Exploring Moiré Excitons in Transition Metal Dichalcogenide and Complex Oxide Heterostructures

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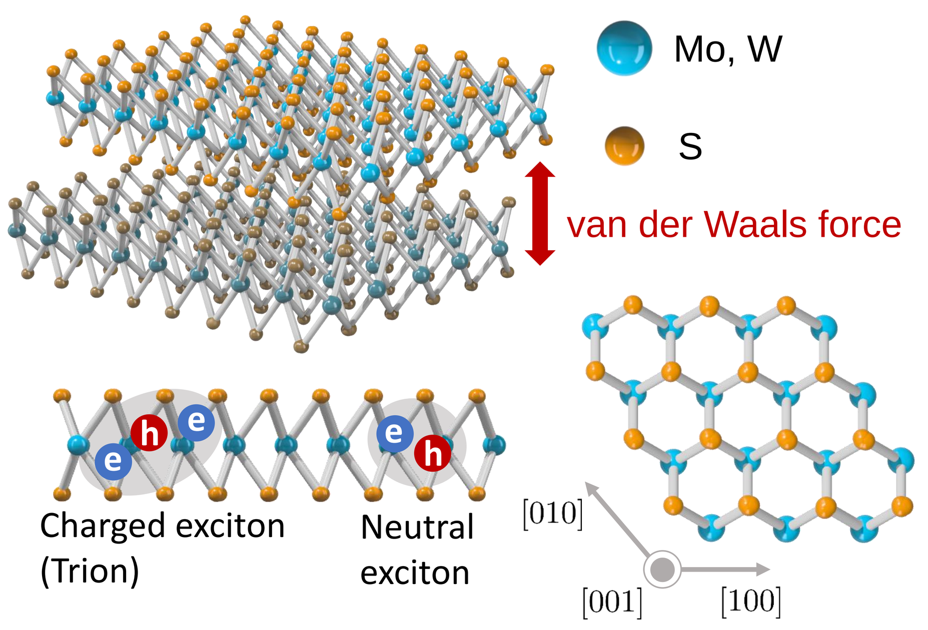
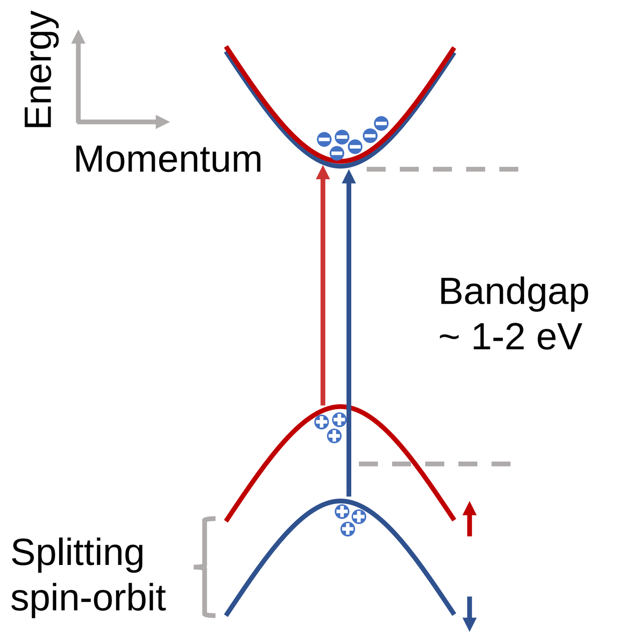
Transition metal dichalcogenides (TMDs) have recently emerged as a promising platform for exploring novel moiré physics. So far, however, moiré excitons have only been observed and studied in semiconducting TMD heterostructures. In this work, we explore the unique properties of moiré excitons formed in heterostructures combining TMDs and complex oxides. By integrating these two material systems, we aim to exploit the multifunctional capabilities of moiré excitons and complex oxides. Utilizing photoluminescence and differential reflectance spectroscopy, we probe the signatures of moiré exciton emissions in these heterostructures. This research paves the way for potential applications in tunable moiré superlattices and optoelectronic devices, while also broadening the understanding of excitonic interactions in hybrid material systems.

INTRODUCTION

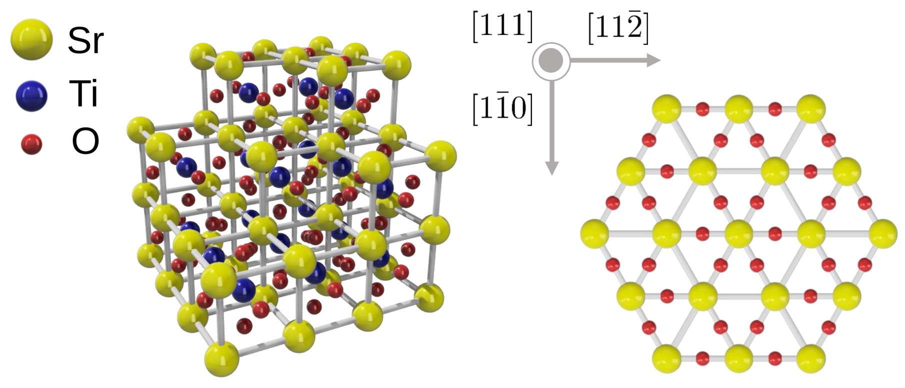
TMDs



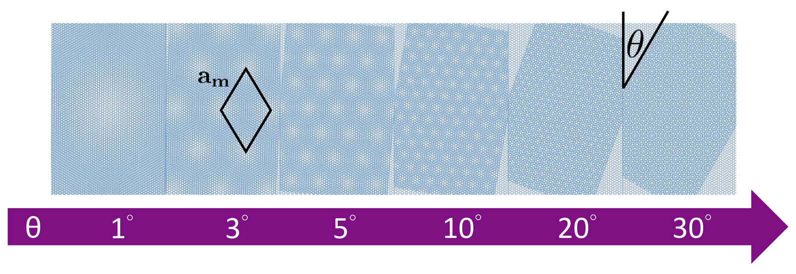
Band Structure



$SrTiO_3$



Moiré Pattern

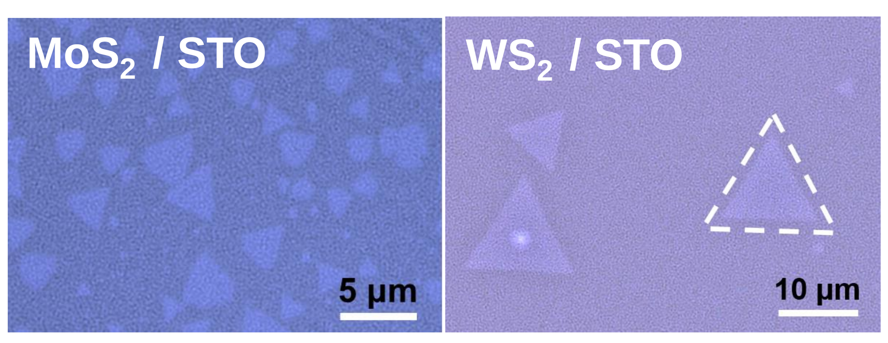


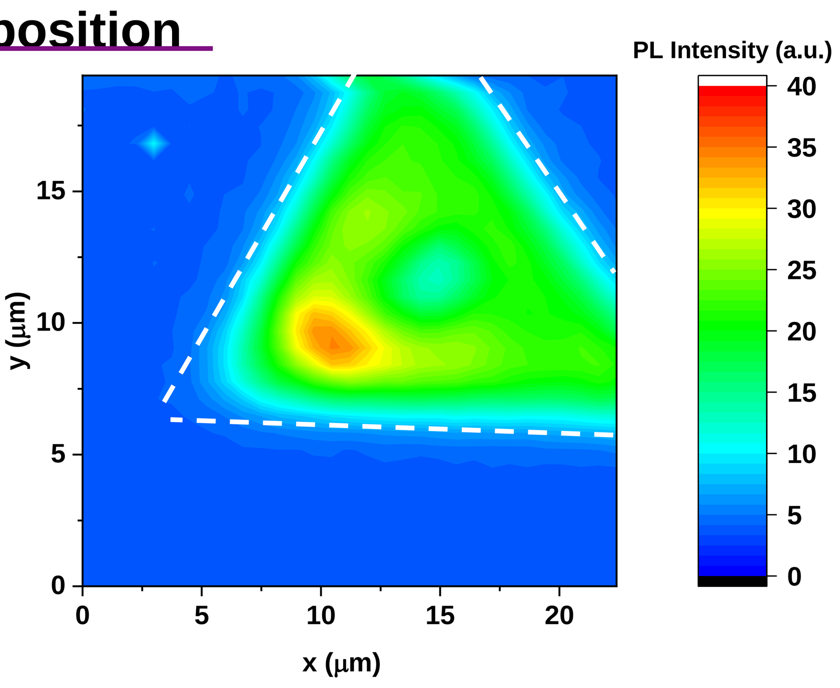
$$a_m \approx \frac{a_0}{\sqrt{\theta^2 + \left(\frac{a_0 - a_0'}{a_0}\right)^2}}$$

- Direct band gaps ≈ 1-2 eV → 2D semiconductor
- Reduced dielectric environment → Excitonic physics
- Similar lattice constants & structures → Moiré pattern

METHOD

TMDs Grown by Chemical Vapor Deposition



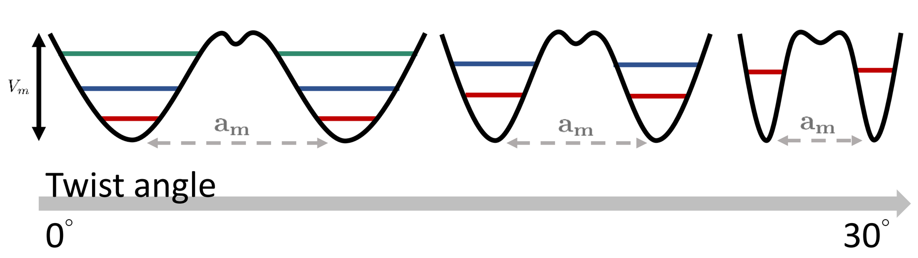


4K Optical Measurement

- Photoluminescence (PL)
- Differential reflectometry (DR)

PHYSICAL MODELING

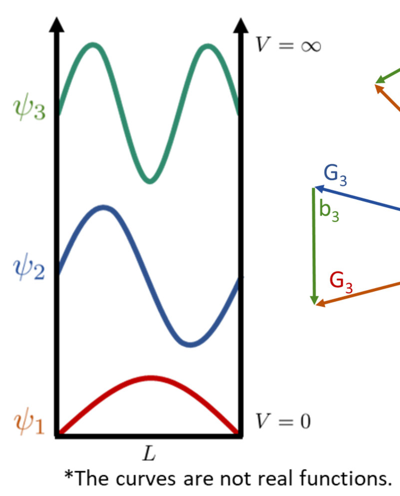
Moiré Potential Approximation

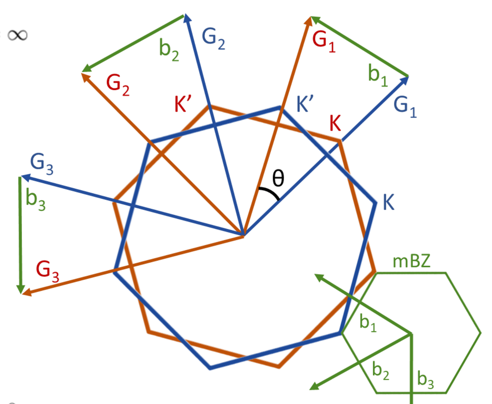


Bloch wave function
$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$

$$\hat{H} = \underbrace{\left(E_0 - \frac{\hbar^2\nabla^2}{2\mu}\right)}_{\hat{H}_0} + \underbrace{\left(V_m \sum_i^6 \exp(i\mathbf{b}_i \cdot \mathbf{r})\right)}_{\hat{H}_m}$$

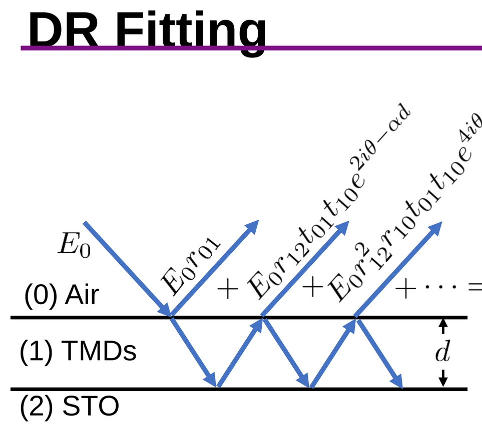
$\mathbf{b}_i = \mathbf{G}_i - \mathbf{G}'_i$
$\mathbf{k} = \mathbf{q} + n_1\mathbf{b}_1 + n_2\mathbf{b}_2, \quad n_i \in \text{integers}$





- $\mathbf{b}_i$: Mini Brillouin zone (mBZ) wavevector
- $\mathbf{k}_i$: Momentum in MoS_2, WS_2
- $\mathbf{q}_i$: Momentum in mBZ

DR Fitting



$$+\cdots = E_0\left(r_{01} + \frac{t_{01}t_{10}r_{12}e^{2i\theta-\alpha d}}{1 - r_{12}r_{10}e^{2i\theta-\alpha d}}\right)$$

Assume normal incidence…

$$\frac{\Delta R}{R} = \frac{R_{WS_2} - R_{STO}}{R_{STO}} = \frac{\left|r_{01} + \frac{t_{01}t_{10}r_{12}e^{i\theta-\alpha d}}{1-r_{12}r_{10}e^{i\theta-\alpha d}}\right|^2 - |r_{02}|^2}{|r_{02}|^2}$$

$$r_{ij} = \frac{n_i - n_j}{n_i + n_j}, \quad t_{ij} = \frac{2n_i}{n_i + n_j}$$

- θ: Phase difference through TMDs
- α: Absorption rate of TMDs

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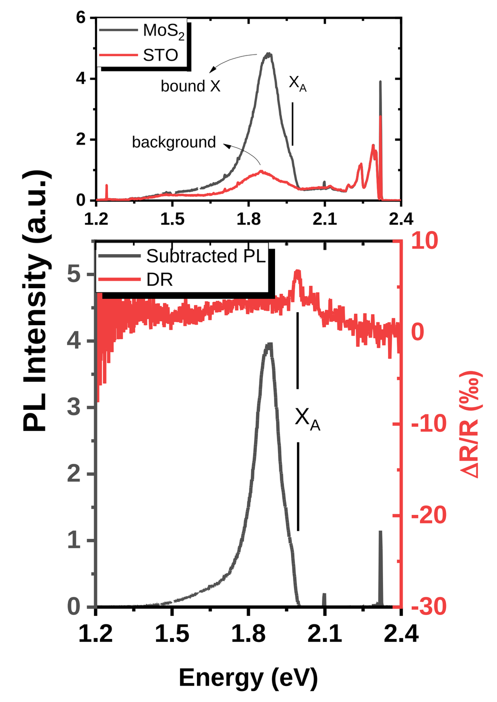
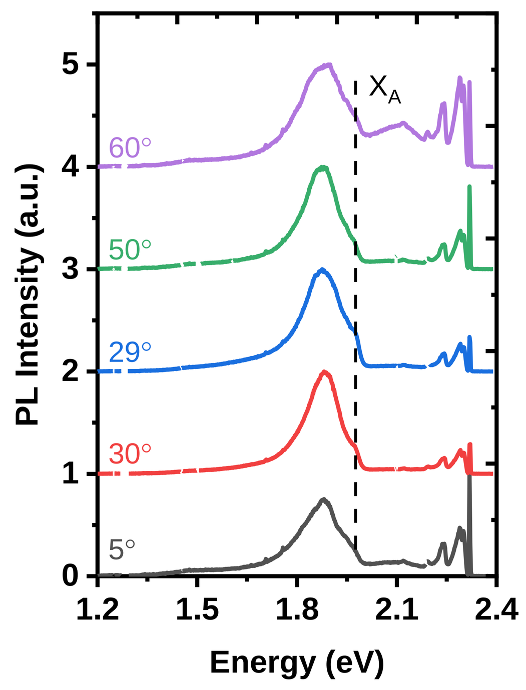
RESULT & DISCUSSION

PL & DR Characteristic

MoS_2 / STO

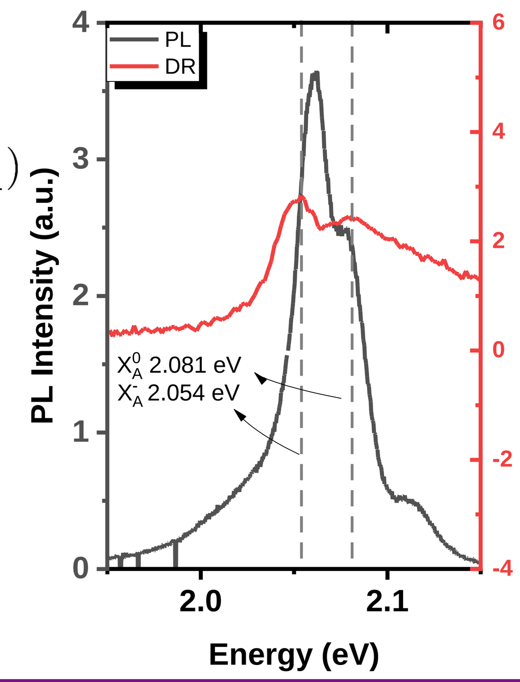
- A exciton $(\mathbf{X_A})$
- Broadband defect states

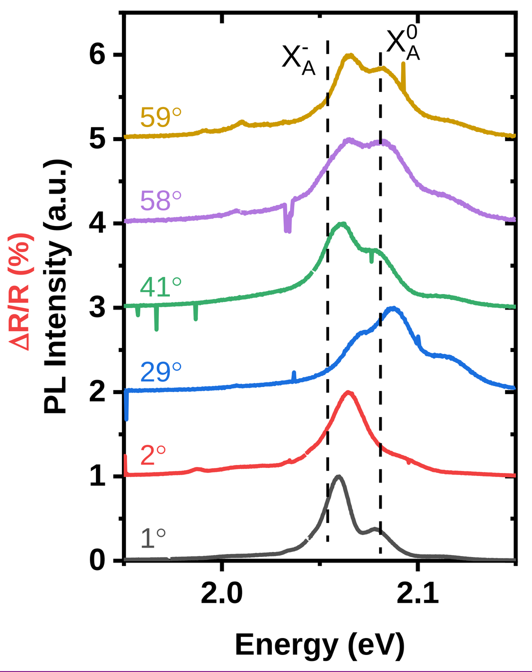




WS_2 / STO

- A neutral exciton $(\mathbf{X_A^0})$
- A trion $(\mathbf{X_A^-})$
- Random defect states

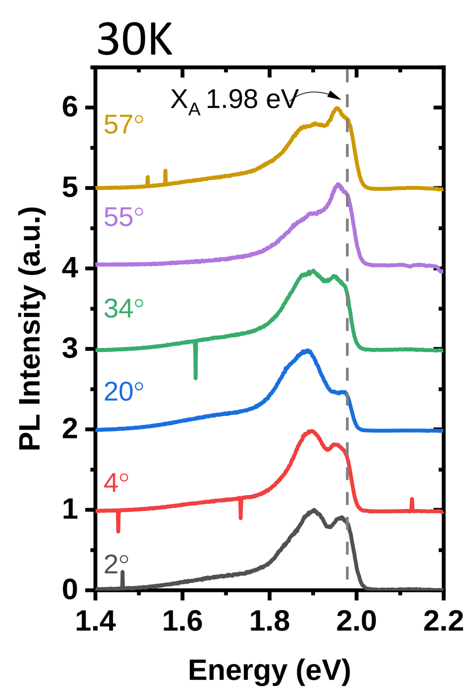


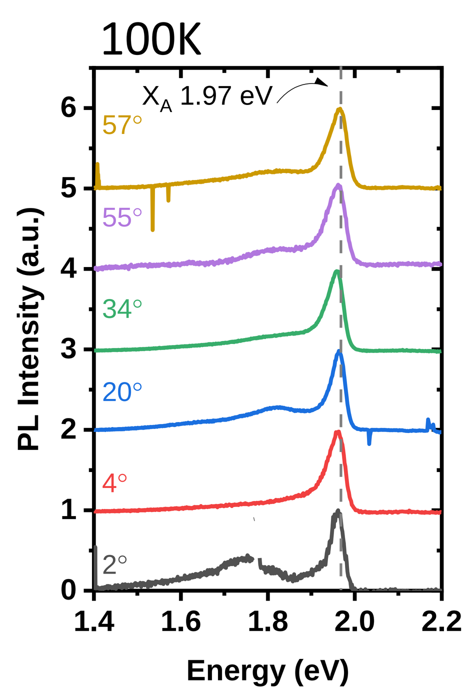


Temperature Dependence

MoS_2 / STO

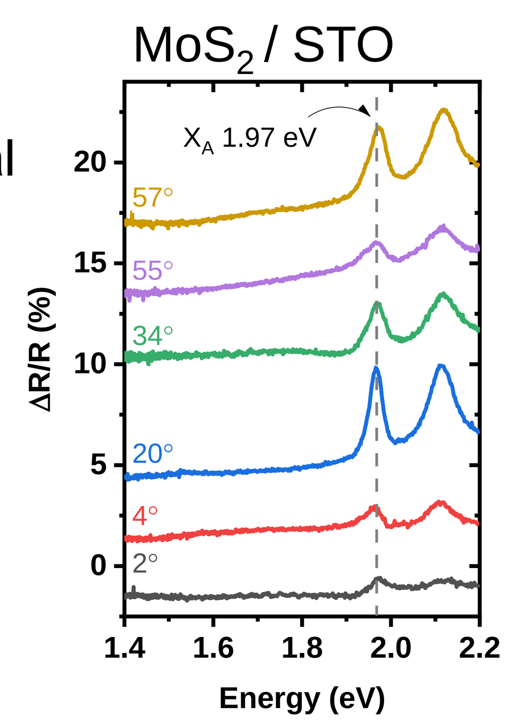
Temperature increases
→ Defects suppressed

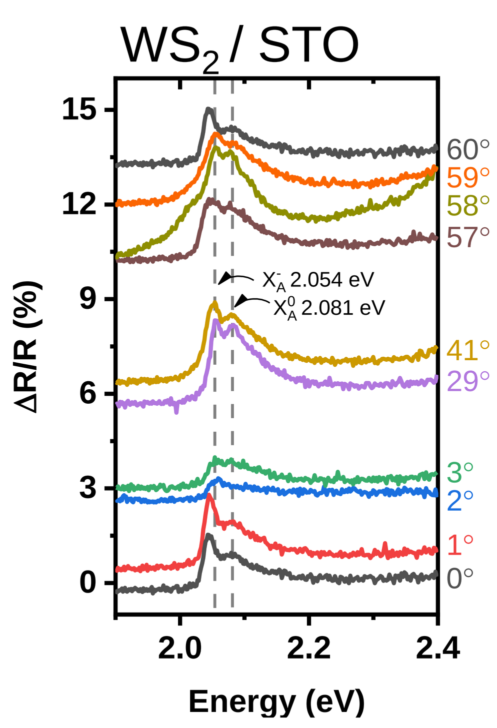




Probing DR Energy Shift

Subtle peak energy shifts
→ Shallow moiré potential





CONCLUSIONS

- To avoid defect states
  1. → DR is better for probing the moiré potential.
  2. → Varying temperature also works.
- Moiré effect seems subtle (shallow potential depth)
  → Quantitative analysis is needed.