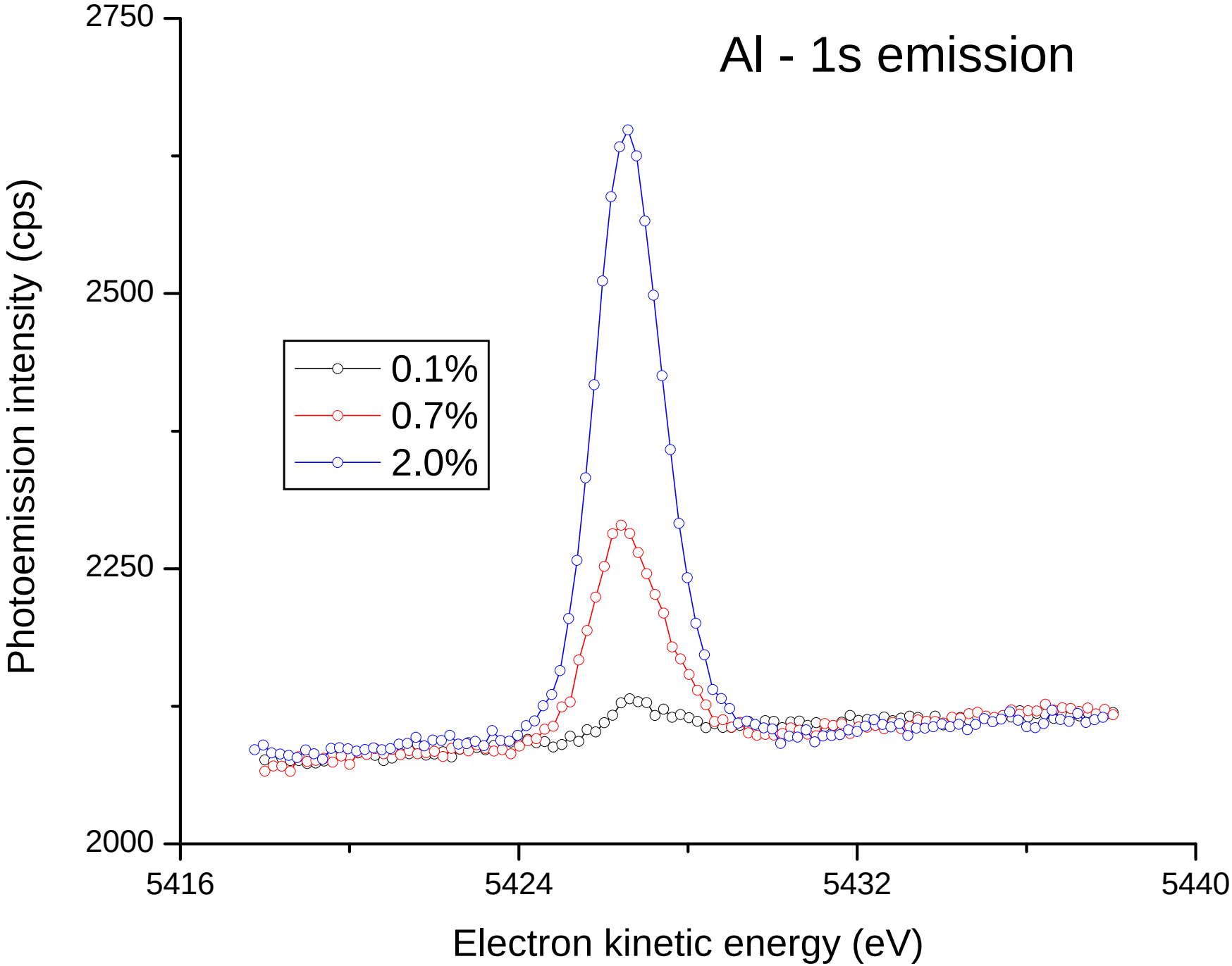
VolPE @ ESRF ID-16

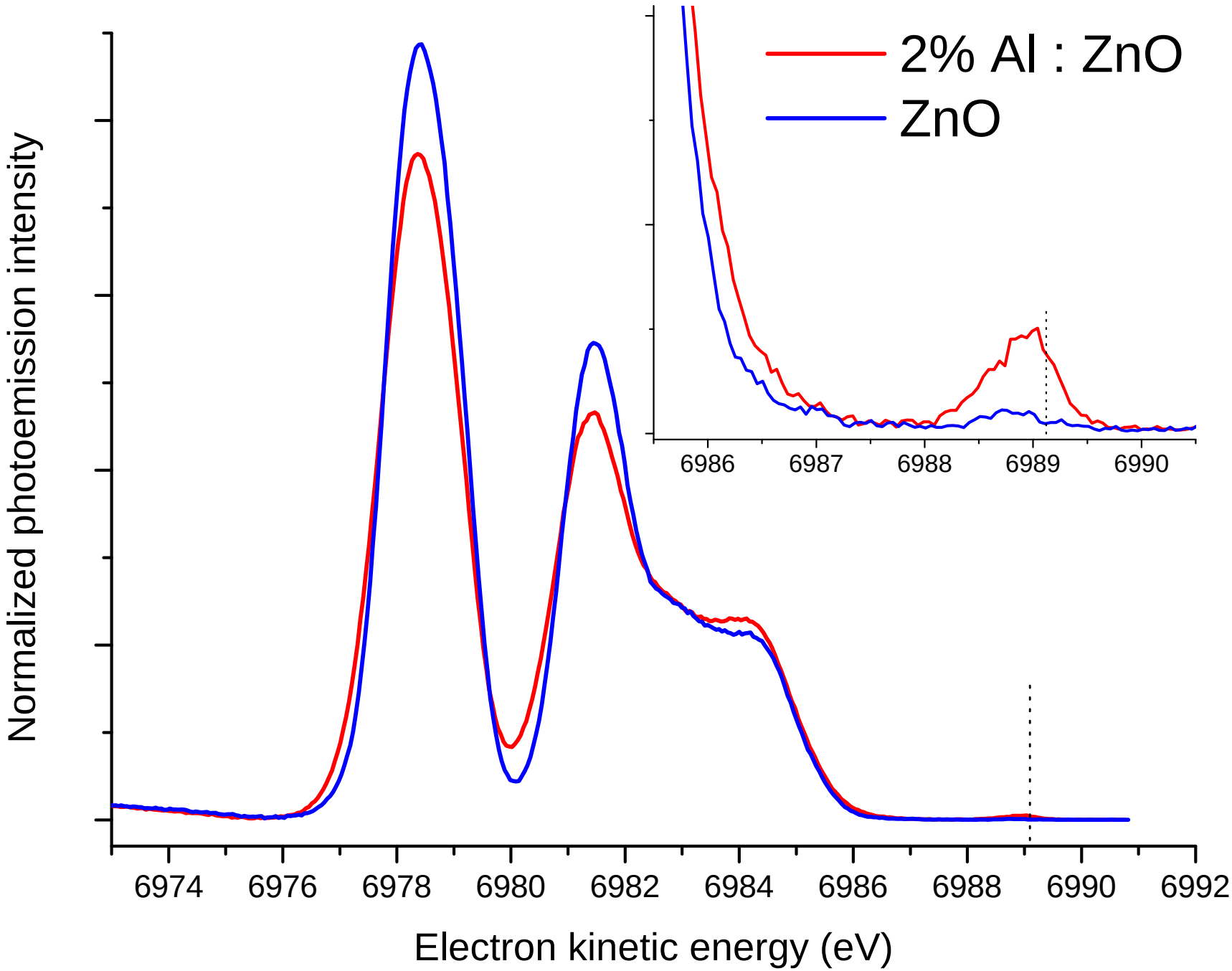
- 7 keV Si(220) 350 meV [Si(440) 160meV] overall resolution

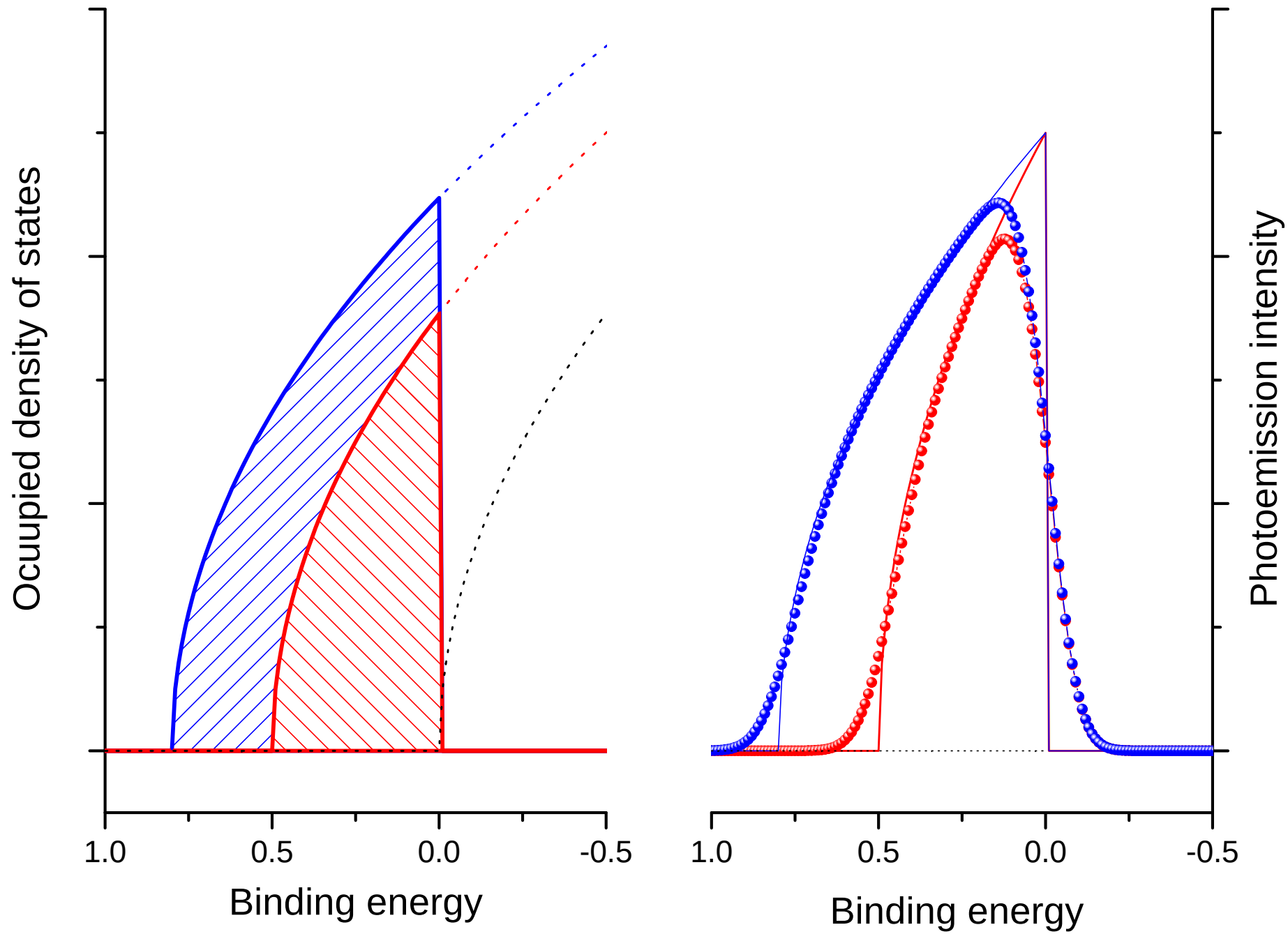
Calculations @ CEA Saclay

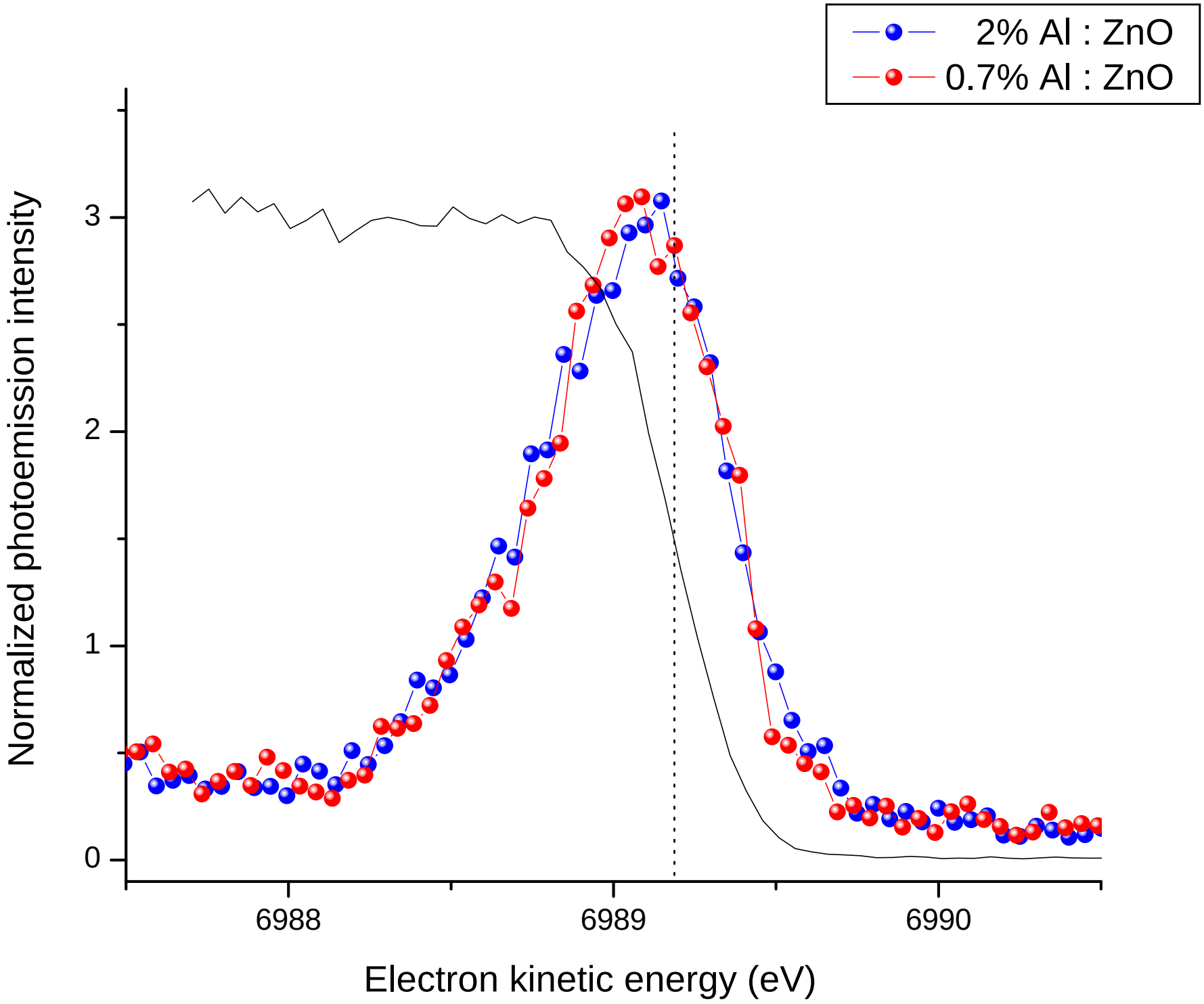
GGA+U model for valence band of AZO


2% Al - ZnO
7 keV
O - 1s
Zn - 2p
Zn - 3s
Al - 1s
Zn - 3p
VB
5400
5600
5800
6000
6200
6400
6600
6800
7000
Electron kinetic energy (eV)

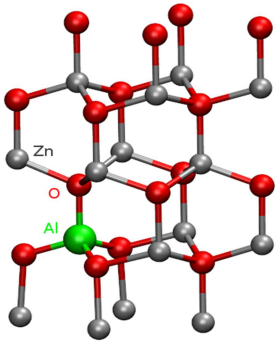

Al - 1s emission
Photoemission intensity (cps)
2750
2500
2250
2000
5416
5424
5432
5440
Electron kinetic energy (eV)
0.1%
0.7%
2.0%

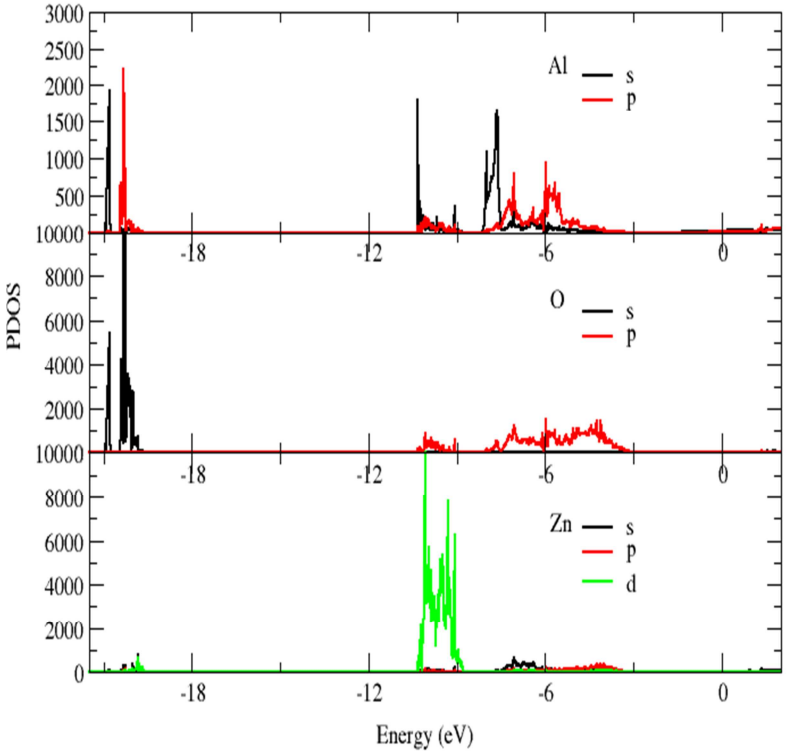

2% Al : ZnO
ZnO
Normalized photoemission intensity
Electron kinetic energy (eV)
6974
6976
6978
6980
6982
6984
6986
6988
6990
6992
6986
6987
6988
6989
6990

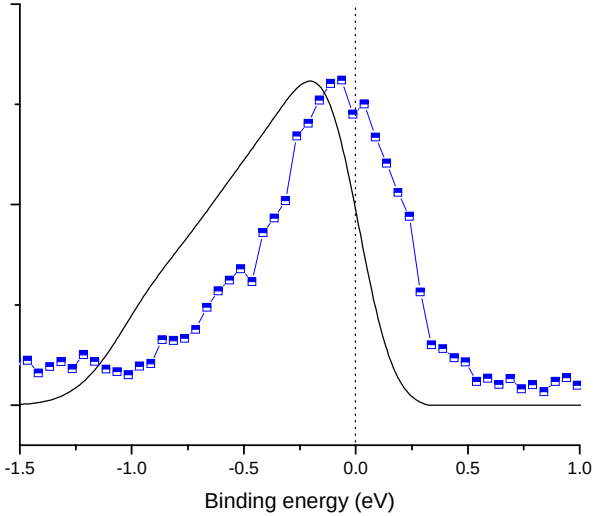

Ocuupied density of states
1.0
0.5
0.0
-0.5
Binding energy
Photoemission intensity
1.0
0.5
0.0
-0.5
Binding energy


2% Al : ZnO
0.7% Al : ZnO
Normalized photoemission intensity
0
1
2
3
6988
6989
6990
Electron kinetic energy (eV)

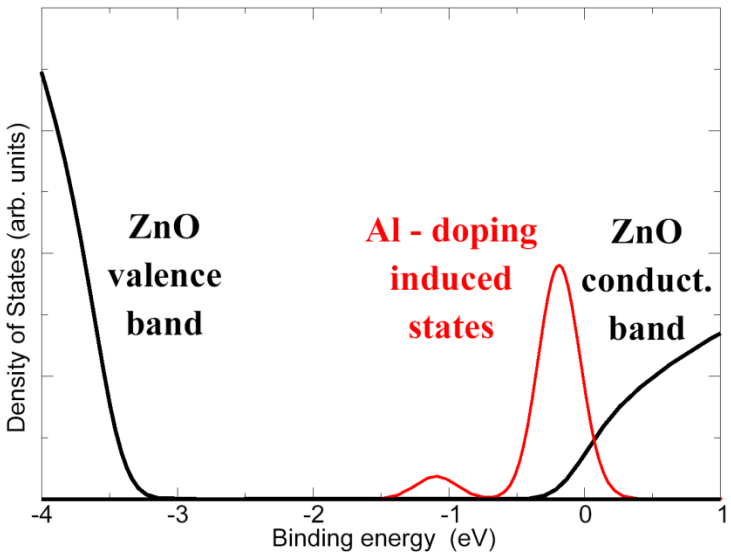
GGA+U

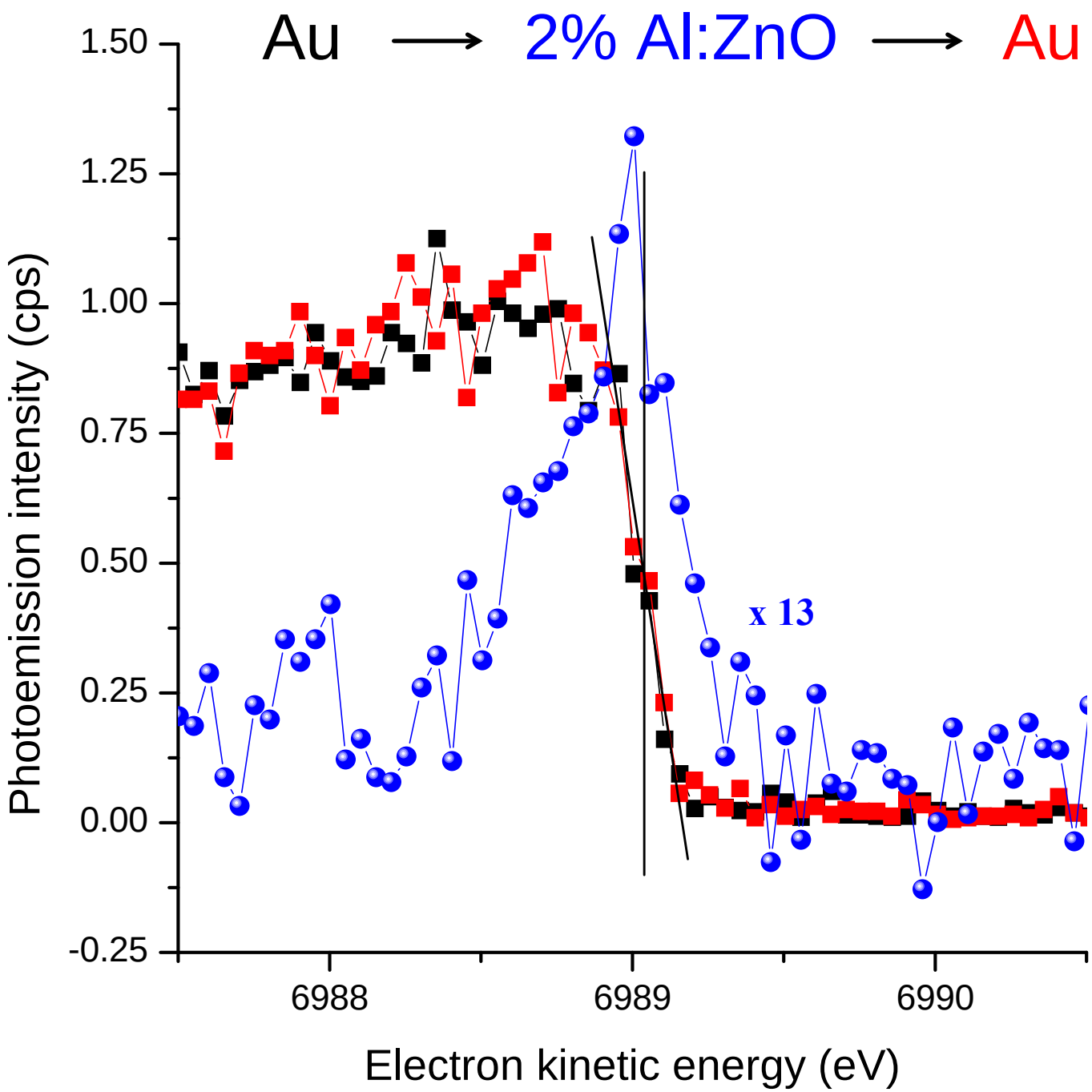






empirical model





160 meV resolution

Photon 100 meV

Si(440)

Analyser 120 meV

Ep=40eV, 0.8mm slit

kT = 25 meV

SUMMARY

- Al-doping of ZnO: a peak grows just below the Fermi level.
- the amount of Al-doping affects the intensity of this peak, not its shape.
- the Fermi level is placed close to the peak maximum

- GGA+U : only a small shift of CB ; Al-doping related states at the FL

Al:ZnO increased conductivity due mainly to doping-related states

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