Modulated Kondo Screening along Magnetic Mirror Twin Boundaries in monolayer MoS_2

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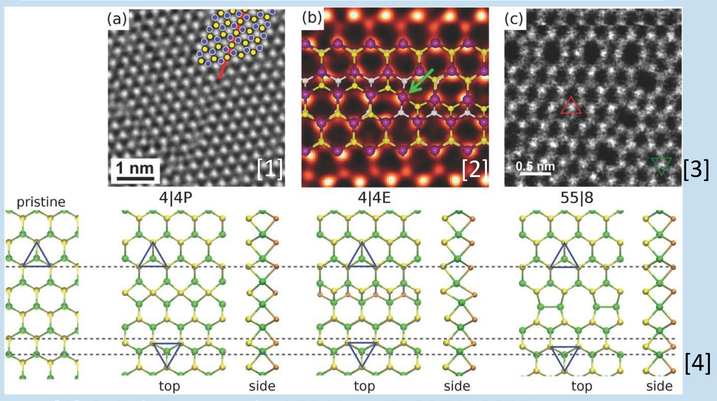
Mirror twin boundaries in semiconducting transition metal dichalcogenides

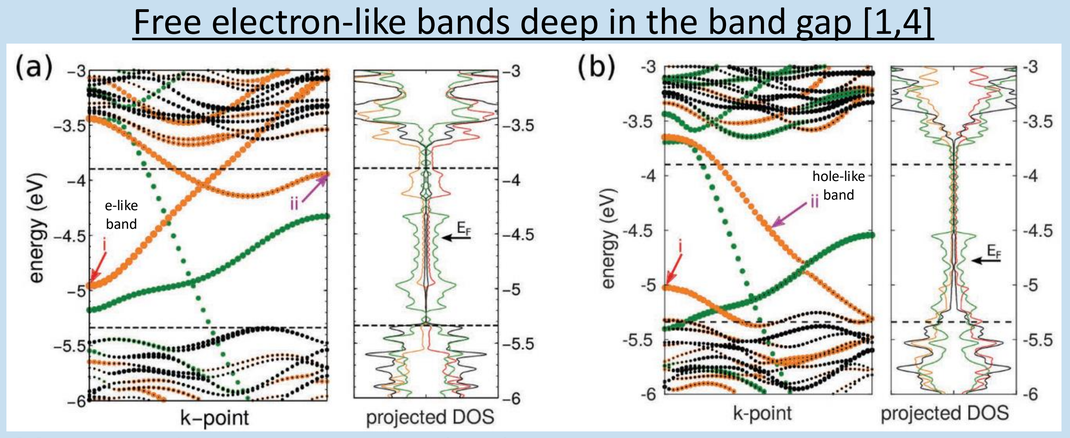
Structure of mirror twin boundaries [1-4]



[1] O. Lehtinen et al., ACS Nano **9**, 3274 (2015)

[2] W. Zhou et al., Nano Lett. **13**, 2615 (2013)

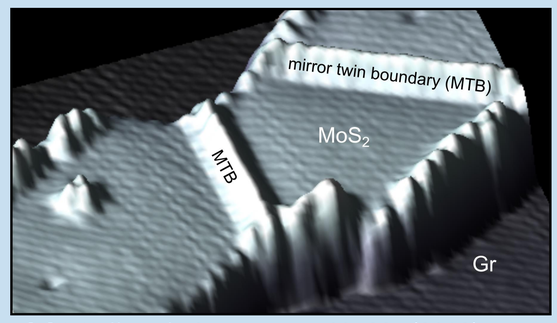
Free electron-like bands deep in the band gap [1,4]



[3] Y.-C. Lin et al., Nat. Commun. **6**, 6736 (2015)

[4] H.-P. Komsa, A. V. Krasheninnikov, Adv. Electron. Mater. **6**, 1600468 (2017)

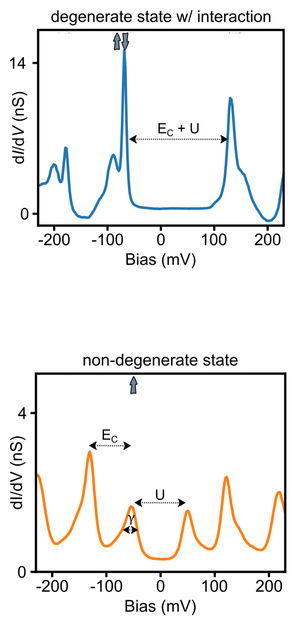
Our system: MoS_2 on graphene/Ir(111) [5]



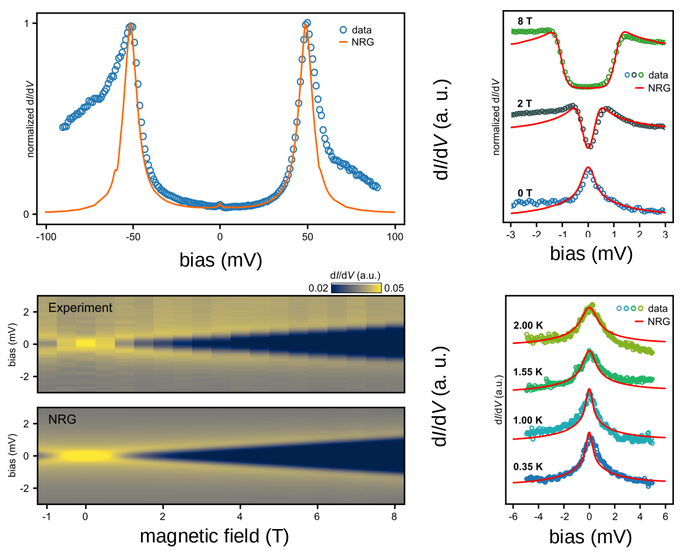
[5] J. Hall et al., 2D Mater. **5**, 025005 (2018)

Strongly Correlated Impurity States and Kondo Resonance in Magnetic Boundaries [6]

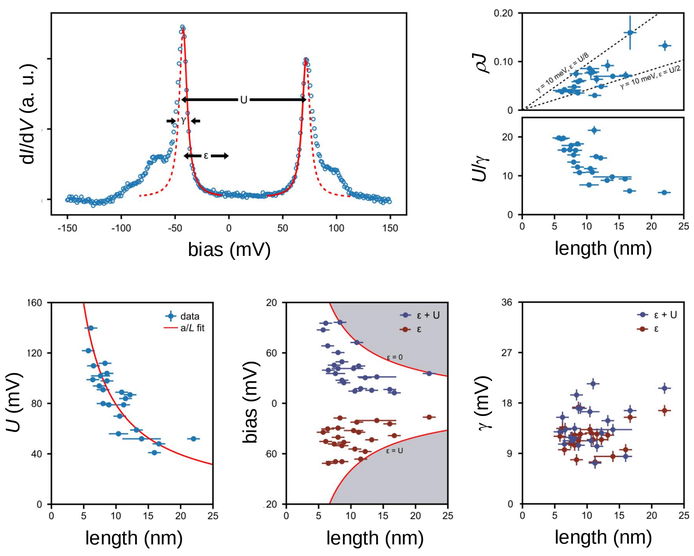
Two ground states



Influence of field and temperature



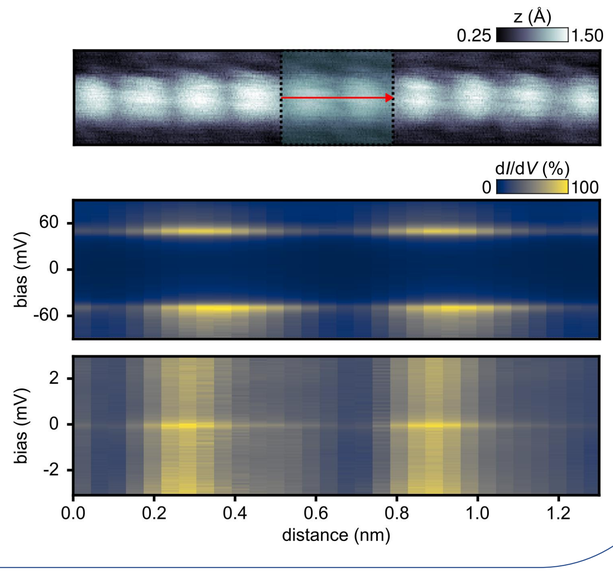
Extracting Anderson model parameters



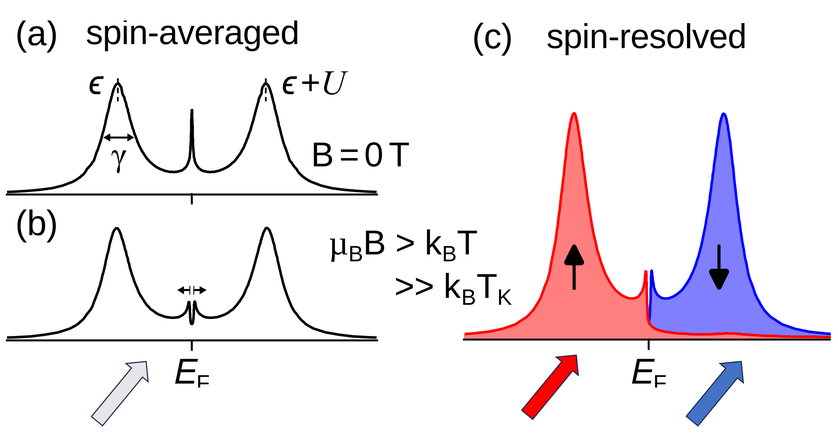
Anderson Hamiltonian

$$H = \sum_{\sigma}(\varepsilon - g\mu_B B\sigma/2)n_\sigma + Un_\uparrow n_\downarrow + \sum_{k\sigma}\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma} + \sum_{k\sigma}V_k(c^\dagger_{k\sigma}d_\sigma + d^\dagger_\sigma c_{k\sigma})$$

Real-space modulations

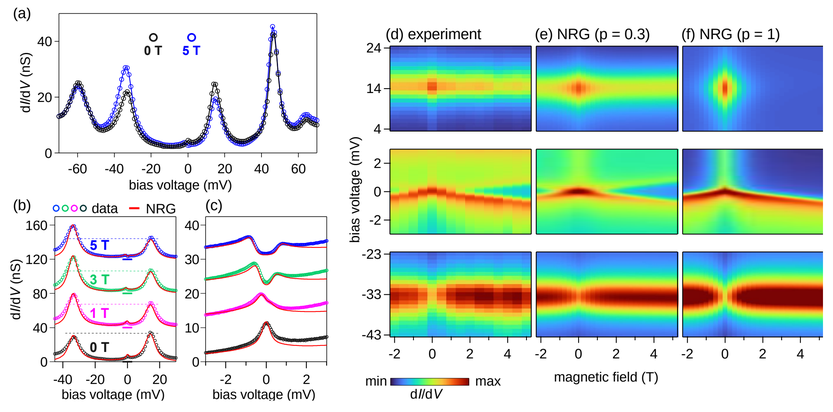


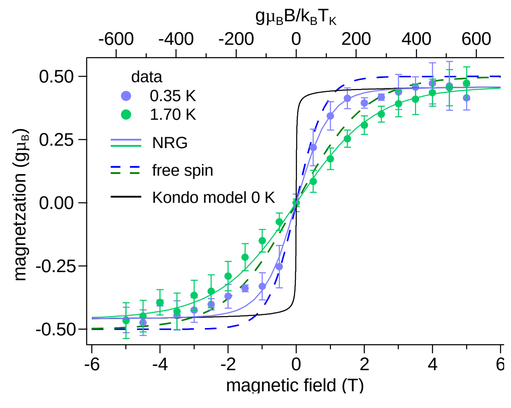
Spin-polarized STM of an Anderson impurity [7]



B-field : **tiny** effect on **spin-averaged** spectra

B-field : **huge** weight rearrangement in **spin-resolved** spectra





$$\frac{dI}{dV} = \frac{1+p}{2}\frac{dI}{dV_\uparrow} + \frac{1-p}{2}\frac{dI}{dV_\downarrow} \quad \Rightarrow \quad m(B,T) = -g\mu_B\left(A^w_{dI/dV}(B,T) - A^w_{dI/dV}(0,T)\right)/2p$$

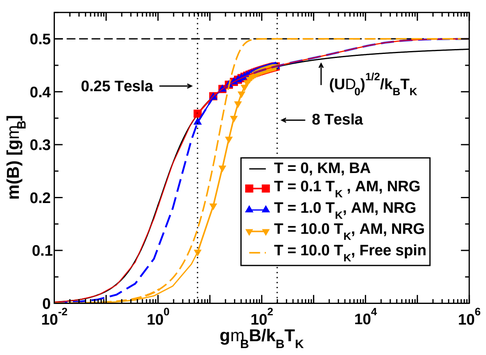
NRG calculations on JURECA: 24 nodes, 192 MPI tasks, 16 OpenMP threads

[6] C. van Efferen et al., Nature Physics, **20**, 82-87 (2024)

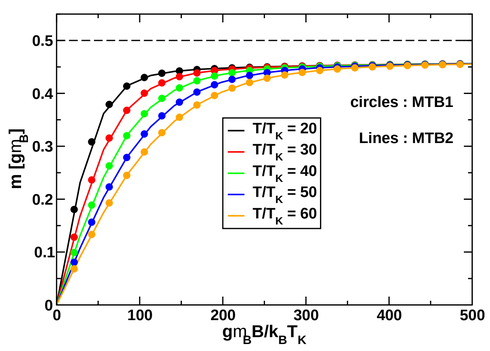
[7] Mahasweta Bagchi, et al., Phys. Rev. Lett. **133**, 246701 (2024)

Magnetization regimes of the Anderson model

Magnetization regimes



Universality



- Low field universal regime $g\mu_B B < (U\Delta_0)^{1/2} \sim 10 - 20\mathrm{meV}$
  - Accessed in the MTBs investigated
  - Allows testing universal predictions of the model against expt.
  - Logarithmic approach to free spin value→ Kondo effect
- High-field regime $g\mu_B B > (U\Delta_0)^{1/2} \sim 10 - 20\mathrm{meV}$
  - Non-universal, dependence on microscopic parameters
  - Rapid approach to free spin value (noninteracting)

Conclusions and outlook

- **Mirror twin boundaries in MoS_2 realize standard model of correlated electrons (Anderson impurity model)**
- Kondo effect
  - Highest confined state occupied by two electrons → non-magnetic
  - Highest confined state occupied by one electron → magnetic (S=1/2)
  - Coupling with substrate states → Kondo effect
  - Anderson impurity states accessible → U, ε, γ → calculation of T_K
  - Excellent agreement to numerical renormalization group simulations
- Spin-polarized spectroscopy of an Anderson impurity
  - Signatures of huge spectral weight shift in spin-polarized spectra
  - Access to impurity states → weight asymmetry → magnetization
  - Kondo effect: suppression of magnetization (asymptotic freedom)
- Outlook
  - MTBs realize tunable Anderson model - testbed for theories
  - Experimental realizations of 2, 3 impurity models (RKKY vs Kondo)
  - Strong coupling regime ($T<T_K$); Impurities in superconductors …