Continuous Tuning of Electronic Correlations by Alkali Adsorption on Layered 1*T*-TaS_2

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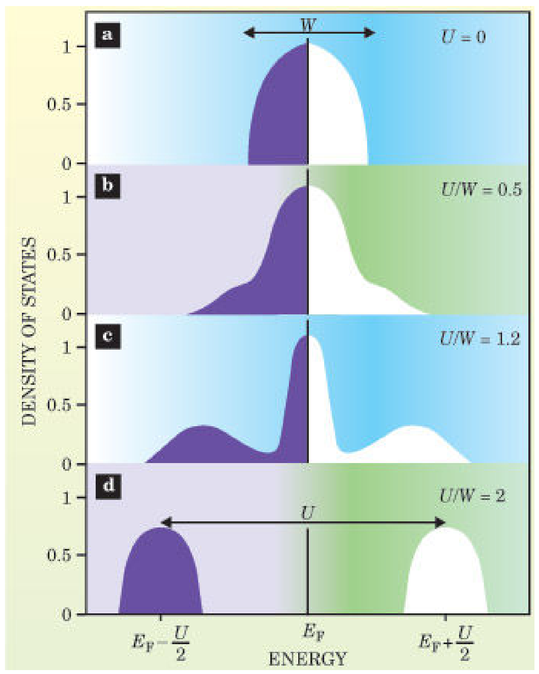
Motivation



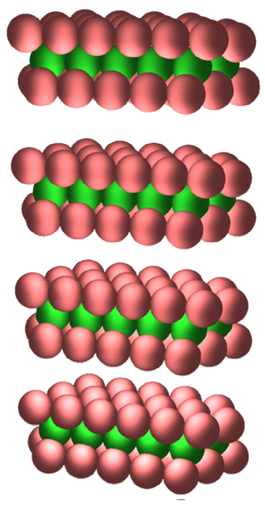
Kotliar & Vollhardt, Physics Today **3**, 53 (2004)

Measure A(**k**, ω) while tuning U / W

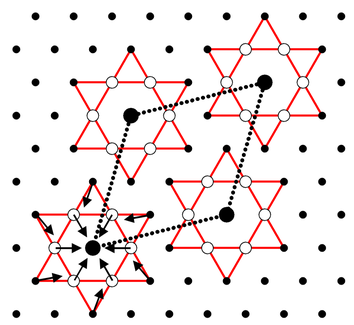
- hydrostatic pressure
- chemical composition
- **alkali adsorption on layered crystals**

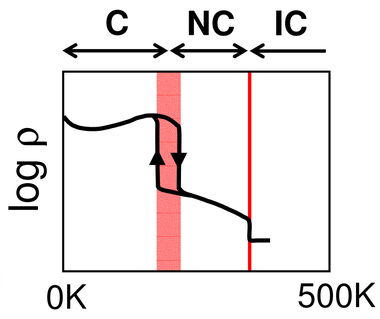
  (charge transfer, CDW, intercalation, …)

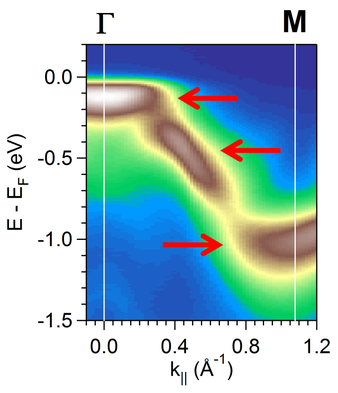
1*T*-TaS_2



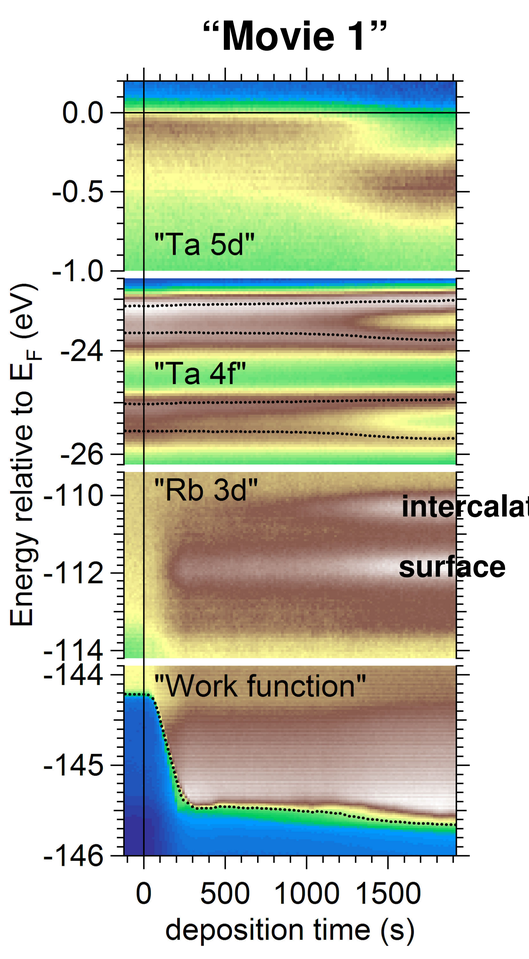
- $\sqrt{13} \times \sqrt{13}$ CDW
- Mott–Hubbard gap
- Anderson localization

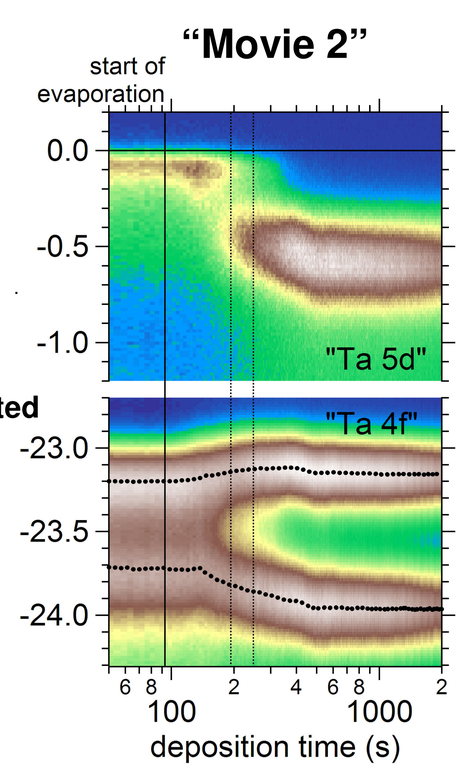


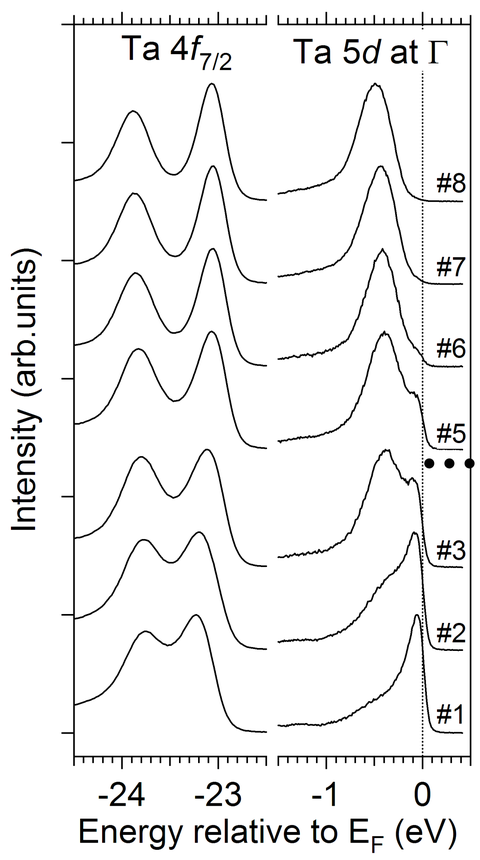




Spectroscopy during Rb deposition

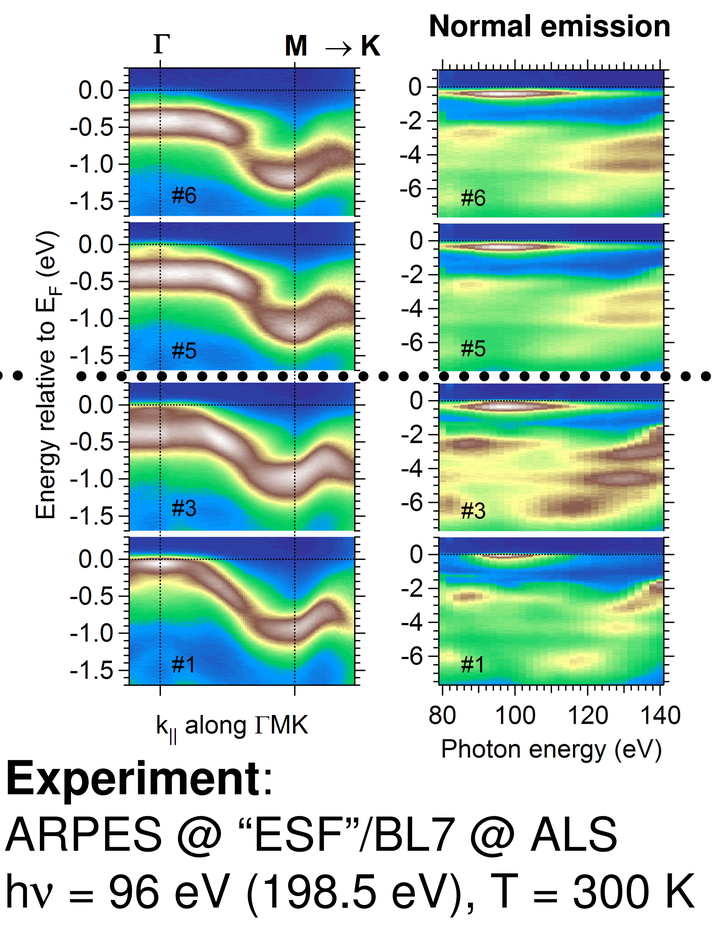






c(2√3 × 4)rect.

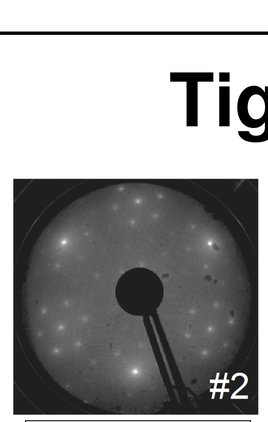
p(√13 × √13)R13.9°

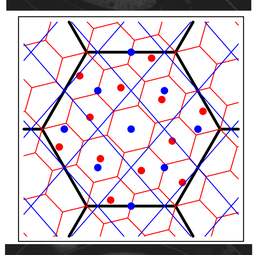


Experiment:
ARPES @ "ESF"/BL7 @ ALS
hν = 96 eV (198.5 eV), T = 300 K

Tight–binding simulation

p(√13 × √13)R13.9°





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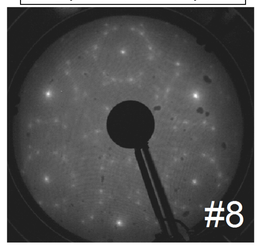

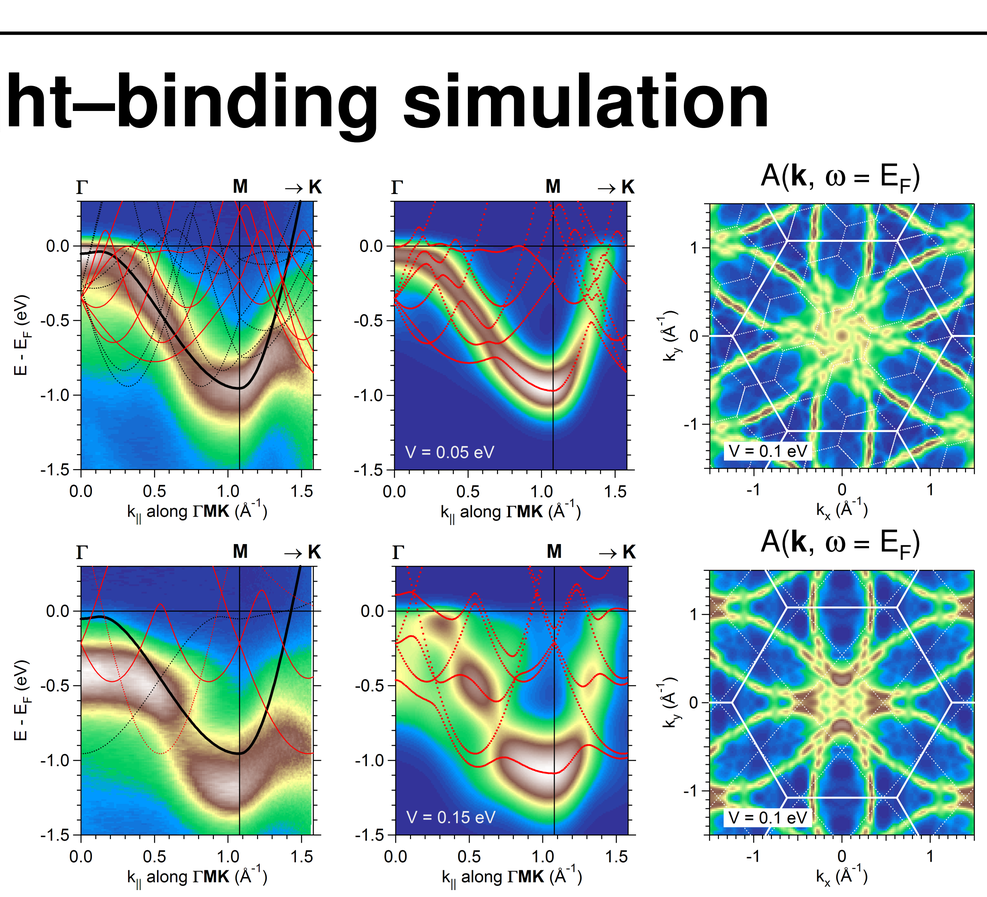

Smith *et al.*, J. Phys. C.: Solid State Phys. **18**, 3175 (1985)
Aiura *et al.*, Phys. Rev. B **69**, 245123 (2004)

Results & discussion

Rb deposition on 1*T*-TaS_2:

- **Metal–insulator transition** (Ta 5d)
  - Mott–Hubbard type + e–ph interaction
- Modification of CDW:
  - Wave vector: $\sqrt{13}$ a → $\sqrt{7}$ a (LEED)
  - Amplitude ~ (Ta 4f splitting, Ta 5d kinks)
- Rb adsorption + **intercalation** (Rb 3d)

Effects on critical parameters:

- Band filling: **n** ≈ 1 ≈ const.
- Correlation energy: **U** ≈ 0.8 eV ≈ const.
- Bandwidth: $\mathbf{W}_{\parallel}$ ⇑ (?), $\mathbf{W}_{\perp}$ ⇓ (!)

Questions:

- Why change of CDW?
- Role of electron–phonon interaction?