

Crystal Structure Characterization of 2D Quantum Materials using LEEM/ μ LEED-IV

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Motivations

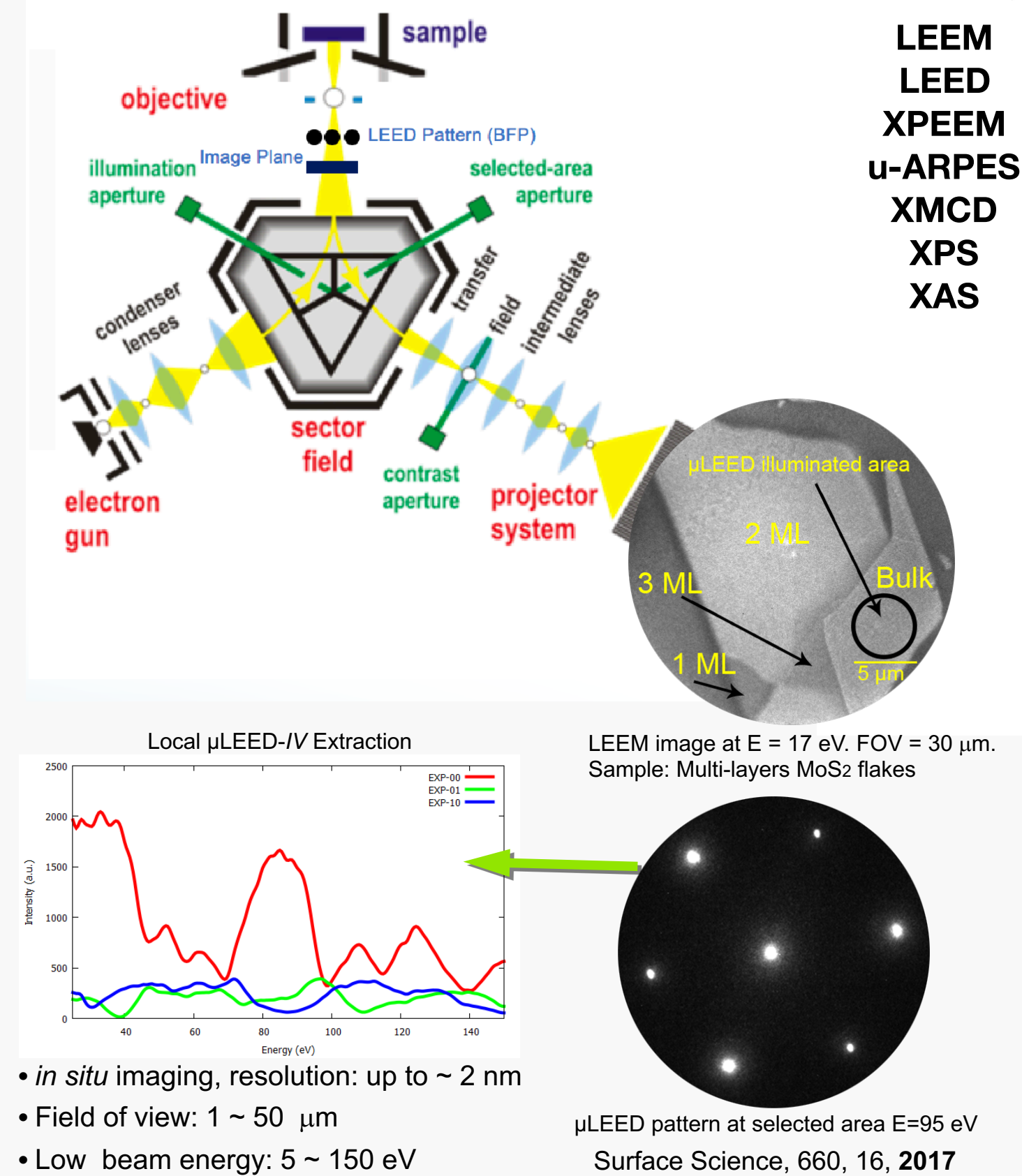
Challenges in crystallography of atomically-thin 2D crystals:

- **Small sampling area.** Commonly mechanically exfoliated using scotch tape method limited the sampling size to a few μm .
- **Thin.** Usually, a few \AA to a few nm in thickness, which requires the characterization technique to be extremely sensitive to surface atomic structures.
- Various 2D materials are **unstable**, thus requires probing technique to be **non-destructive**.

Experiments

Low Energy Electron Microscopy (LEEM) and Diffraction

Aberration -corrected LEEM system

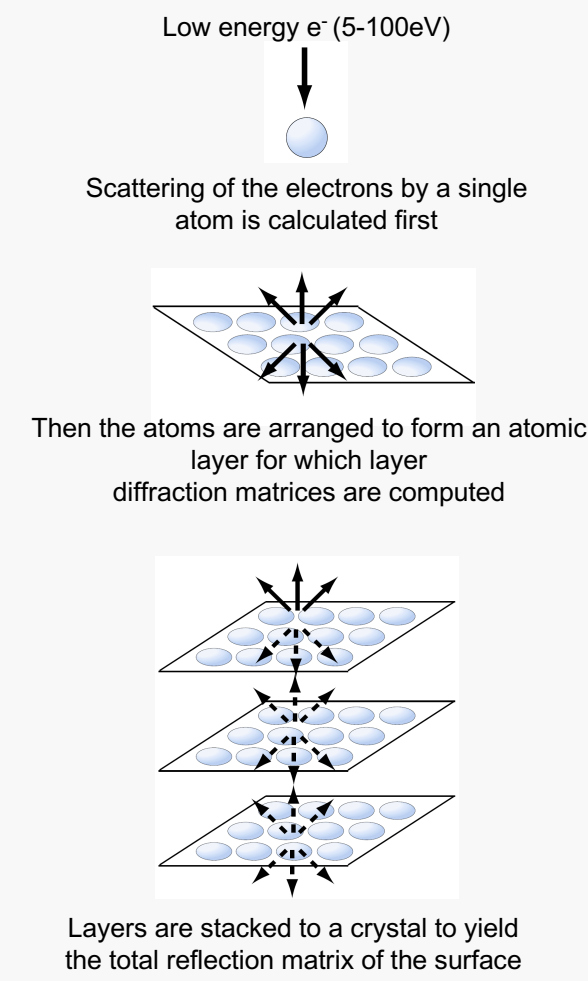


- *in situ* imaging, resolution: up to ~ 2 nm
- Field of view: $1 \sim 50 \mu\text{m}$
- Low beam energy: $5 \sim 150$ eV

μ LEED pattern at selected area $E = 95$ eV
Surface Science, 660, 16, 2017

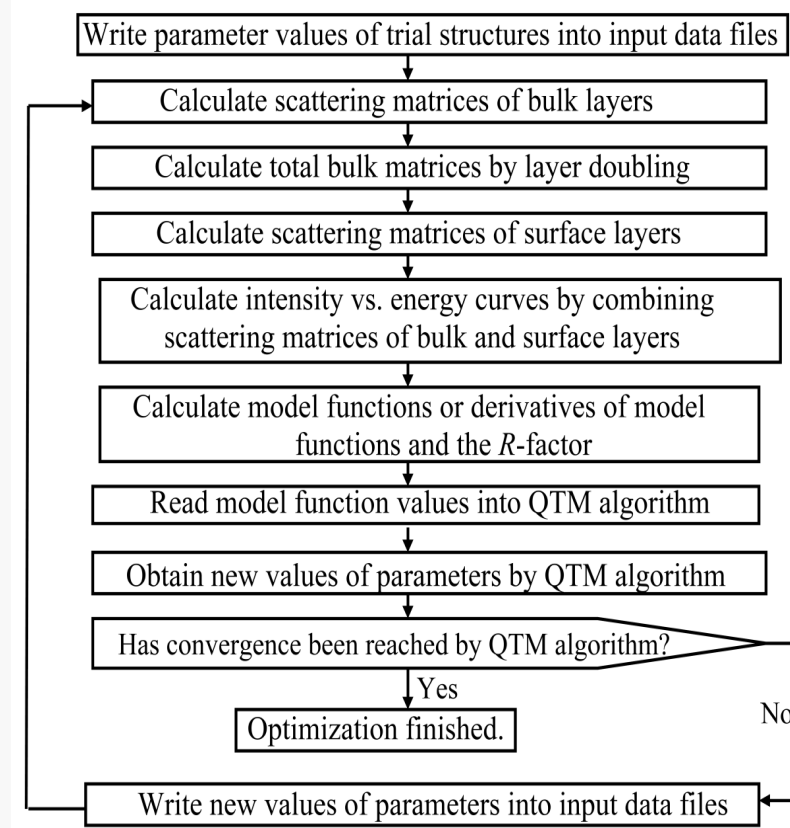
Simulations

IV spectra calculation



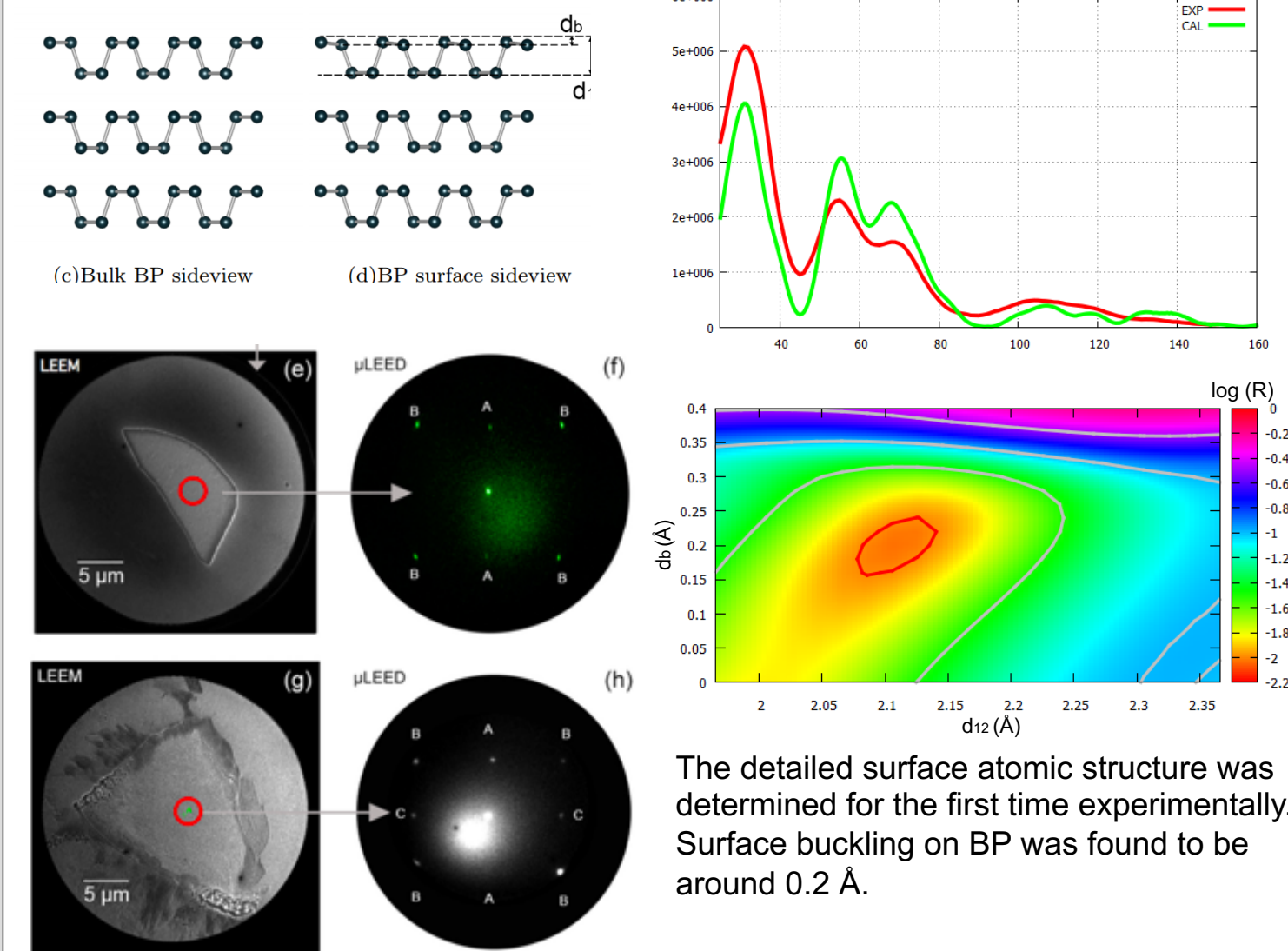
The electron multiple scattering IV calculations are based on the muffin-tin model of the crystal potential

Iterative structural optimization



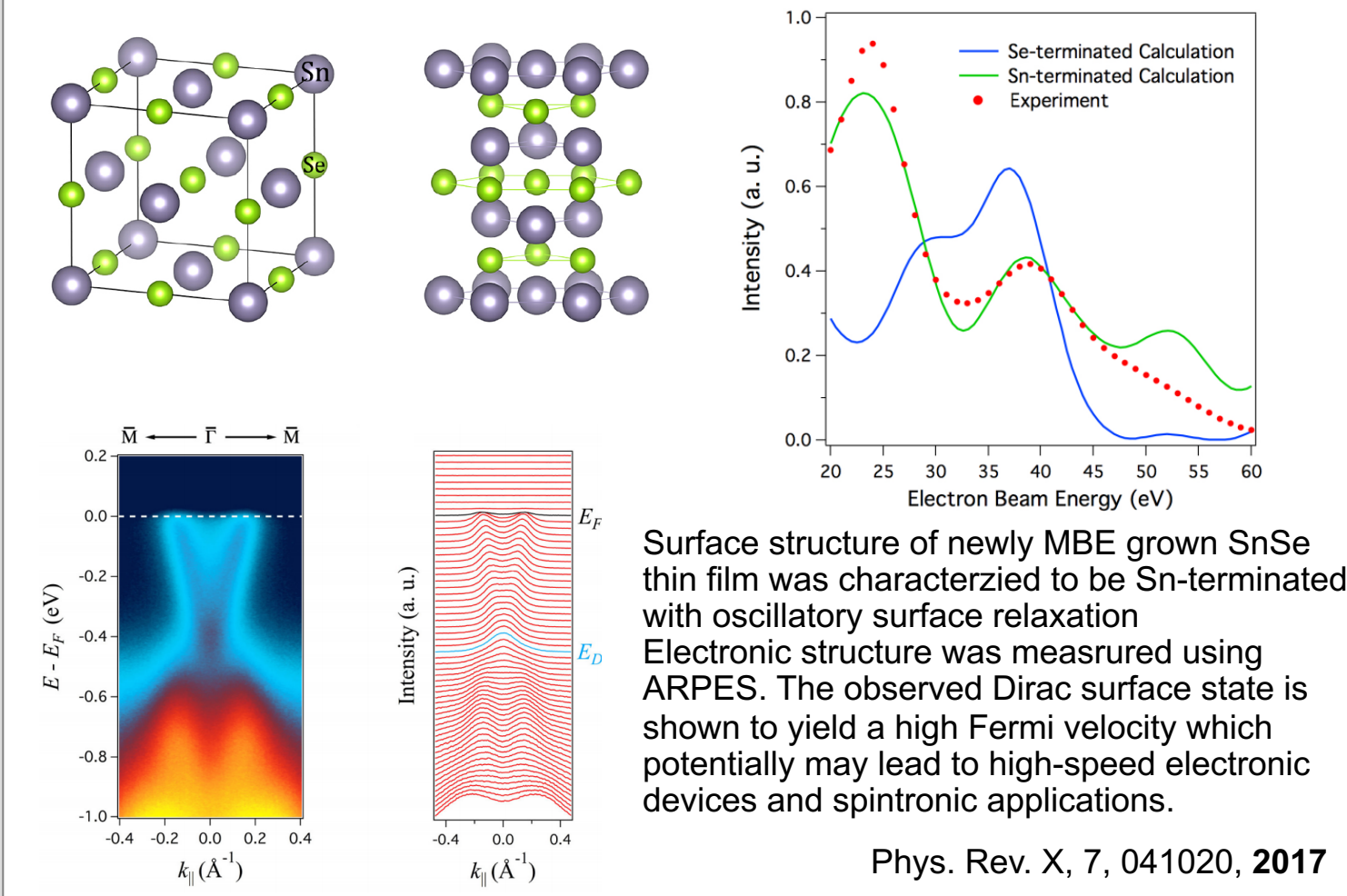
Results

Black phosphorus surface buckling



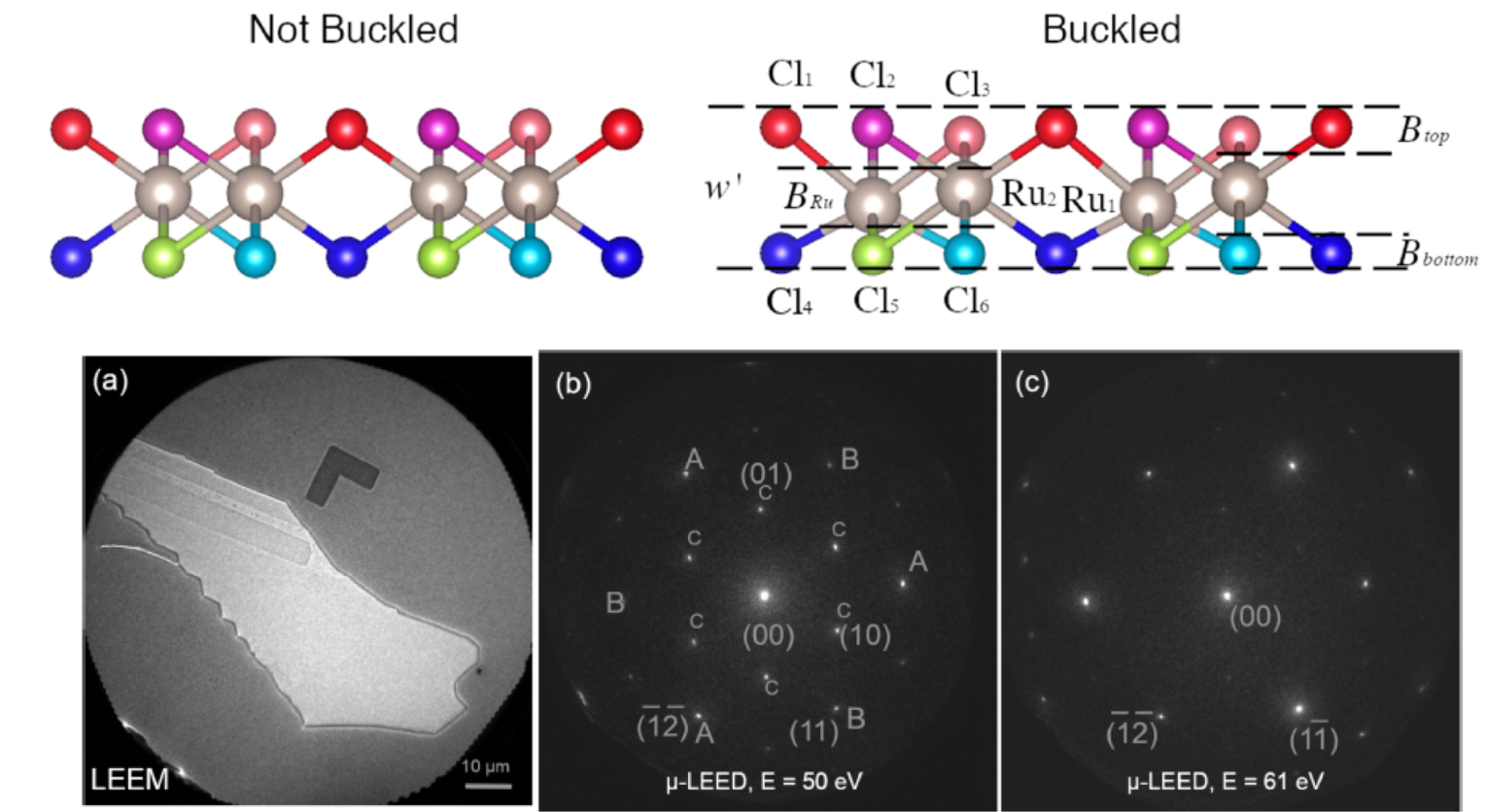
Phys. Rev. Mater., 1, 074003, 2017

TCI SnSe, Sn- or Se- termination?



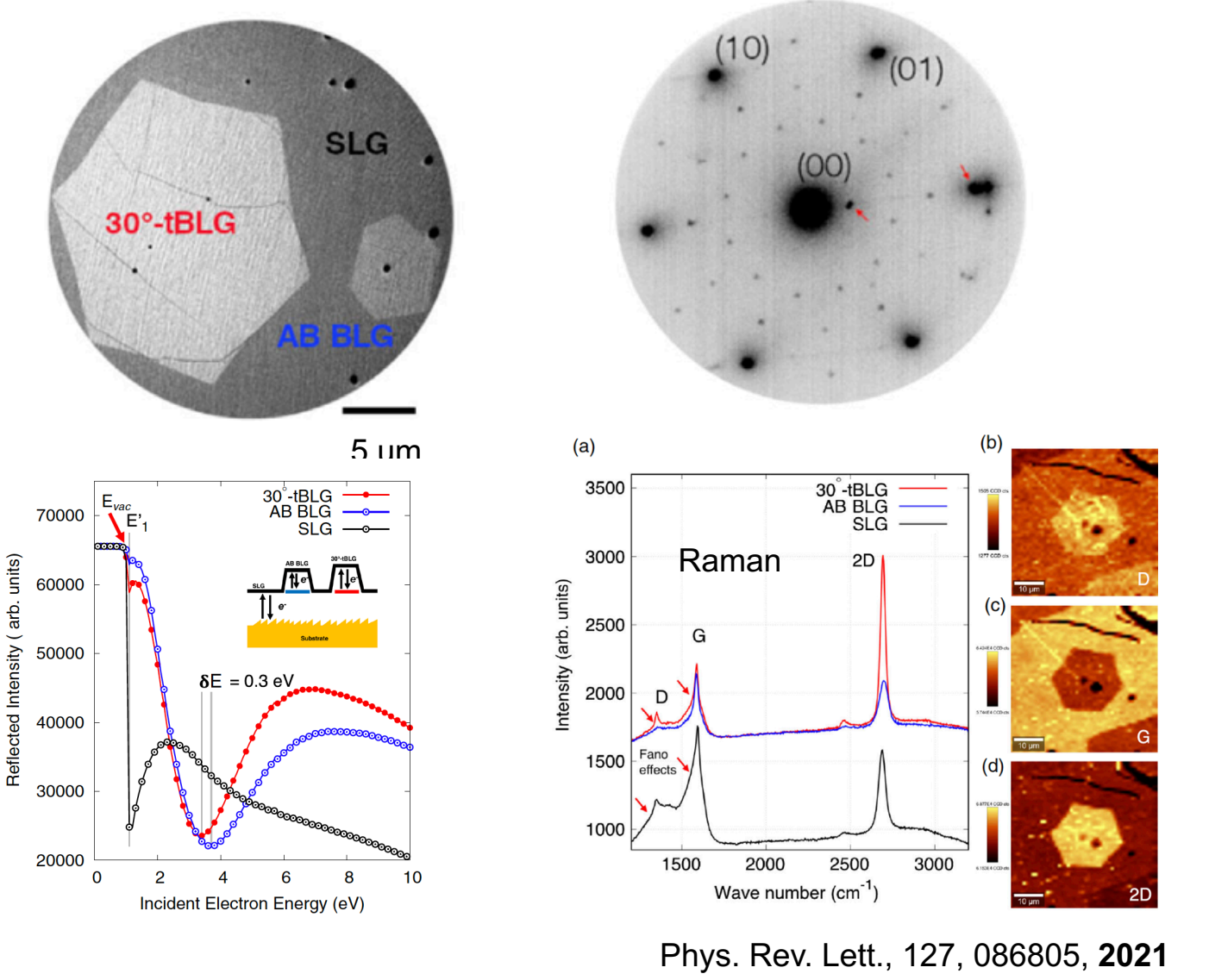
Phys. Rev. X, 7, 041020, 2017

Quantum spin liquid candidate: α -RuCl₃



2D Mater., 7, 035004, 2020

30° twisted bilayer graphene



Phys. Rev. Lett., 127, 086805, 2021

Conclusions

- μ LEED-IV was applied to study the crystal structures of various 2D materials, with sub- \AA precision.
- Lattice structural variations are distinct in atomically thin 2D materials, comparing to their parent bulk crystals.
- Twisted 2D systems present unique platforms to study quantum well, confinement, localization and potential applications in QIS.

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- *Now at the Molecular Foundry, Lawrence Berkeley National Lab, e-mail: zhongwei@lbl.gov #Now at the Hong Kong University of Science and Technology

Prof. Karsten Pohl Scholarship Fund needs your help!

We are approaching the deadline (Oct. 25th) to raise \$50,000, in order to perpetuate Prof. Karsten Pohl's legacy and establish a scholarship to help the students in needs, at the University of New Hampshire. Please scan to donate, we appreciate your support!



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