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Growth of Metallic TaSe₂ on GaP(111)_B Substrates

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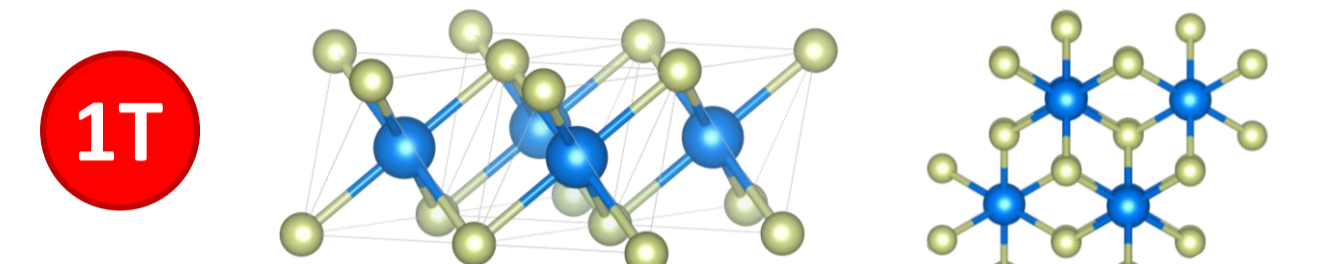
Motivations

Context: TaSe₂ is a group V metallic transition metal dichalcogenide which also exhibits **charge density waves (CDW)**, superconductivity and **Mott insulating** states. Since the occurrence of these properties largely depends on the polytype, understanding the phase formation in TaSe₂ grown by **molecular beam epitaxy (MBE)** may be required for applications. However, the selective growth of 1T and 1H-TaSe₂ monolayers has only been demonstrated on graphene [1] and the phase diagram of few-layers TaSe₂ remains scarcely explored yet.

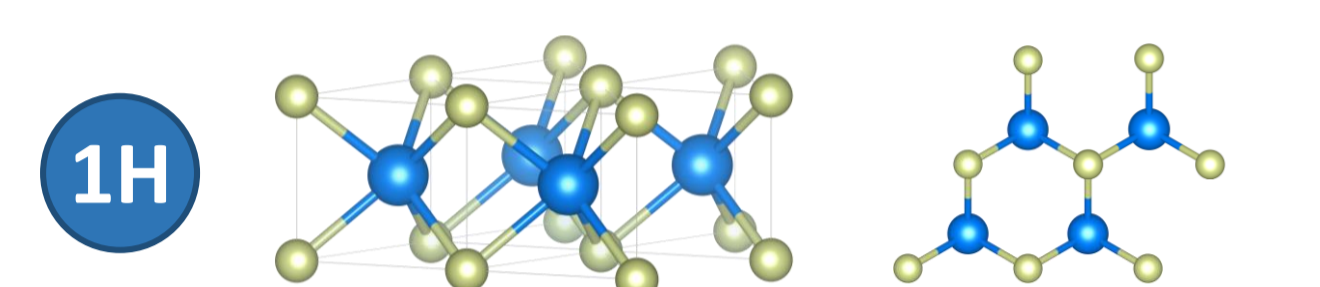
Goals:

- Propose a commercially available III-V semiconducting substrate (gallium phosphide) which enables electrical characterisations.
- Investigate the growth of TaSe₂ multilayers and its possible use as high work function metallic contacts.

1T-TaSe₂
Mott insulator in monolayer
CDW at room temperature



1H-TaSe₂
Always metallic
CDW below 122K

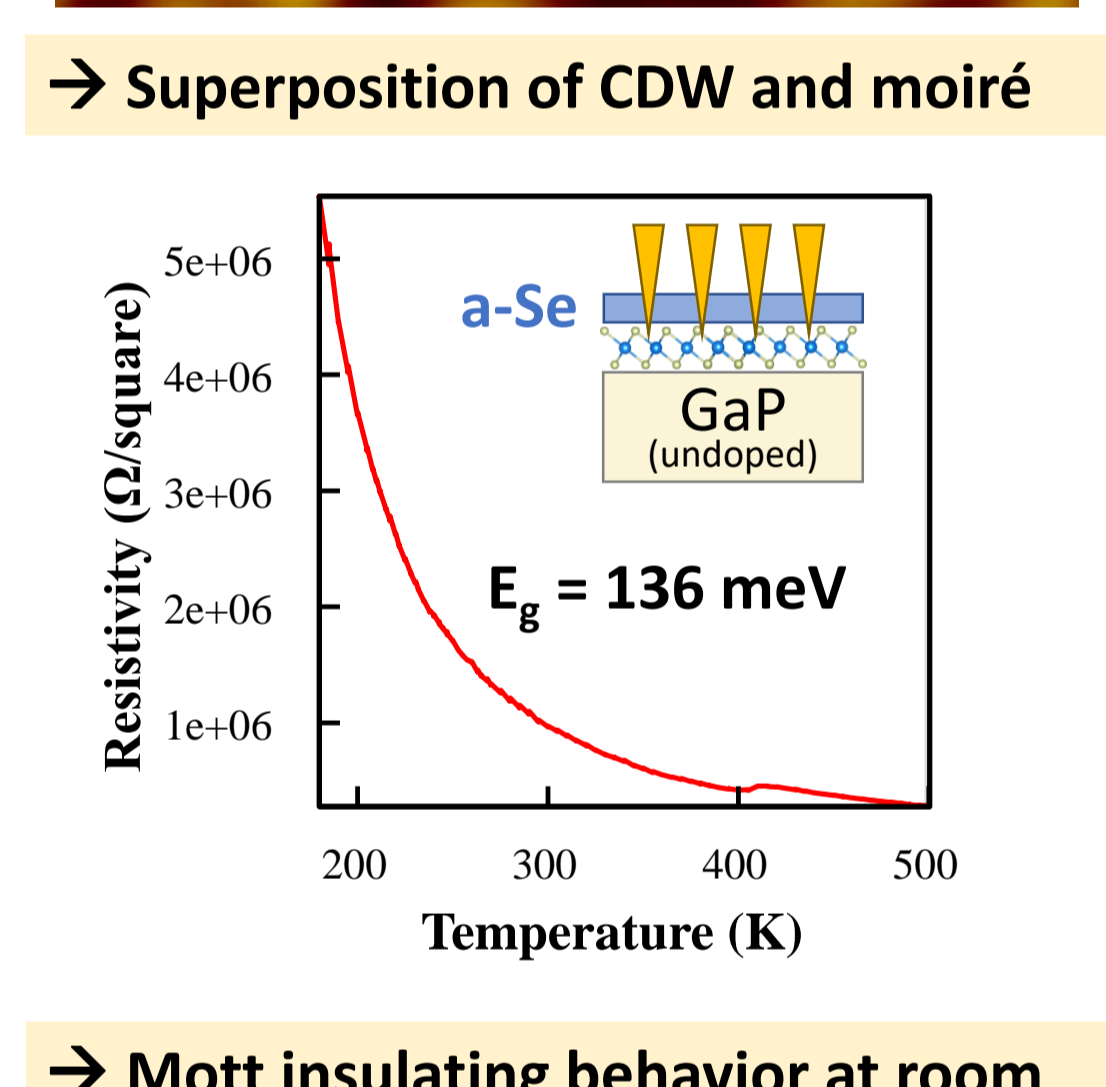
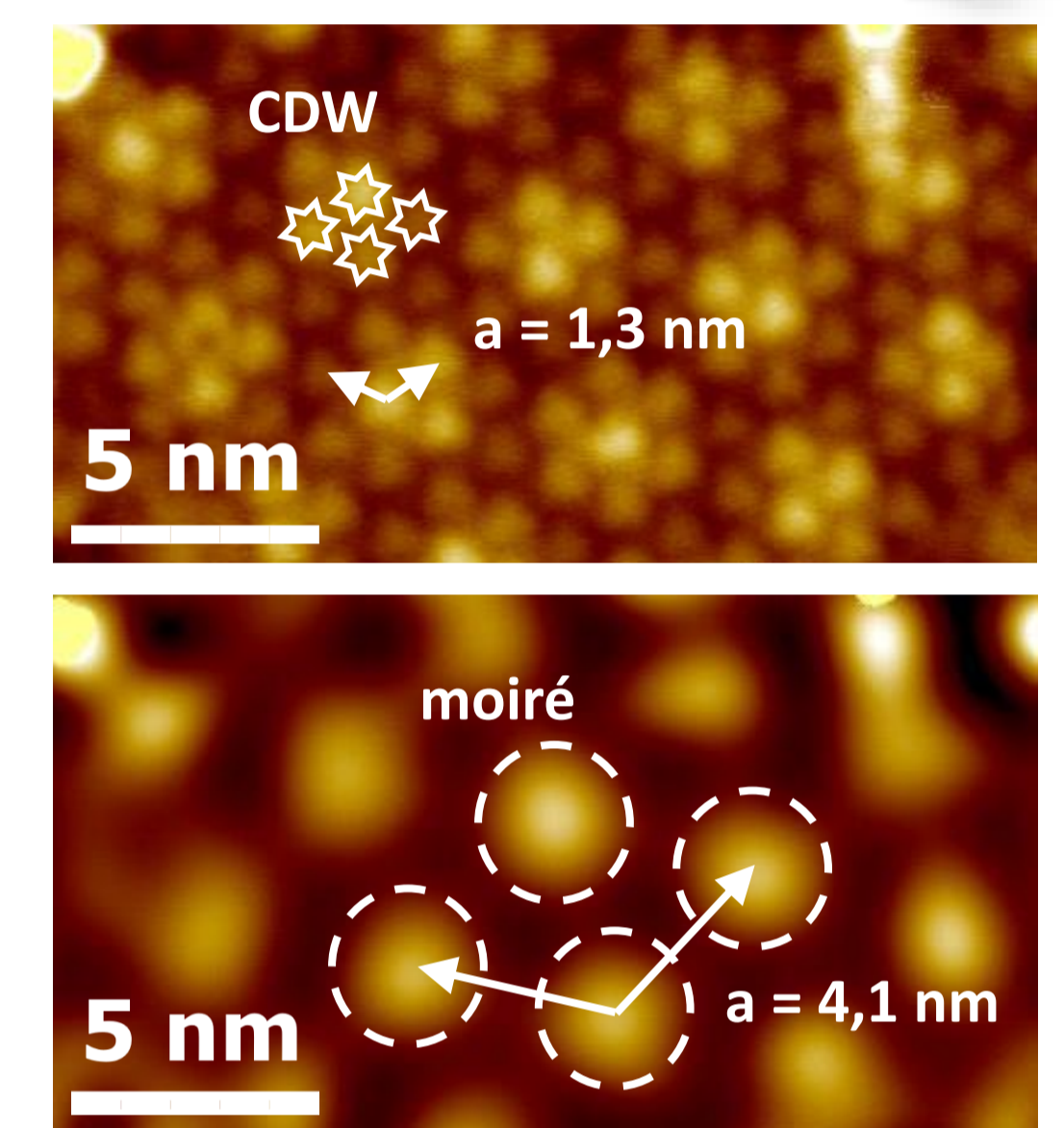
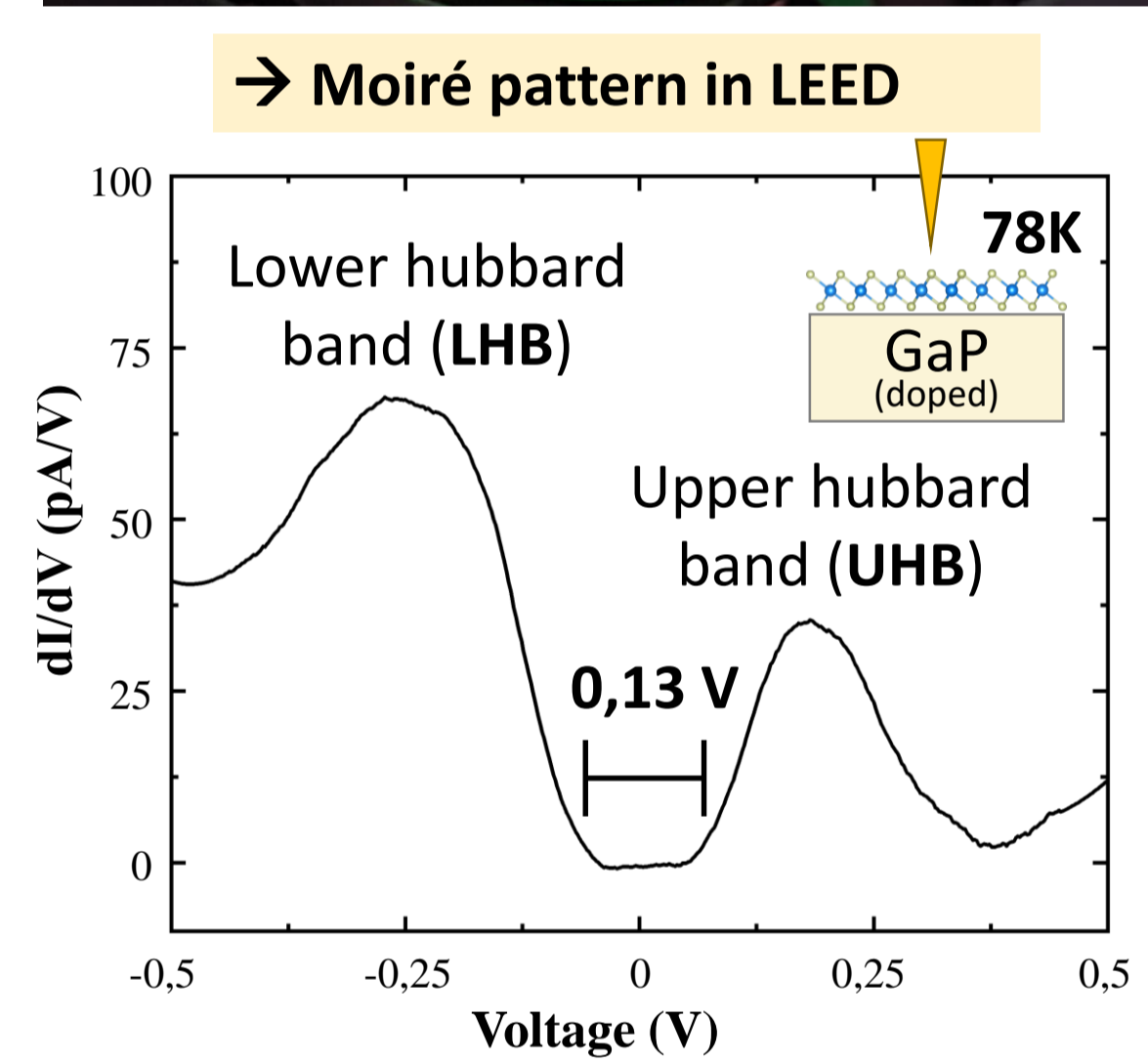
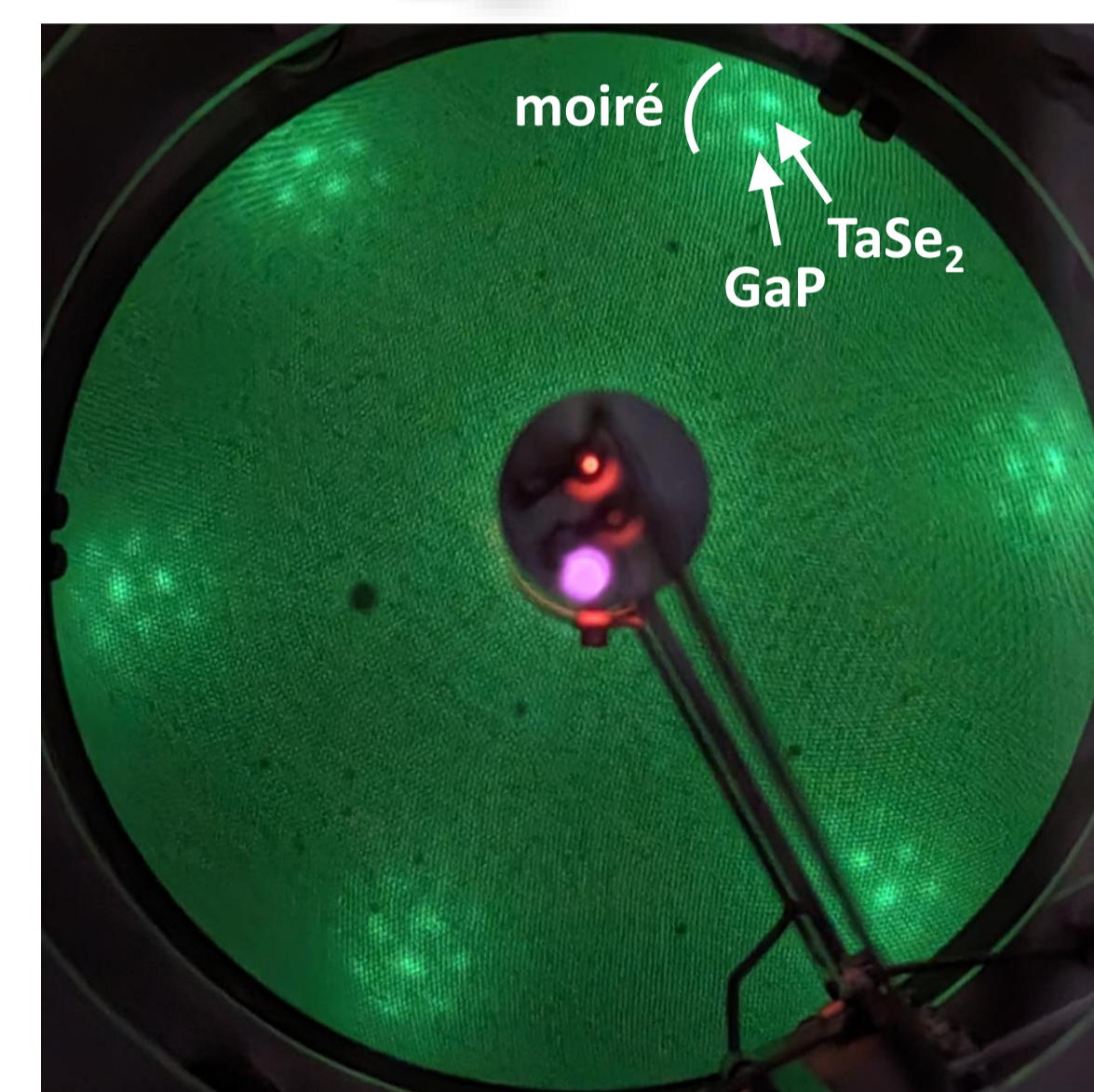
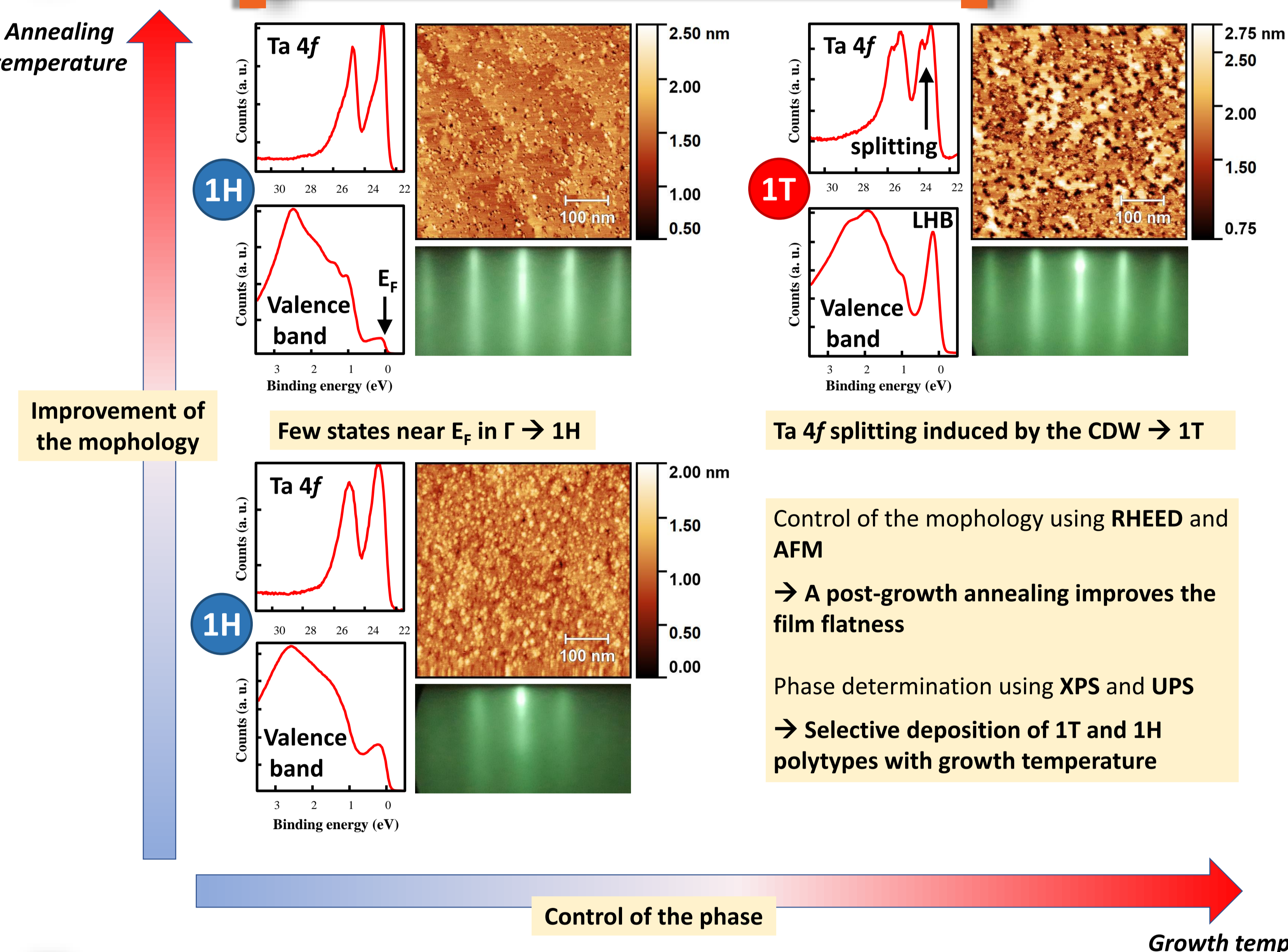


[1] Y. Nakata, T. Yoshizawa, K. Sugawara, et al. "Selective fabrication of Mott-insulating and metallic monolayer TaSe₂". ACS Applied Nano Materials 1.4 (2018), pp. 1456–1460.

Phase and morphology (XPS, UPS, AFM, RHEED)

TaSe₂ monolayers

Properties of 1T-TaSe₂ (LEED, STM, STS, 4-point probe)

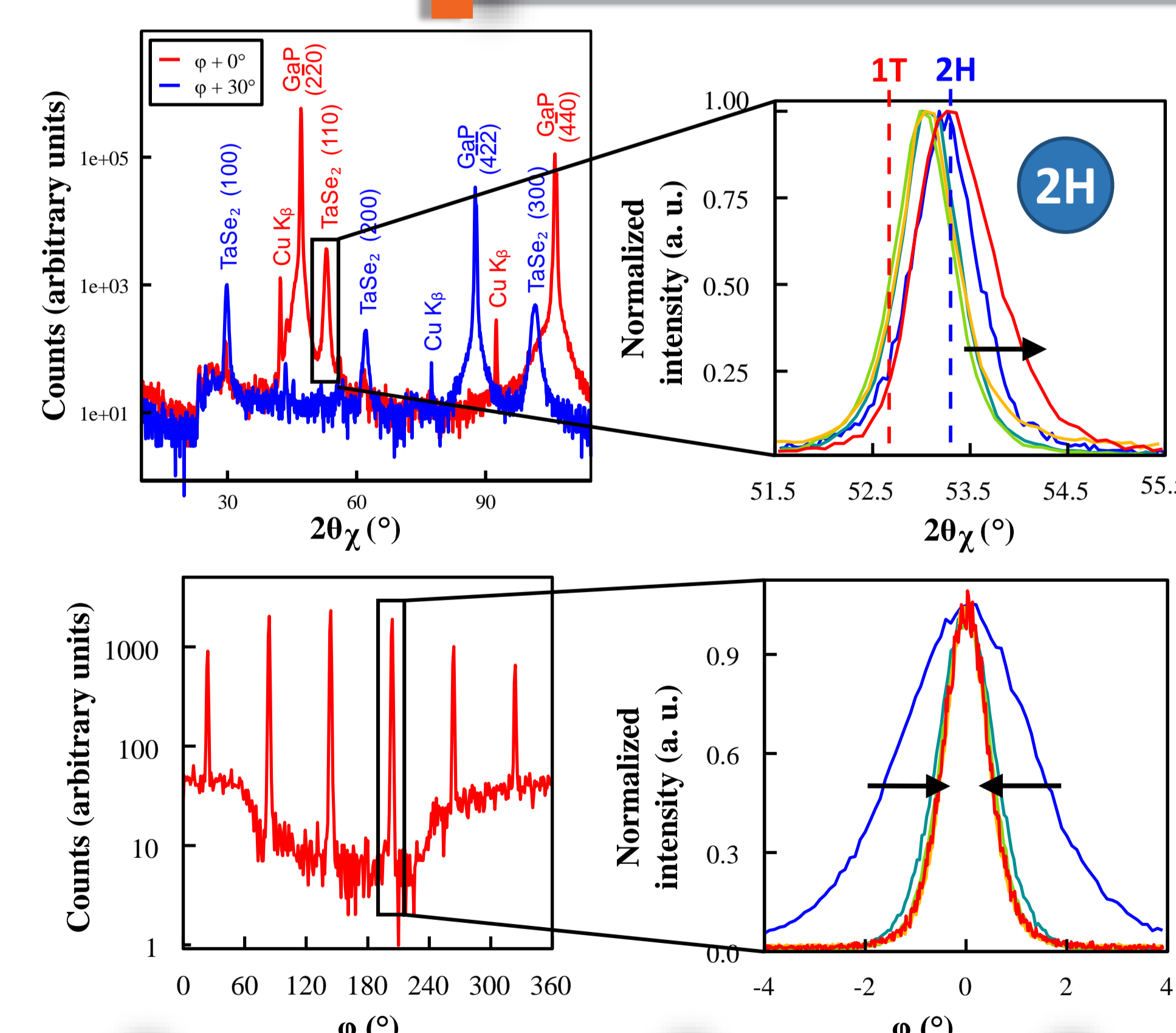
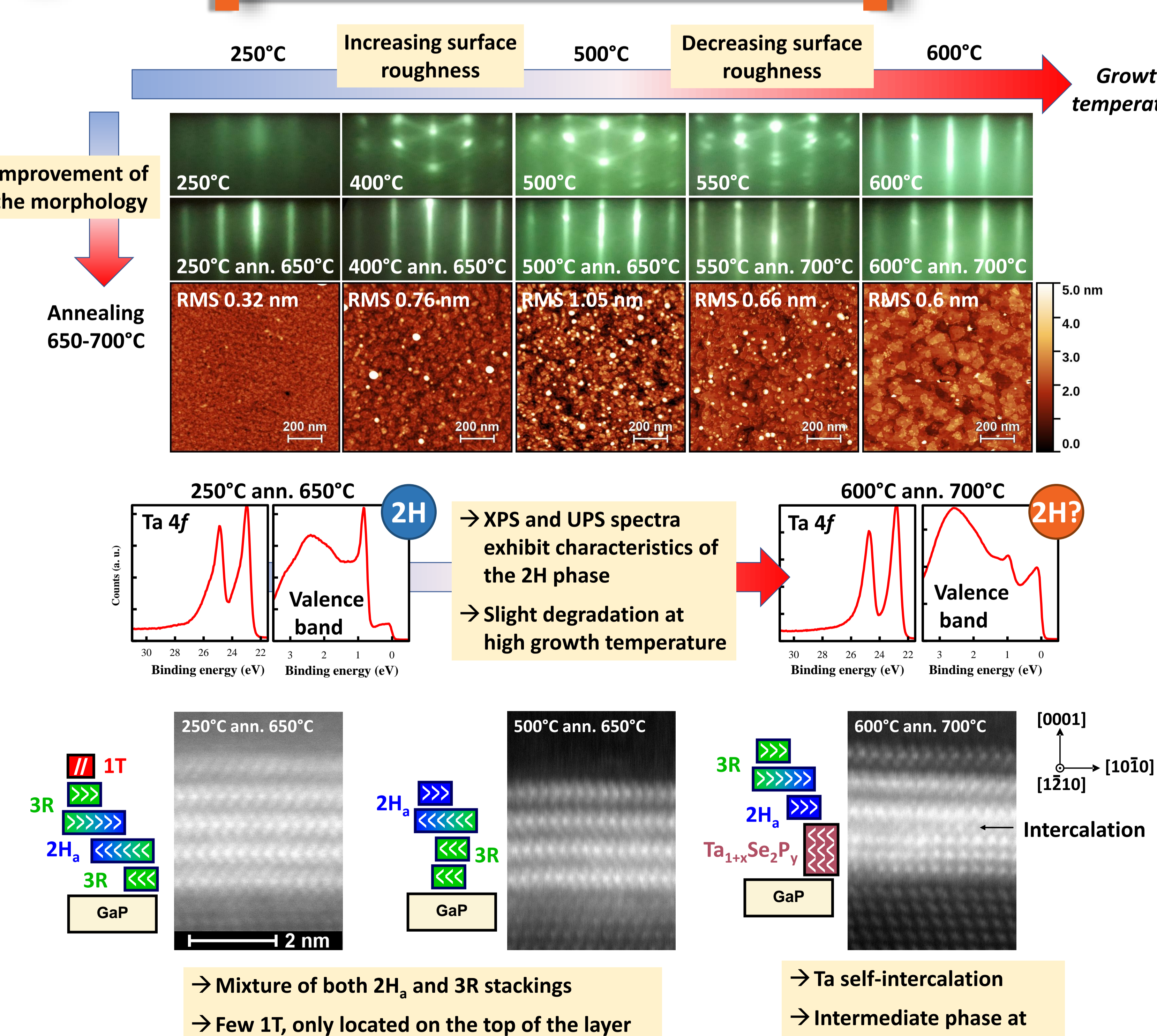


H. Koussir, Y. Chernukha, C. Sthiou, et al. "Large-area epitaxial Mott insulating 1T-TaSe₂ monolayer on GaP(111)B". Nano Letters 23.20 (2023), pp. 9413–9419.

Phase and morphology (XPS, UPS, AFM, RHEED, STEM)

TaSe₂ multilayers

Structure (In-plane grazing-incidence XRD)



→ Lattice parameter in agreement with the 2H phase
→ Slight shift related to variations of the layer composition
→ Asymmetry at the highest growth temperature

→ The film reproduces the 6 fold-symmetry of the substrate.
→ In-plane misorientation below 1° at 400°C and above

Composition (XPS)

Electrical properties (UPS, 4-point-probe)

