

# Exploring novel materials for future electronic devices

## Multi technique approach for synthesis and characterization of 2D TMDCs

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Two dimensional transition metal dichalcogenides (TMDCs) have captured the interest of materials science research due to their outstanding properties and prospective applications in next generation devices.<sup>[1]</sup> Here we present the growth and characterisation of MoS<sub>2</sub> and WS<sub>2</sub> which are the most well-known TMDC materials.

They are part of the family of the 2D materials presenting a variety of properties.

- energy band gap depending on the structure and the number of layers
- valley polarization due to absence of inversion symmetry and strong spin-orbit interactions
- existence of stable structures

### TMDCs

Transition metal dichalcogenides

Two dimensional TMDCs monolayers are atomically thin crystalline materials of the type **MX<sub>2</sub>**,

Where one layer of transition metal (**M** = Mo, W etc.) atoms is sandwiched between two layers of chalcogen (**X** = S, Se etc.) atoms.

#### TMDC-based piezoelectronics

self-powering nano-robots and body-implanted devices<sup>[2]</sup>

#### Low-power and high-performance integrated circuits

nanoscale circuits contributing towards green electronics<sup>[3]</sup>

#### Sensors

enhanced sensitivity to functionalisation<sup>[4]</sup>

#### Optoelectronics

direct band gap in near Infrared and visible range<sup>[5]</sup>

#### Valleytronics

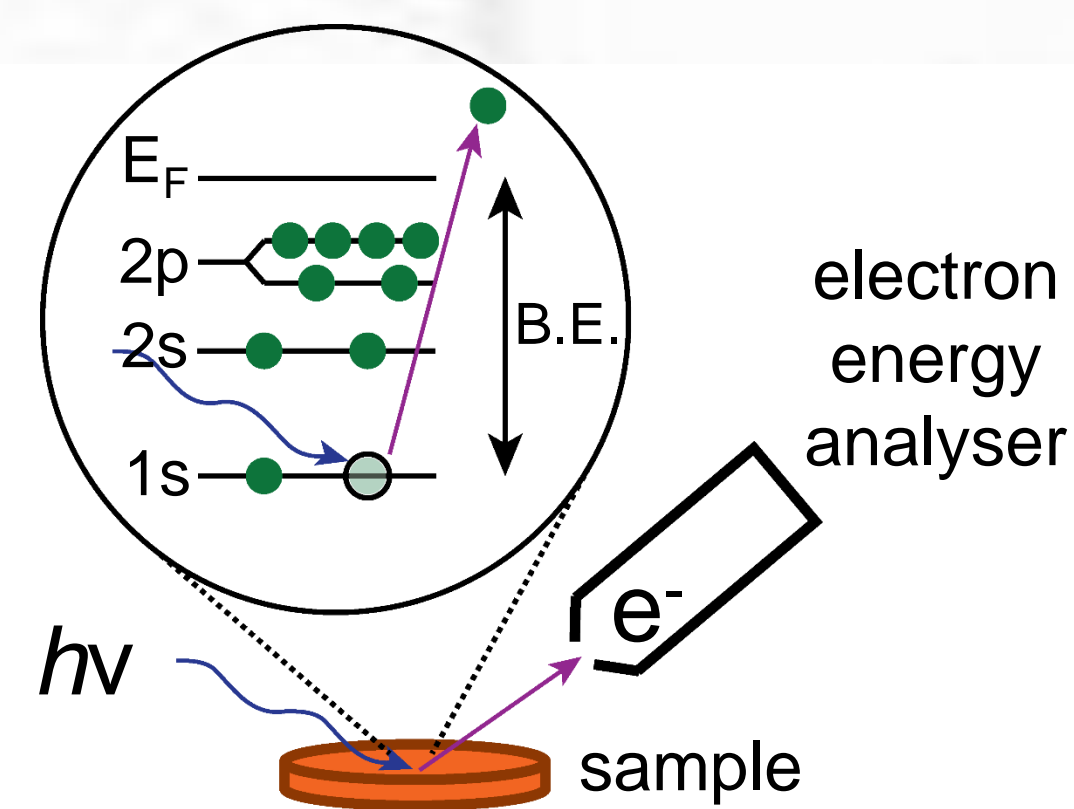
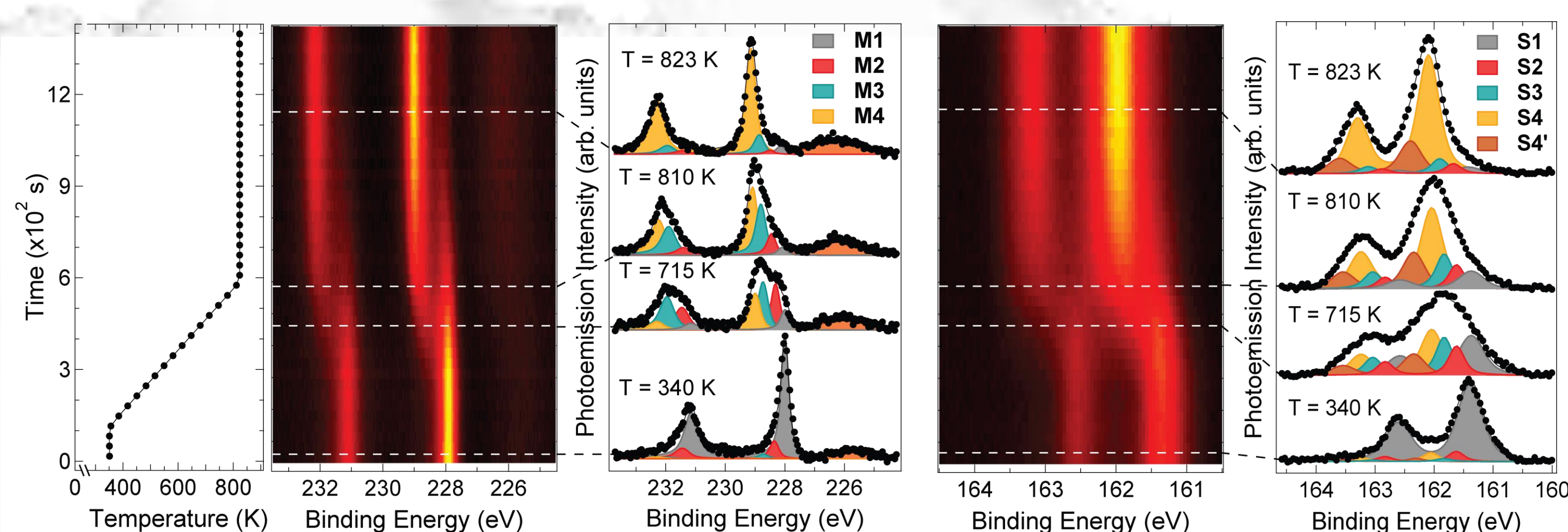
degenerate valleys of energy bands well separated in momentum space<sup>[6]</sup>

## Fast XPS - investigation of the growth of MoS<sub>2</sub> on Au(111)

Fast-XPS (X-ray Photoelectron Spectroscopy) allows to

- monitor the sample growth in real time.
- study the growth dynamics.
- avoid the growth of unwanted species by carefully tuning the growth parameters.

Mo 3d and S 2p core level spectra simultaneously acquired for the study of the growth of single layer MoS<sub>2</sub>.<sup>[7]</sup>

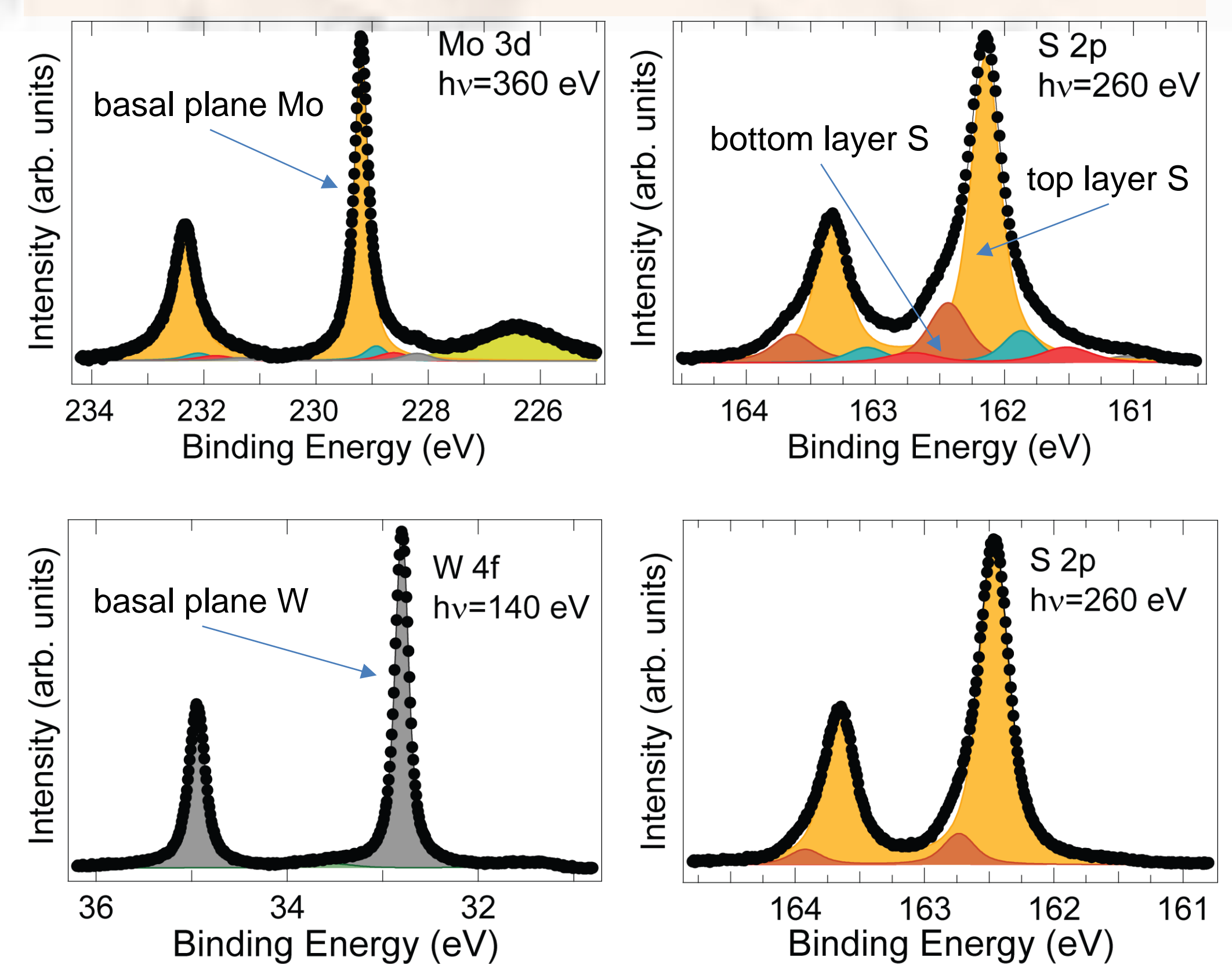


## High resolution XPS

HR-XPS is

- element specific and quantitative.
- sensitive to chemical and structural environment.

High resolution spectra of Mo 3d, S 2p and W 4f show the core level components of single layer MoS<sub>2</sub> and WS<sub>2</sub>.

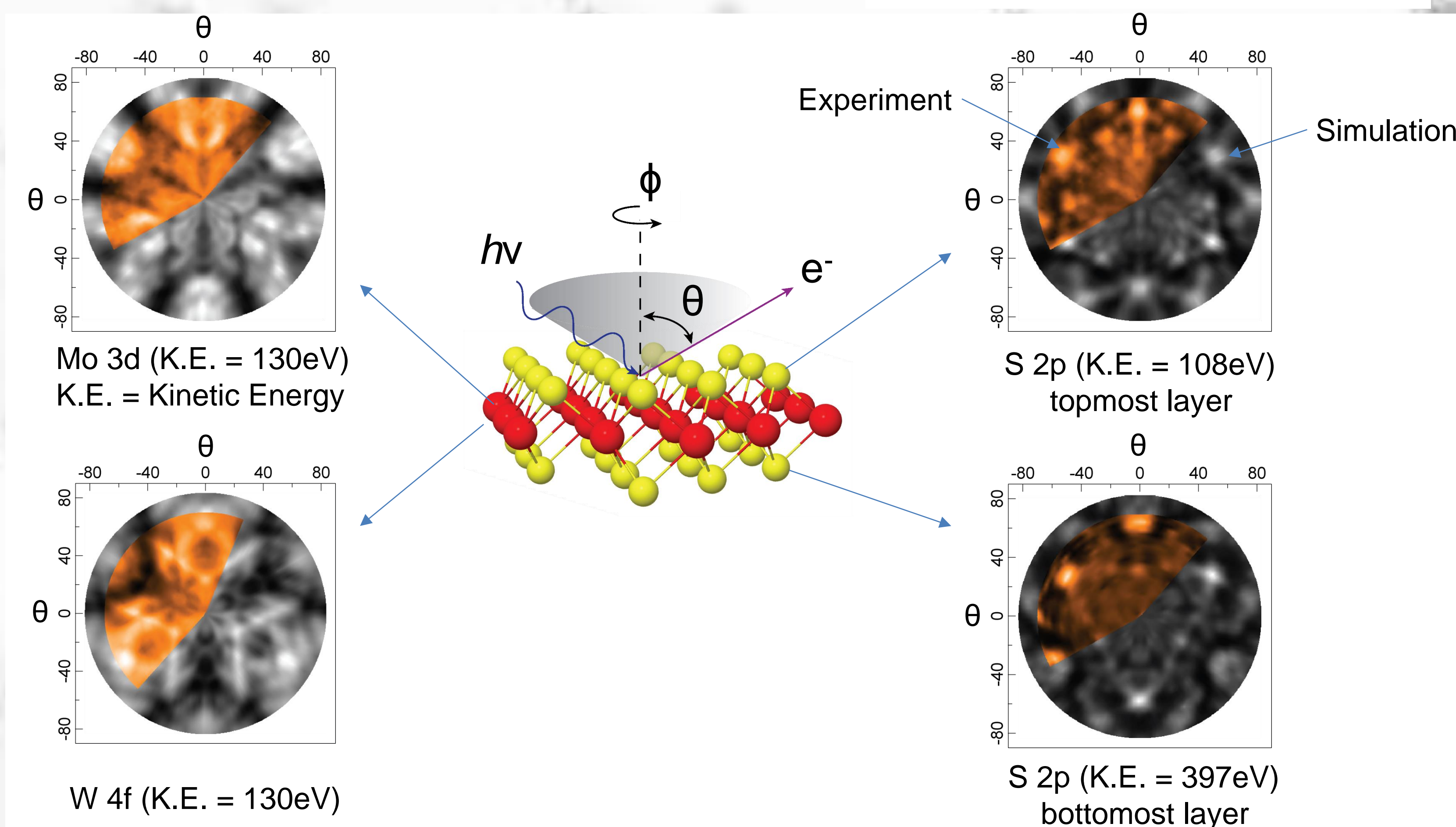
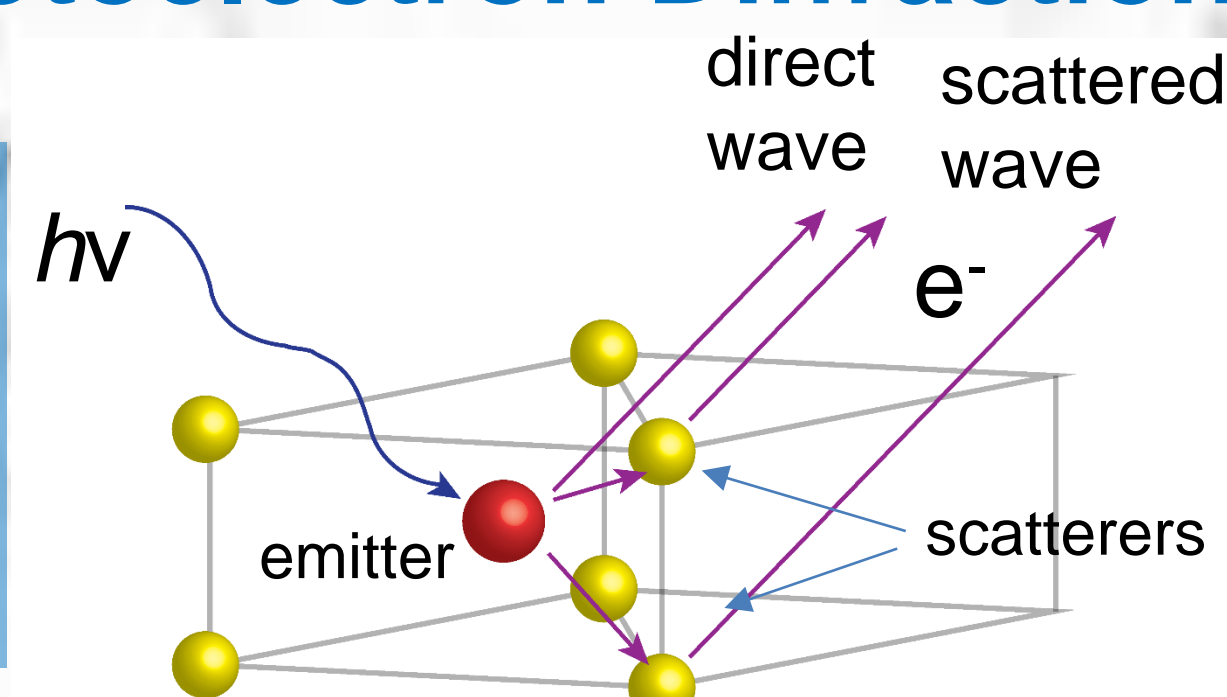


## Structure determination: X-ray Photoelectron Diffraction

XPD is a powerful tool to

- examine local order.
- determine crystal structure and orientation.

XPD patterns are in excellent agreement with the simulations for single layer MoS<sub>2</sub> and WS<sub>2</sub>.

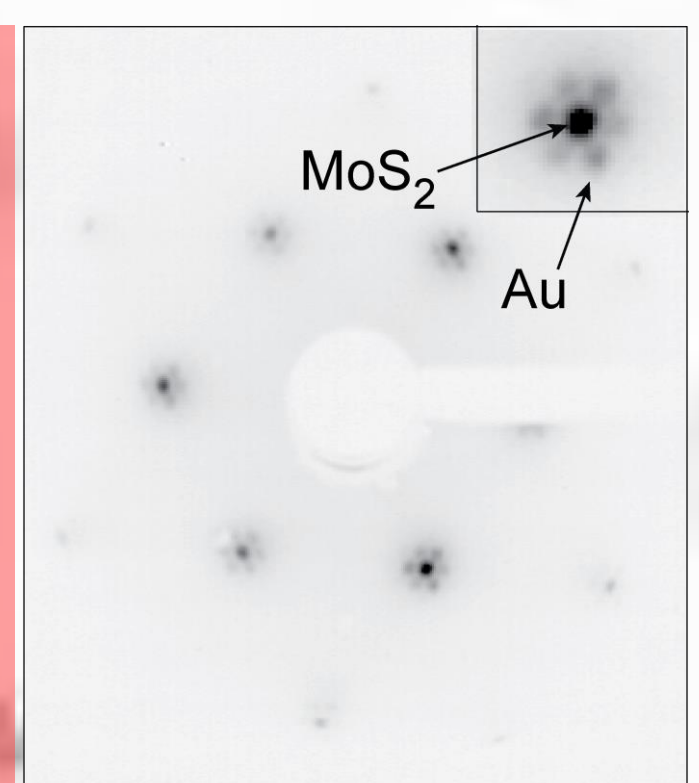


## Low Energy Electron Diffraction

LEED is used to

- determine long range order.
- study symmetry and rotational alignment of the adsorbate

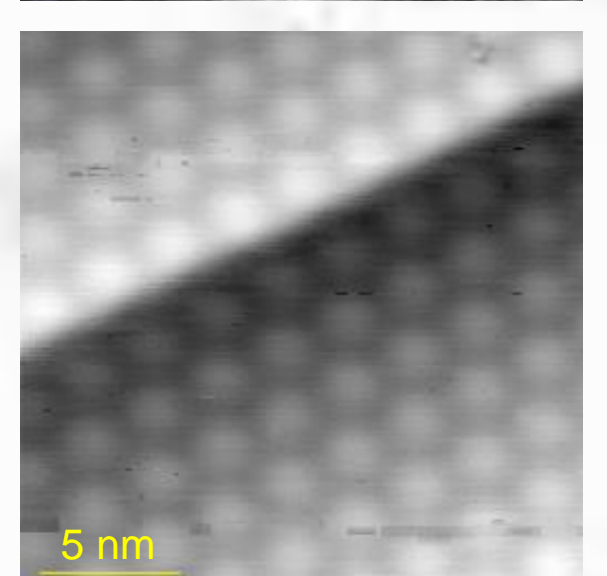
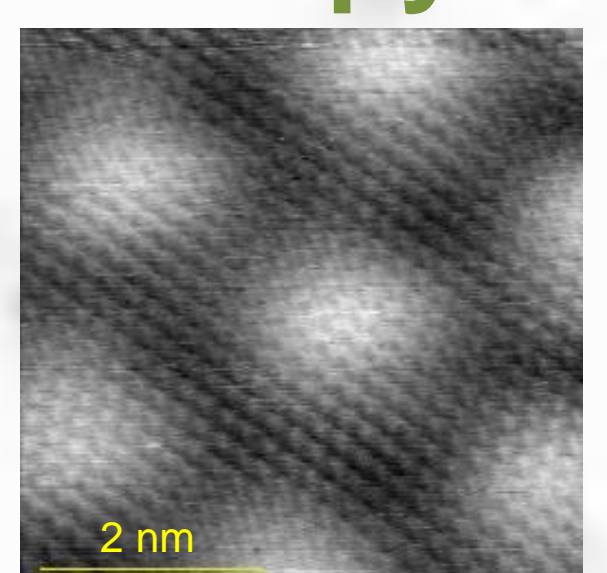
LEED image (at 117eV) for MoS<sub>2</sub> on Au(111) showing the moiré pattern due to lattice mismatch between MoS<sub>2</sub> and the substrate.



## Scanning Tunnelling Microscopy

The atomically-resolved STM image on the top shows the topmost S atoms exhibiting moiré periodicity of 3.4 nm, visible in the form of bright hexagonal protrusions.

Image at the bottom shows the single layer MoS<sub>2</sub> nano-island carpeting over an Ag terrace.



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