

The Center for Integrated Nanotechnologies

Nanomaterials

Integration

A U.S. DOE Nanoscale Science Research Center

LEEM-PEEM: a new tool to study...

Taisuke Ohta

Band alignment in transition metal dichalcogenides: Kuntal Keyshar^{1,2}, Morgann Berg^{3,4}, Gautam Gupta², T. E. Beechem³, Pulickel Ajayan¹, Calvin Chan³, Aditya Mohite^{2,4}

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⁴ Center for Integrated Nanotechnologies, Sandia National Laboratories & Los Alamos National Laboratory, New Mexico, United States

Local variation of the electronic properties in polycrystalline CdTe: M. Berg^{3,4}, C. Chan³, Jason M. Kephart⁵, Walajabad S. Sampath⁵

⁵ Dept. of Mechanical Engineering, Colorado State University, Fort Collins, Colorado, United States

Atomic arrangement in twisted bilayer graphene: Jeremy T. Robinson⁶, T. E. Beechem³, B. Diaconescu³, S. W. Schmucker⁶, J. P. Long⁶, J. C. Culbertson⁶, A. L. Friedman⁶, P. J. Feibelman³, G. L. Kellogg³

⁶ Naval Research Laboratory, Washington, District of Columbia, United States

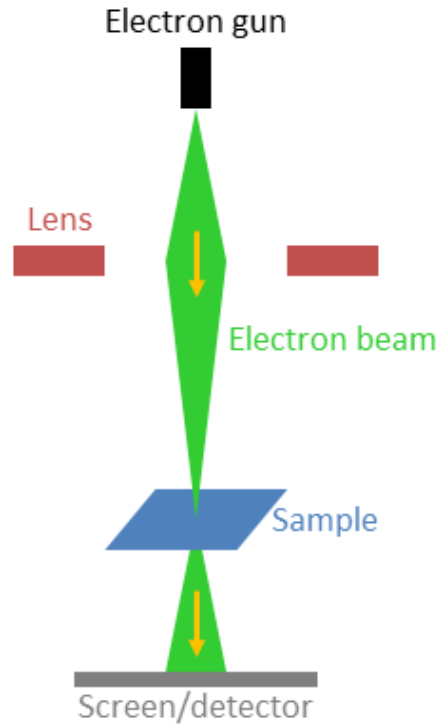
2017-10-09

Informal discussion with a small group from the University of Maryland

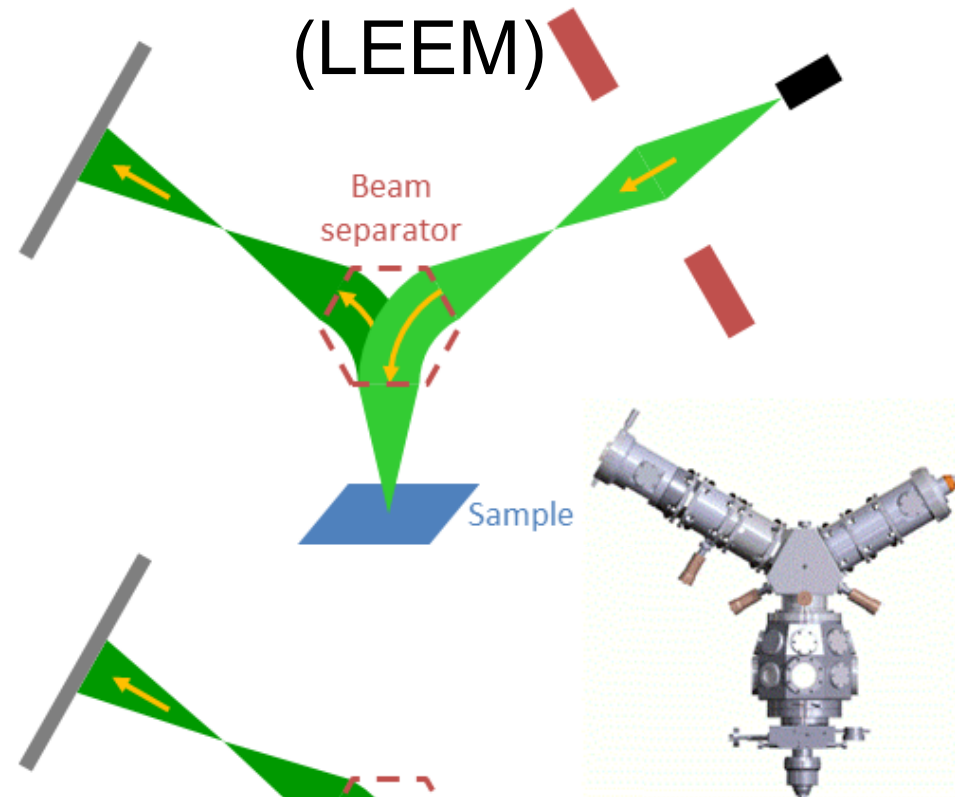


Electron microscopies come in various geometries

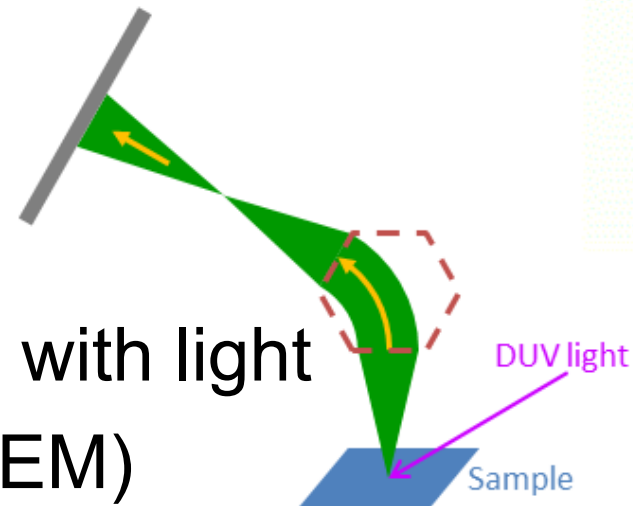
- Transmission geometry



- Reflection geometry

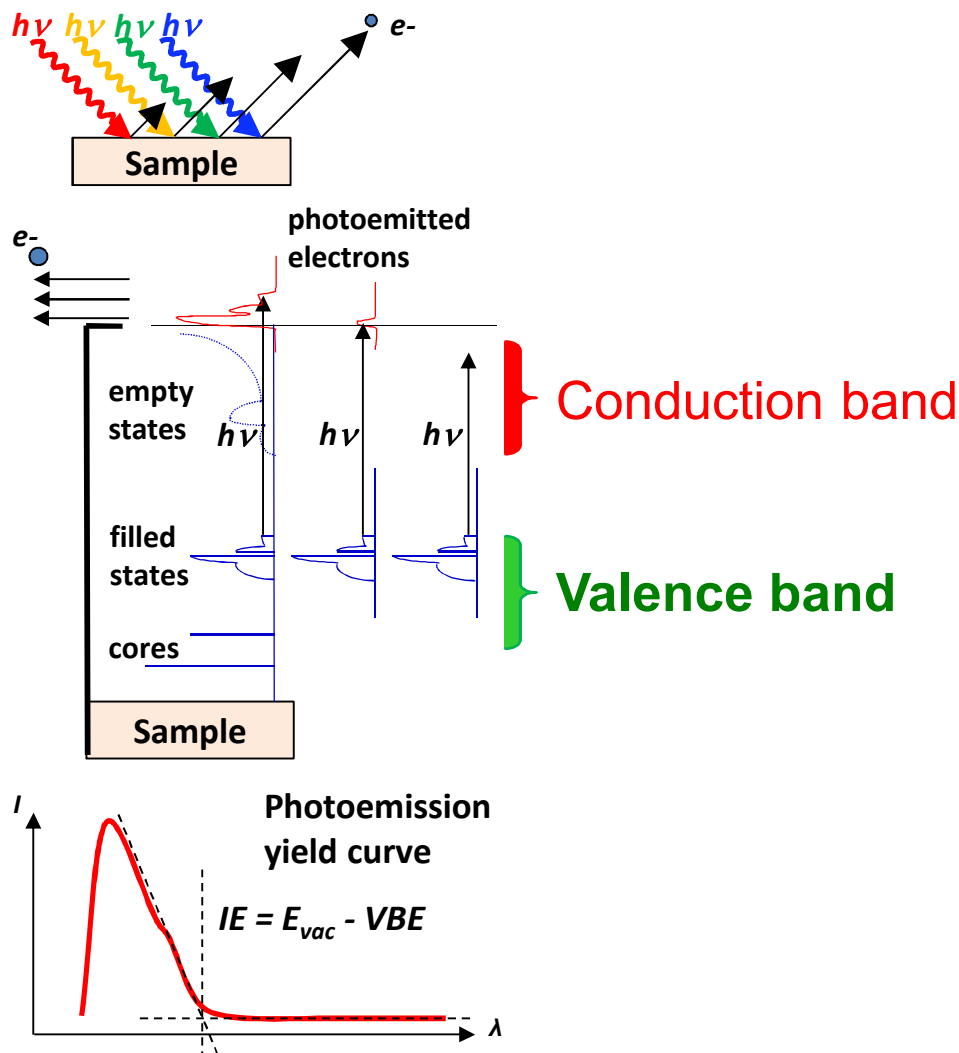
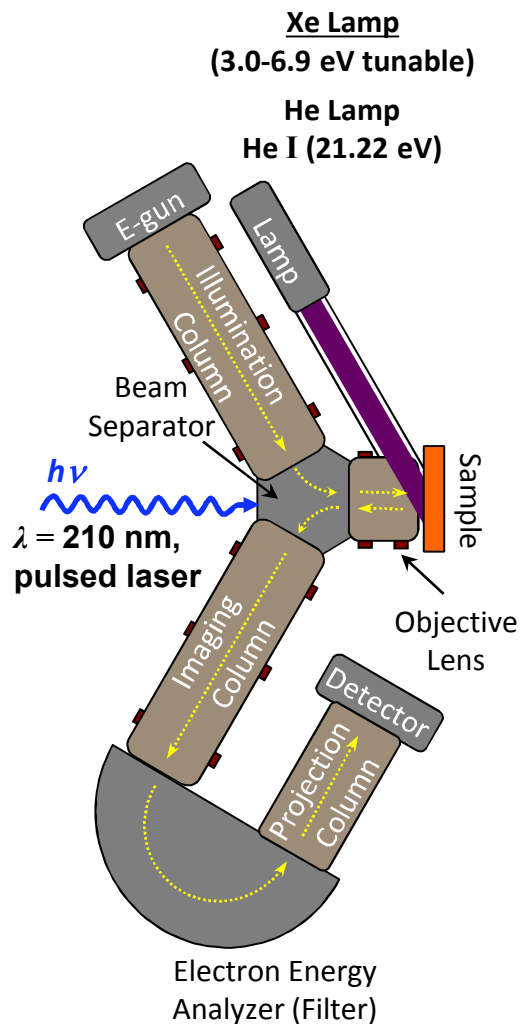


- Excitation with light (PEEM)

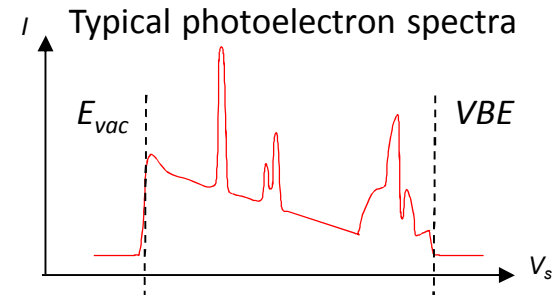
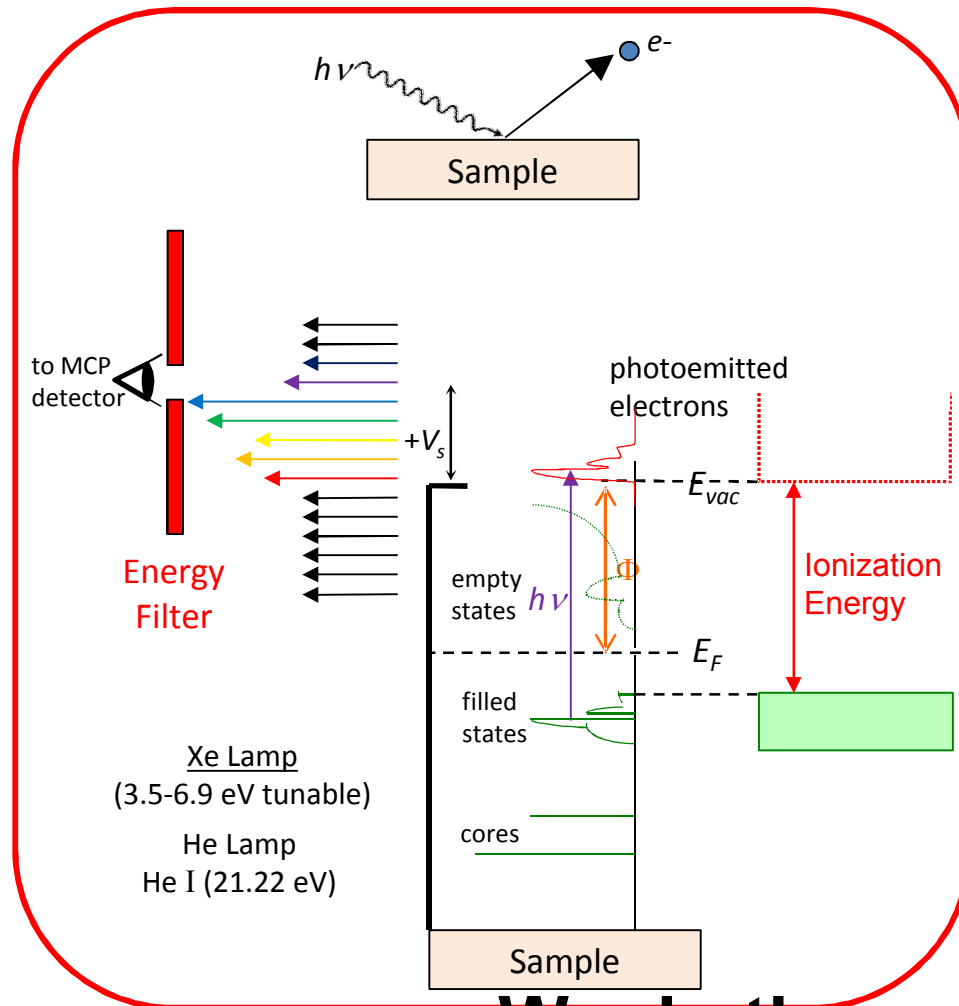




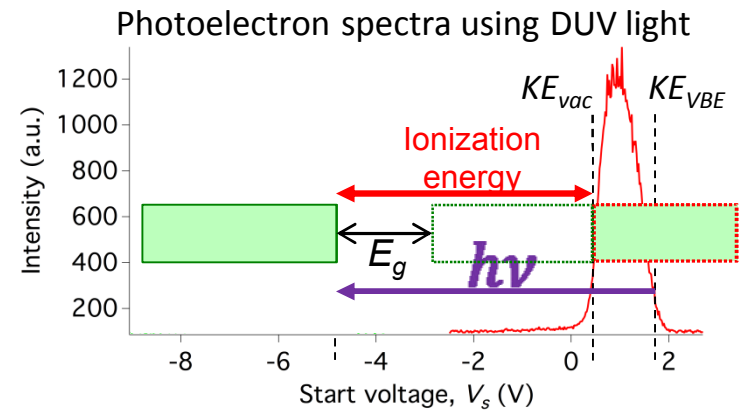
Photoemission threshold tells us about the work function or the ionization energy



Photoemission spectroscopy enables determining the vacuum level & highest occupied state



- We extract E_{vac} & valence band edge at Brillouin zone center from photoelectron (or photoemission) spectra

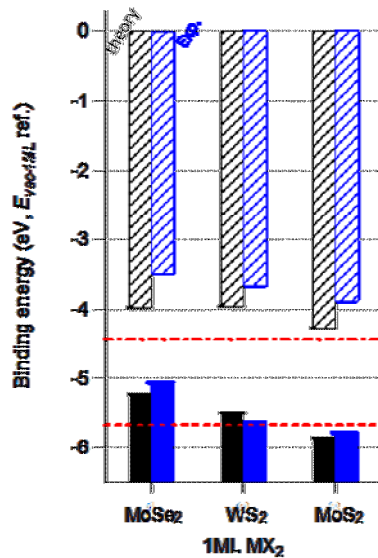


$$BE = KE - hv$$

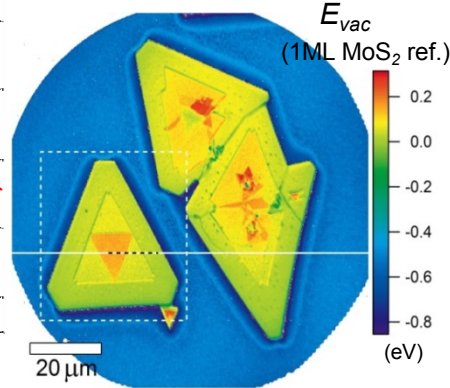
• We do these photoemission measurements with spatial resolution



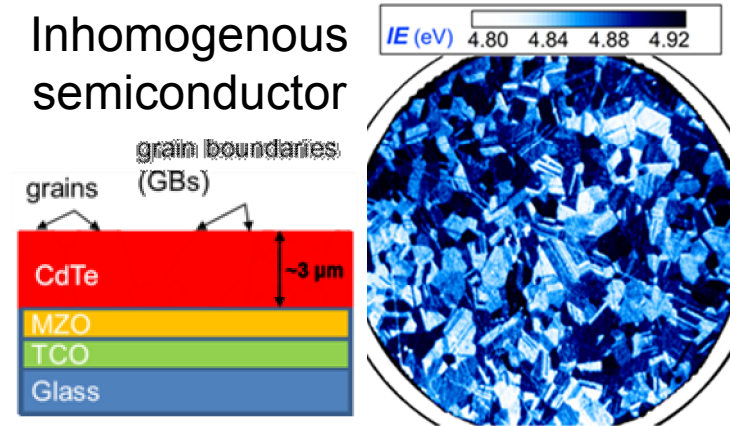
Four studies using LEEM-PEEM



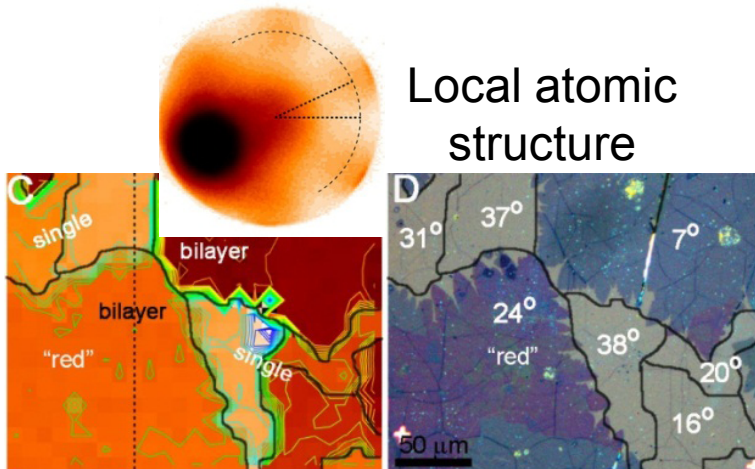
Semiconductor heterostructure



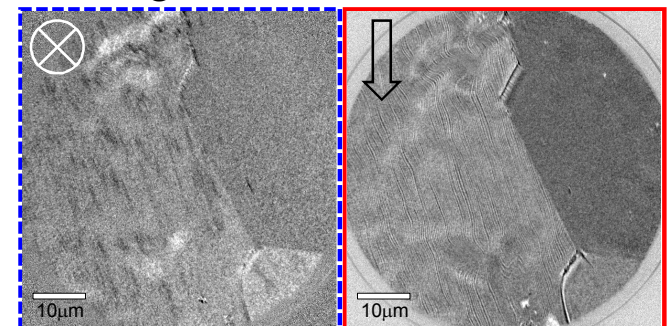
Inhomogeneous semiconductor



Local atomic structure

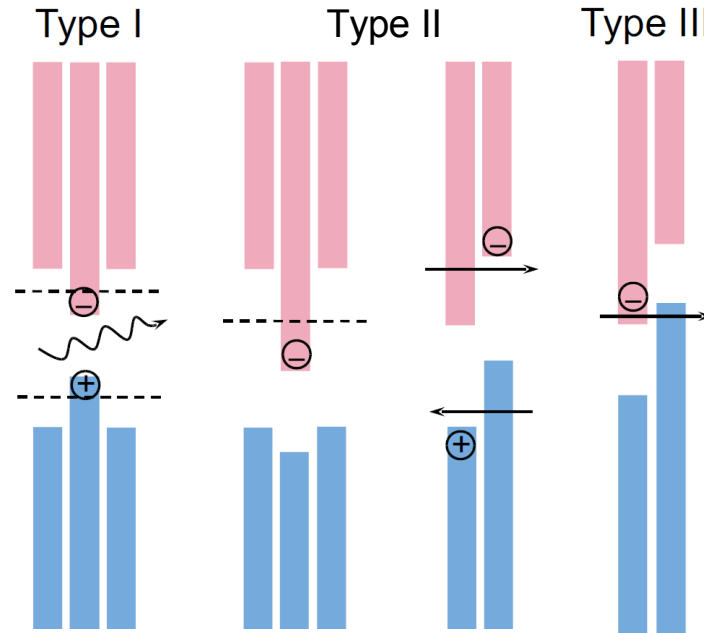
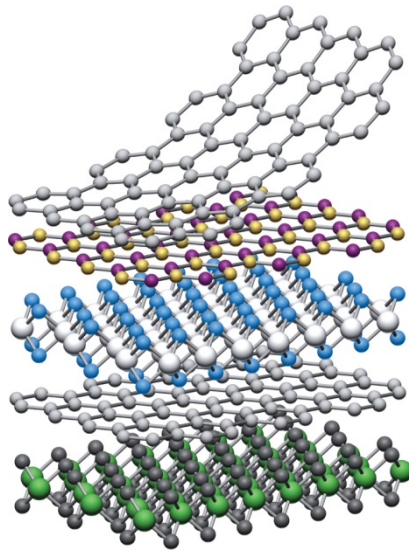


Magnetic nanostructures





Ionization energies govern the band alignment of TMD heterostructures



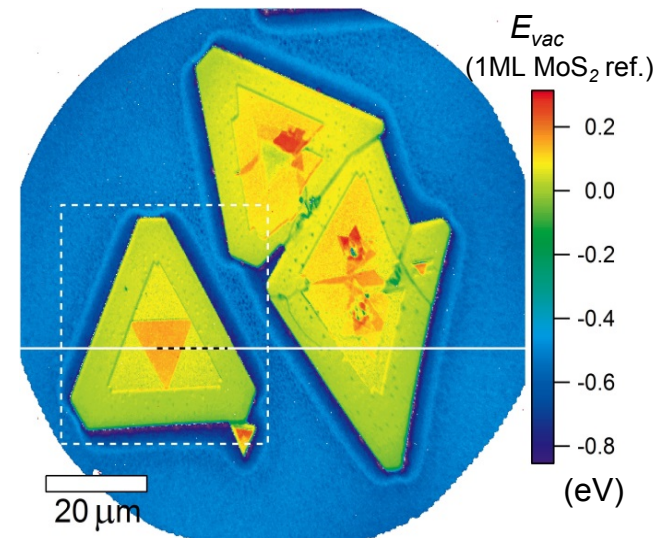
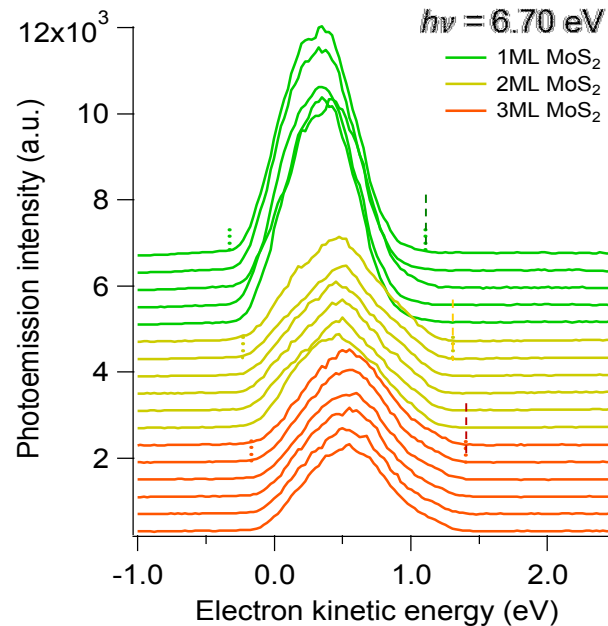
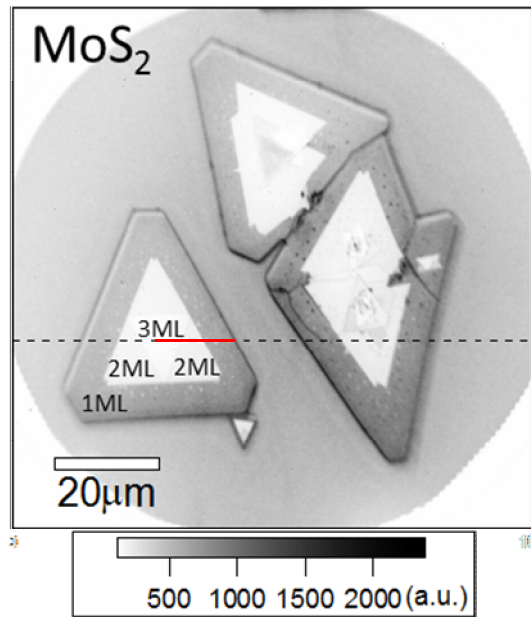
Özçelik, et al., Phys. Rev. B 94, 035125 (2016)

Question: How do the states align when stacked into 2D crystal heterostructures?

Approach: relative positions of the states



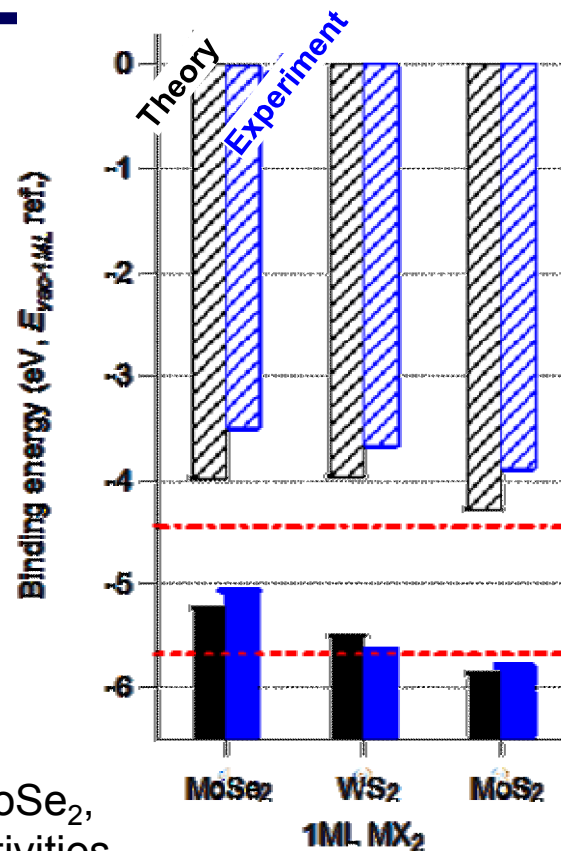
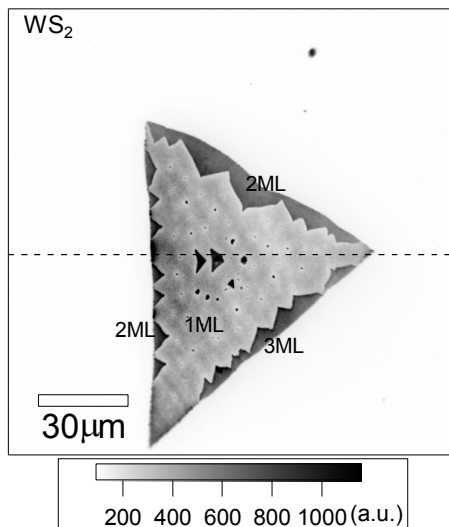
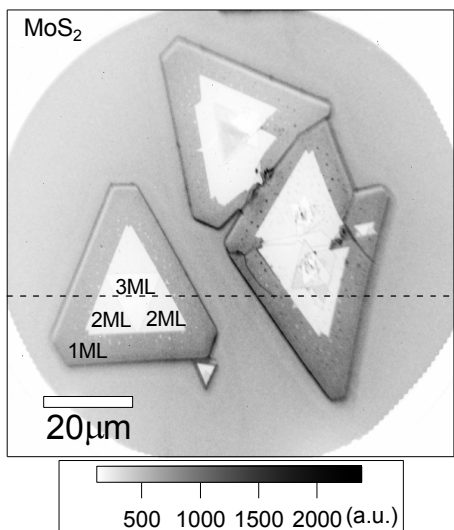
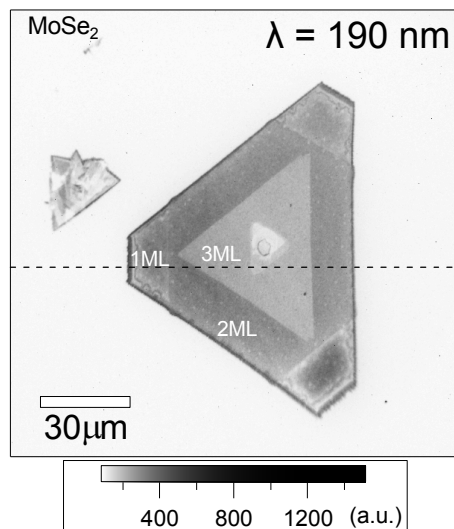
We determine E_{vac} & valence band edge on MoS_2 multi layers



- **Concurrent imaging and spectroscopy**



Experimentally determined ionization energies match well with DFT calculations

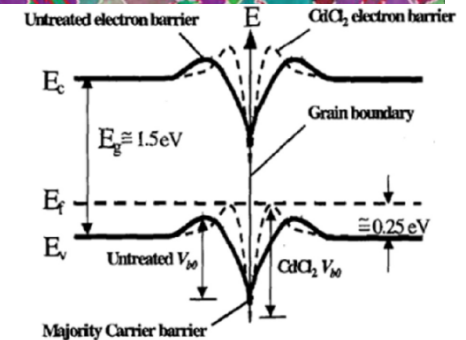
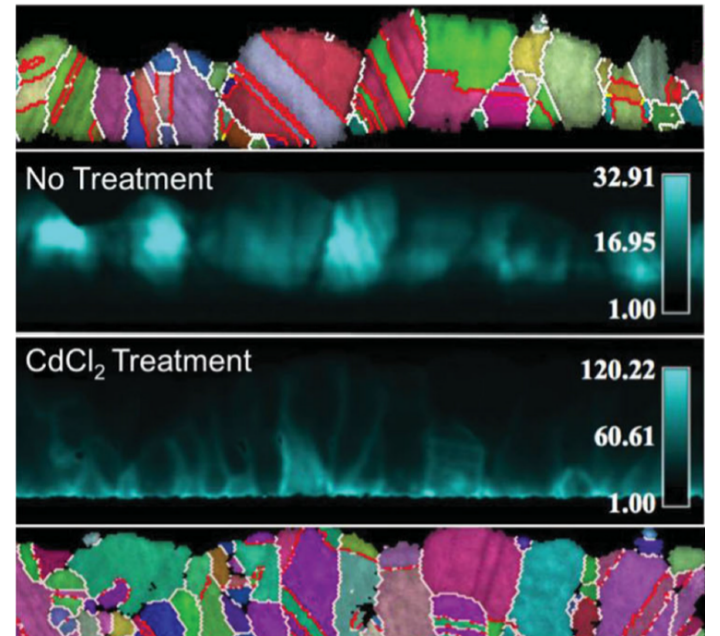
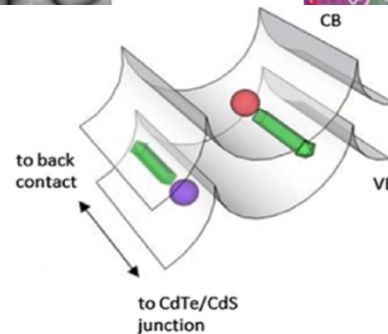
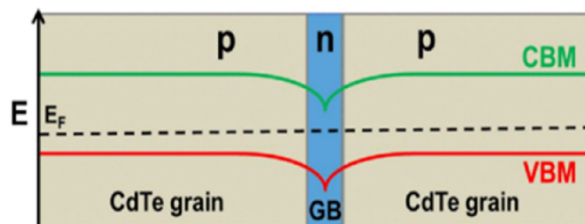
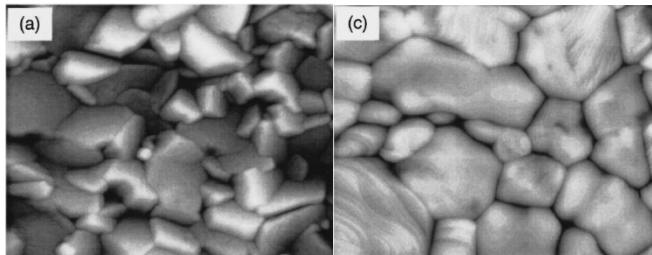


- Decrease from MoS₂, WS₂, to MoSe₂, anticipated from the electronegativities of the constituent atoms
- Very good agreement with DFT with GW approximation
- Heterostructures containing MoS₂, WS₂, to MoSe₂ are likely to display type II alignment



Photovoltaic efficiency of polycrystalline CdTe improves with CdCl_2 treatment

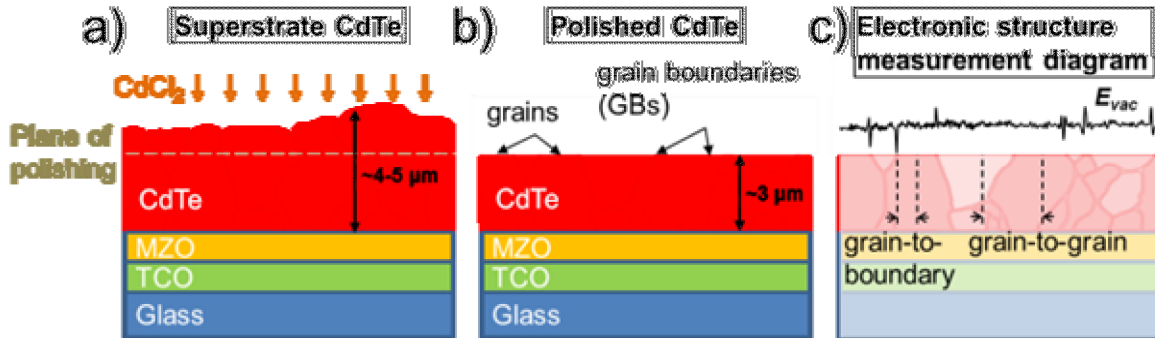
- Polycrystalline cadmium-telluride (CdTe) photovoltaics reaching 21.5% efficiency
 - Serious alternative to silicon-based photovoltaics



Major, Semicond. Sci. Technol. 31 (2016) 093001

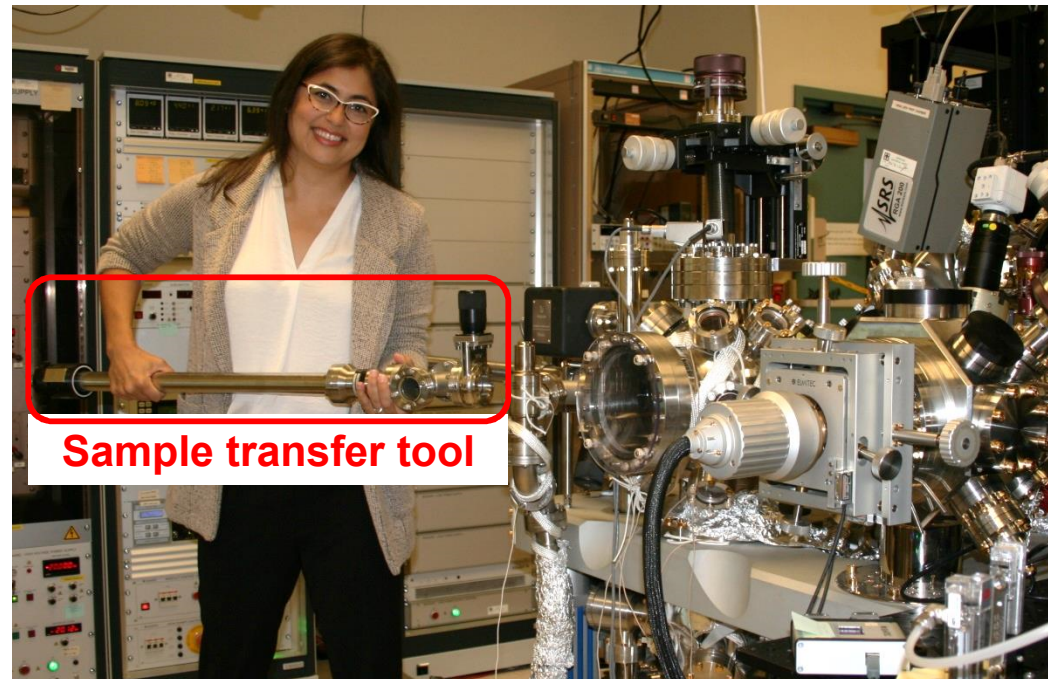
Electronic structure variation under debate

Clean surface of polycrystalline CdTe is prepared by polishing, sputtering, and inert atmosphere transfer



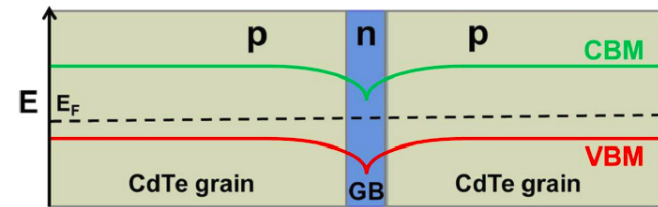
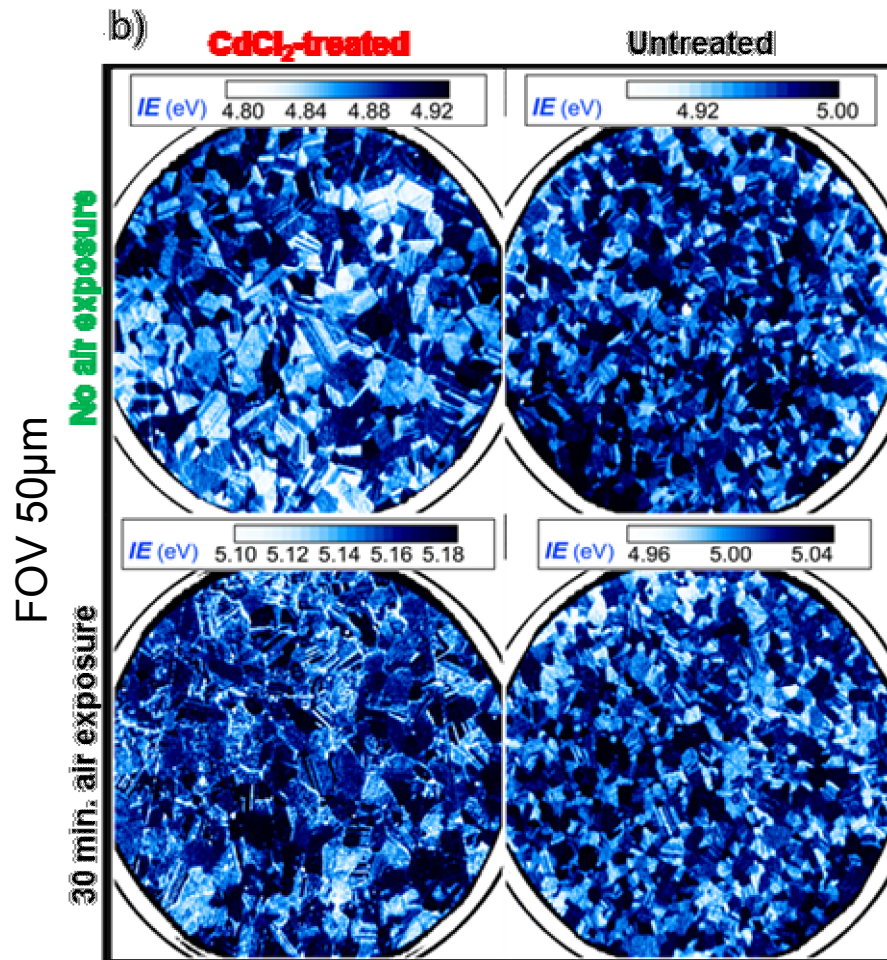
- Flat surface ensures minimum impact of morphology to the PEEM experiments
- Sputtering remove oxide layer and unwanted water

- Inert atmosphere transfer prevents exposure to oxygen





Polycrystalline CdTe changes its electronic structure by CdCl_2 treatment and air exposure



Li, et al., Phys. Rev. Lett. 112, 156103 (2014)

- CdCl_2 treatment has clear influence on the grain size and the electronic properties of grain boundaries
 - Electronic properties not only vary between grain and grain boundaries, but also between grains
- CdCl_2 treatment and air exposure have separate role in activating the grain boundaries



Moiré superlattice changes the optical absorption of twisted bilayer graphene

CVD graphene on Cu foil

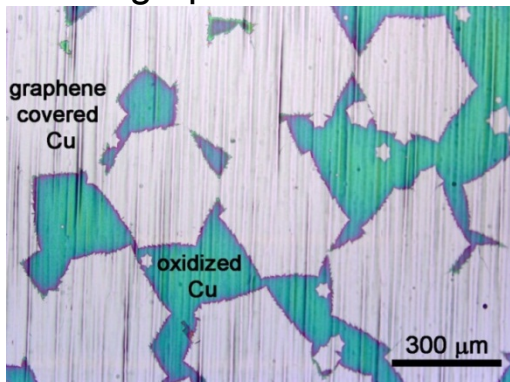
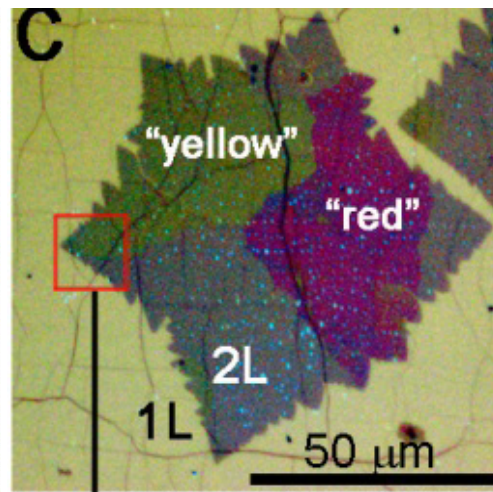
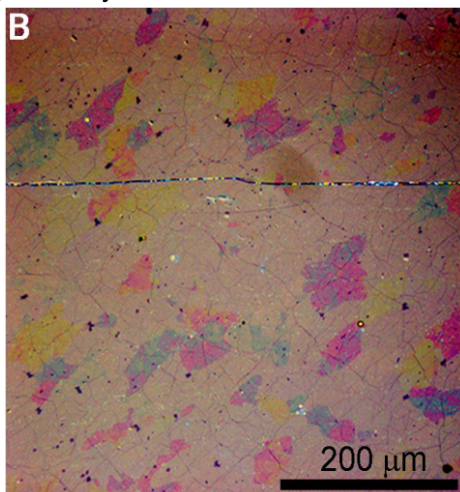
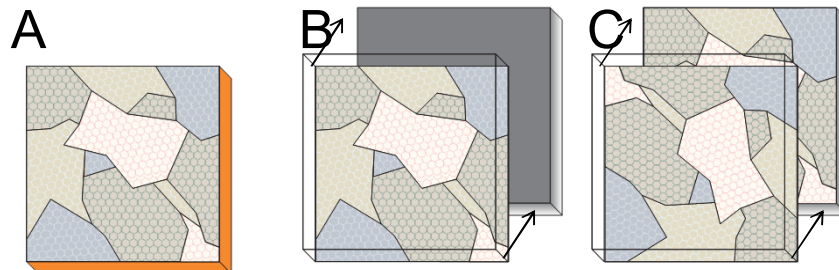


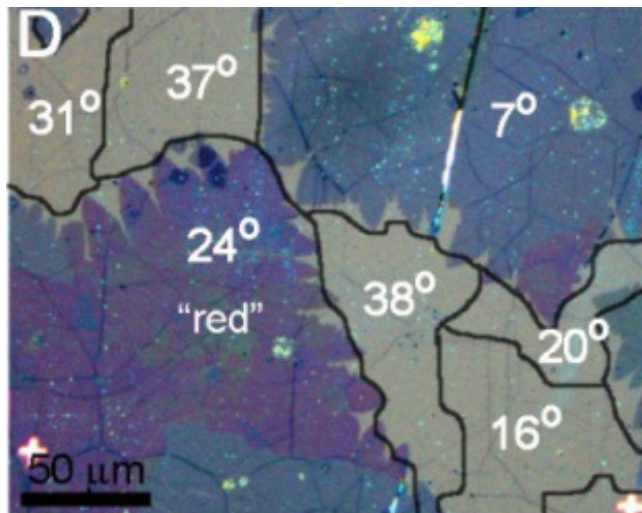
Figure courtesy: Jeremy Robinson



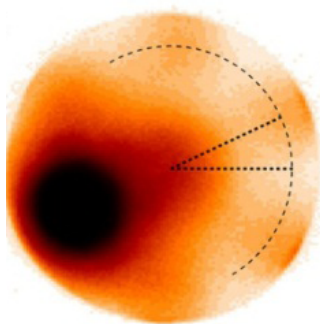
Direct probe to address the atomic arrangement?



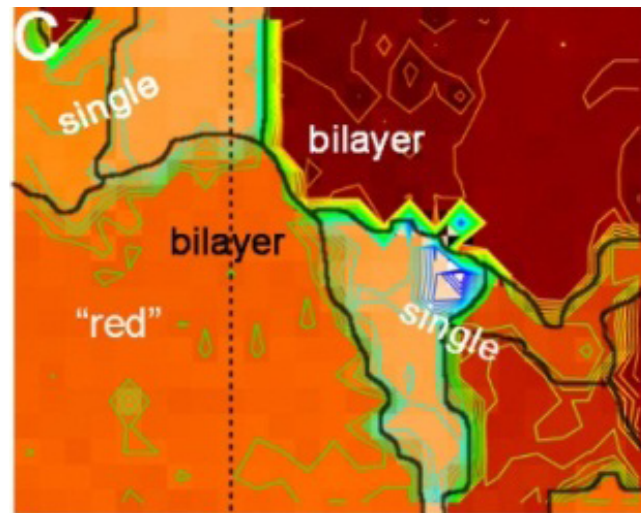
We show the correlation between the atomic arrangement and the color of TBG



Optical micrograph of the same area



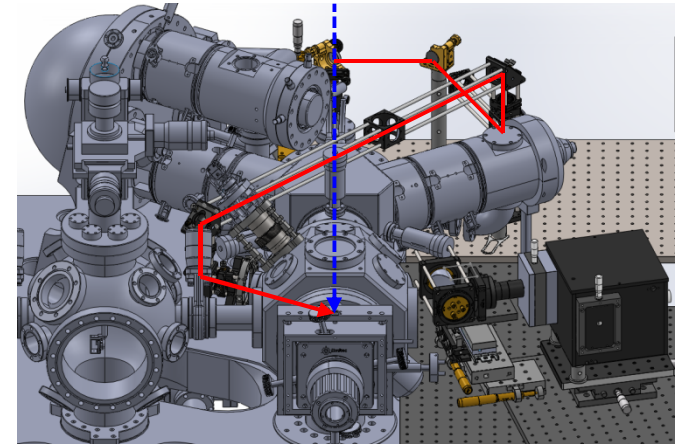
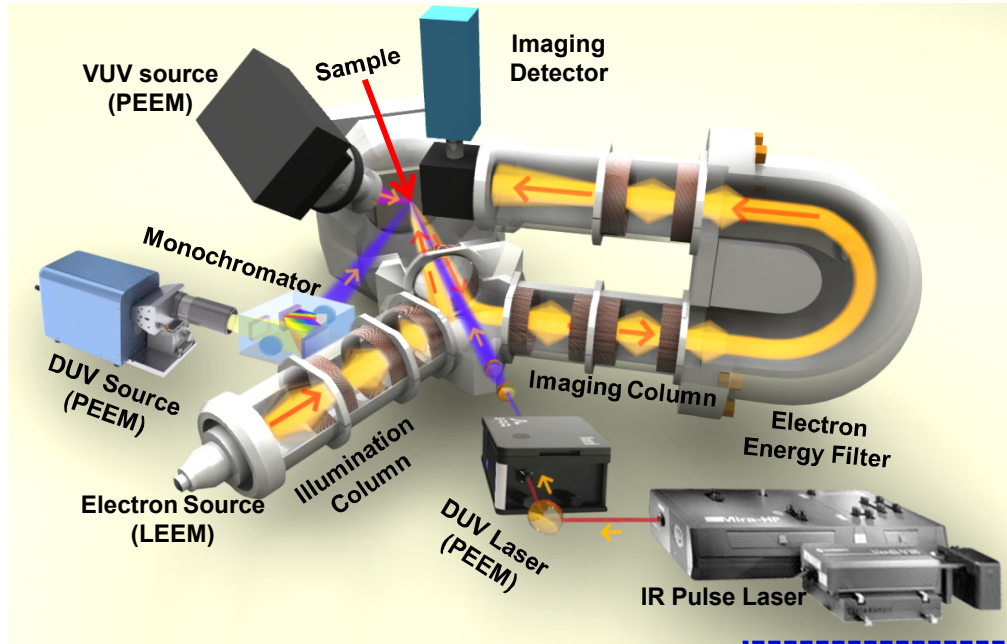
Typical μ -LEED pattern of TBG



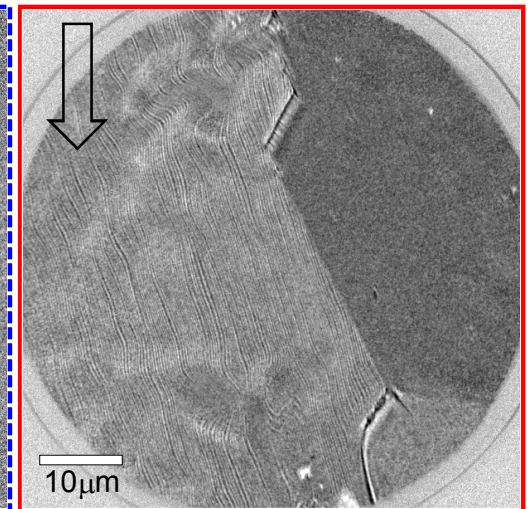
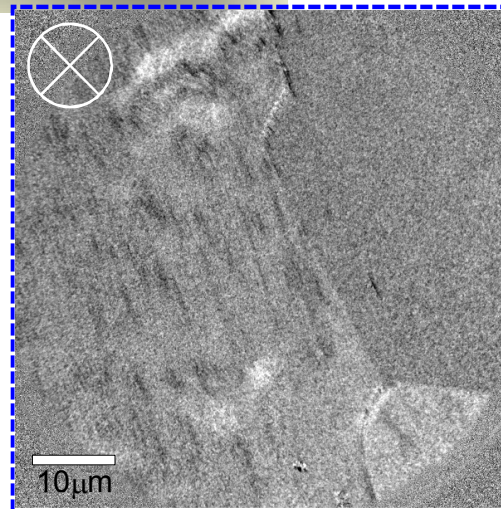
Map of LEED pattern orientations across the sample surface



Preliminary magnetic imaging based on circular dichroism using deep ultraviolet PEEM



- magnetic domain of cobalt film on polycrystalline nickel



Acknowledgements

- TMDs: Kunttal Keyshar
 - Mohite group, Los Alamos National Lab.
 - Ajayan group, Rice Univ.
 - Berg, Beechem, Chan, Sandia National Labs.
- CdTe: Morgann Berg
 - Berg & Chan, Sandia National Labs.
 - Kephart & Sampath, Colorado State Univ.
- Graphene: Jeremy T. Robinson
 - Robinson, Naval Research Lab.
 - T. E. Beechem, P. J. Feibelman, Sandia National Labs.
- Magnetic imaging:
 - R. G. Copeland, Tzu-Ming Lu, Sandia National Labs.
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 - Sandia LDRD

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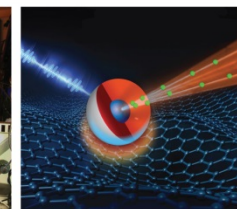
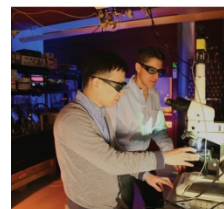
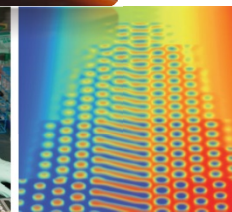
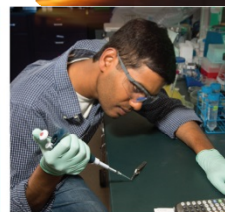
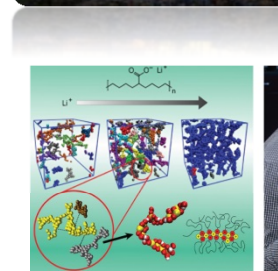


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