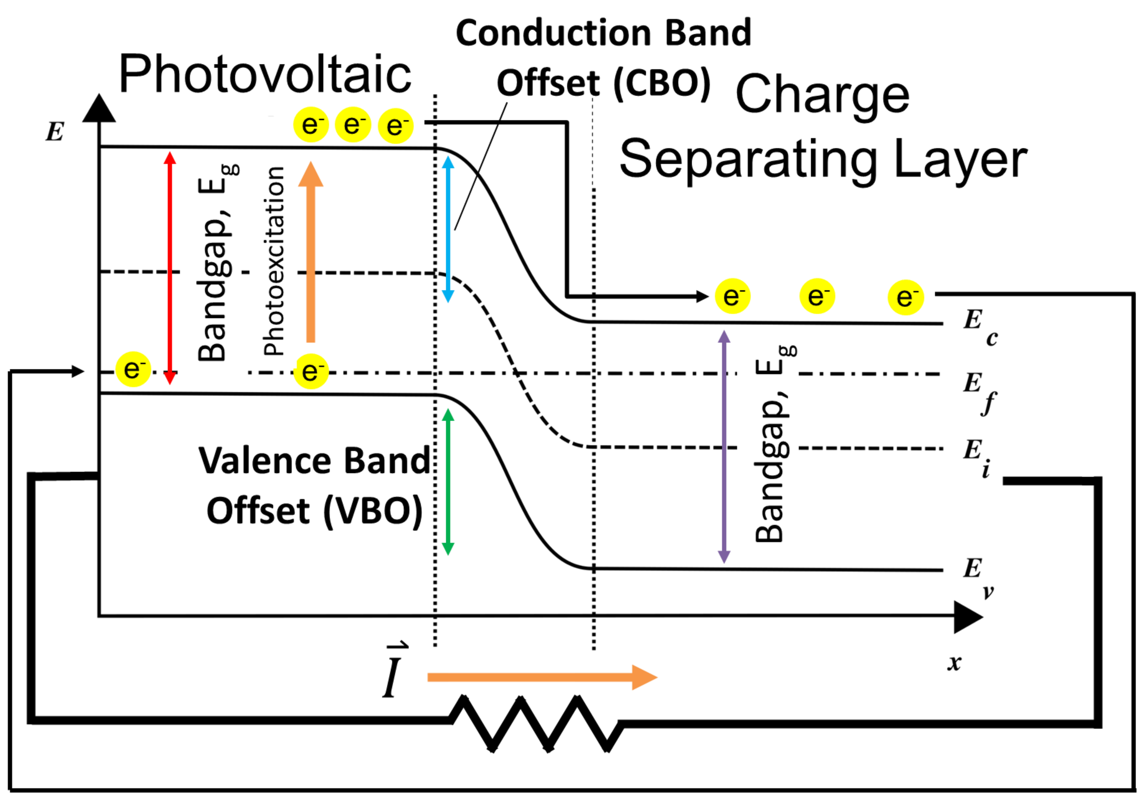
Electronic Band Structure of ALD $MoTe_2/TiO_2$ Heterostructures

Thomas Theiner, Vamseedhara Vemuri, Ben Garland, Robert Hamburger, Ryan Thorpe, Elizabeth Young, Nicholas Strandwitz, Lehigh University Departments of Materials Science and Engineering and Chemistry

Background

Solar Cell Operations

A solar cell absorbs photons to excite electrons, then pass these through a circuit to generate electrical power. This requires a photovoltaic and a layer to separate out excited electrons before they decay.

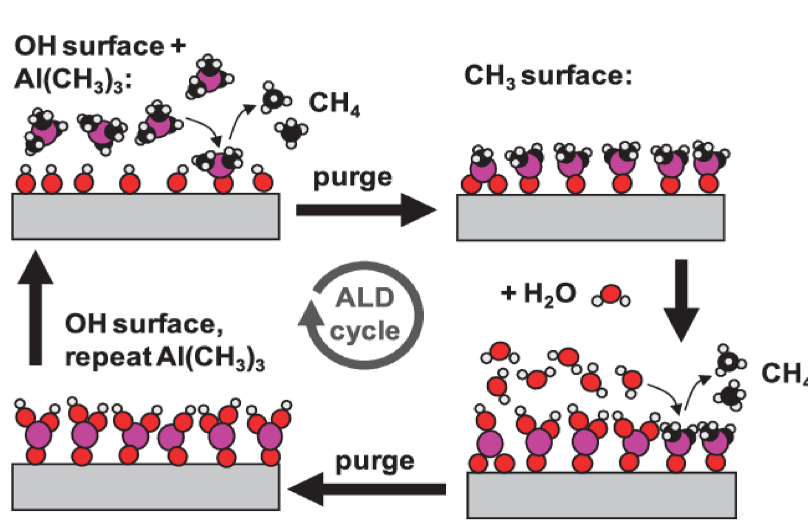


The diagram to the left shows the alignment of the valence bands (EV, valence electrons' "ground state") and conduction bands (EC, first excited state) in such a device. Important parameters for the operation of the device are labeled.

Atomic Layer Deposition

In Atomic Layer Deposition (ALD), a substrate is alternately exposed to low-vacuum pressures of two precursors, which react to form a desired surface species in a self-limiting way. Films can be made as thin as one atom

DAVID AND LORRAINE FREED UNDERGRADUATE RESEARCH SYMPOSIUM



Schematic of one of the most common ALD Processes, for Al_2O_3[1]

This work

Characterizing the chemical and electronic properties of ALD $MoTe_2/TiO_2$ heterostructures

- Observe alignment of E_V and E_C, Observe chemical effects at the interface between $MoTe_2$ and TiO_2

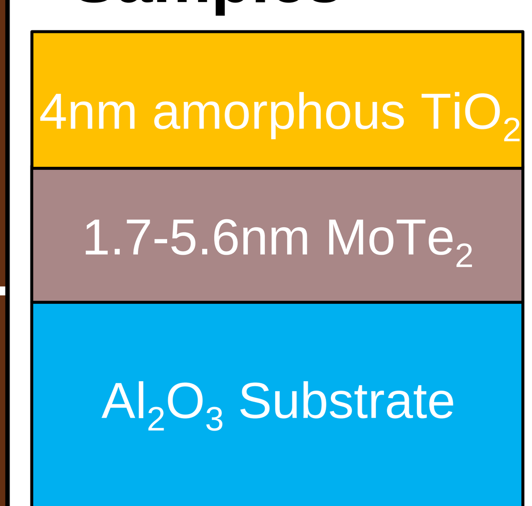
$MoTe_2$

$MoTe_2$ is a promising photovoltaic which very strongly absorbs visible light (films a few nanometers thick appear black). It also has unique properties as a 2D material. A single atomic layer of $MoTe_2$ has a direct E_g = ~1.15 eV, while thicker films have an indirect E_g = ~1.00 eV[2]

TiO_2

TiO_2 is a transparent insulating oxide with E_g = ~3.2 eV used as an electron collecting layer for $MoTe_2$. Amorphous TiO_2 can be deposited using a well studied and effective ALD process[3]

Samples



- Deposited 89 ALD cycles of TiO_2
- Constant thickness of 4nm used[4]

- 15, 25, 50, 80, or 120 cycles of MoO_x deposited via ALD
- Annealed in Te vapor atmosphere at 500°C[2]

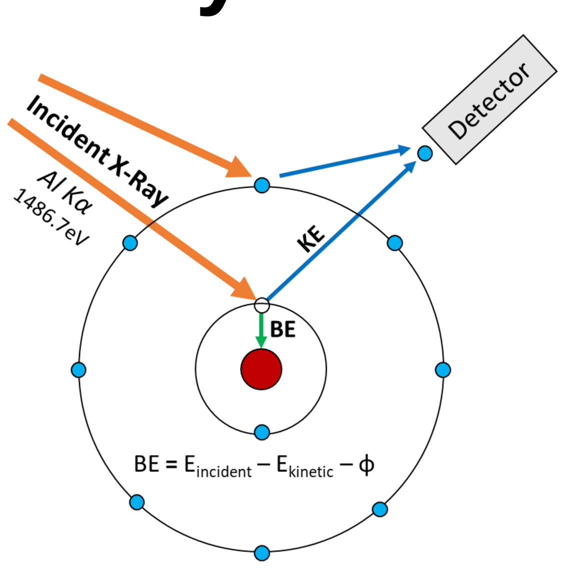
Commercially Available single-crystal sapphire substrate

Heterostructures with and without TiO_2 at a range of $MoTe_2$ thicknesses were prepared and analyzed using XPS and UV-VIS Spectroscopy

Future Work

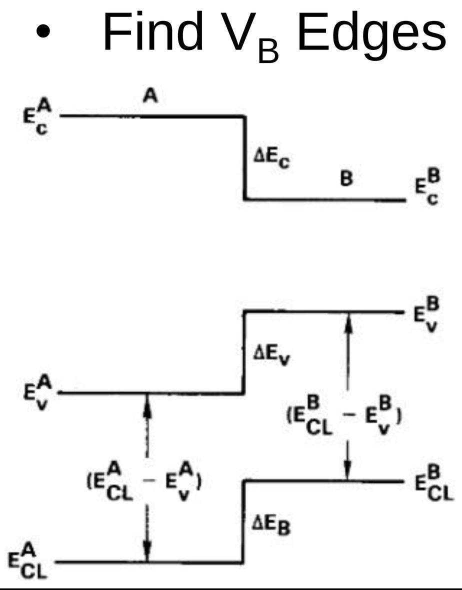
- Repeat experiments on more samples to confirm findings
- Knowledge of Energy levels in $MoTe_2/TiO_2$ heterostructures will be used to inform further study of excitons in $MoTe_2$
  - Applying Transient Absorption Spectroscopy, a pump-probe method identifying energy levels and lifetimes of excited states

X-ray Photoelectron Spectroscopy (XPS)



- XPS spectra taken of Mo3d, Te3d, Te4d, VB edge, and Ti2p on post deposition samples, different peaks for unique chemical species
- Can identify E_V energy relative to core levels
- Find V_B Edges via the Kraut method:

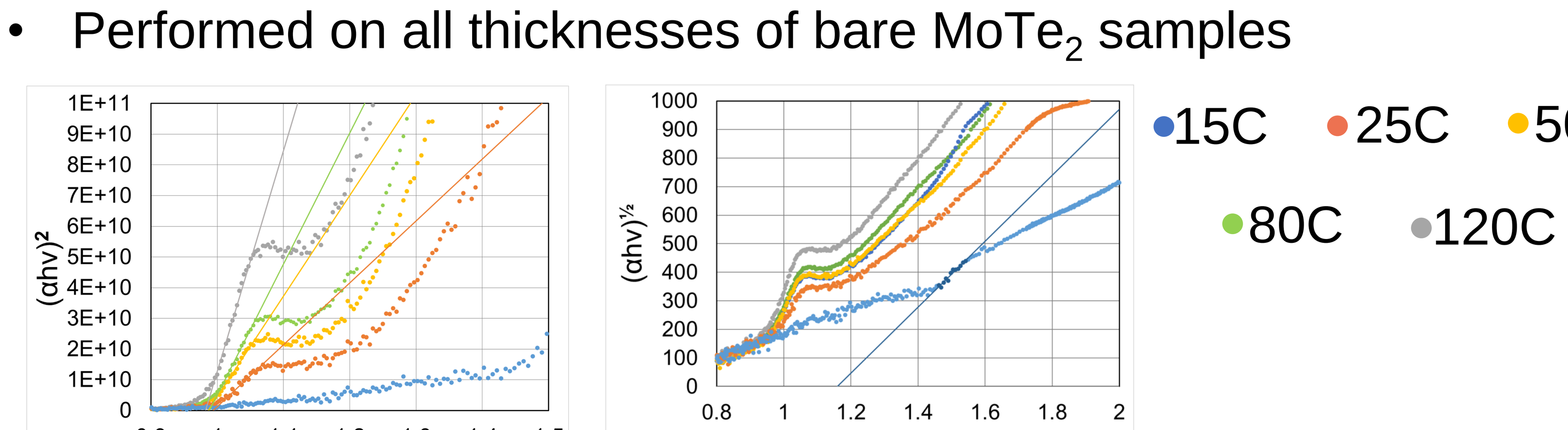
- Measures e^- binding energy (BE)



- ΔE_B, $E_{CL}{}^B - E_V{}^B$, and $E_{CL}{}^B - E_V{}^B$ measured directly,
- ΔE_V follows from these
- ΔE_C follows from ΔE_V and E_g

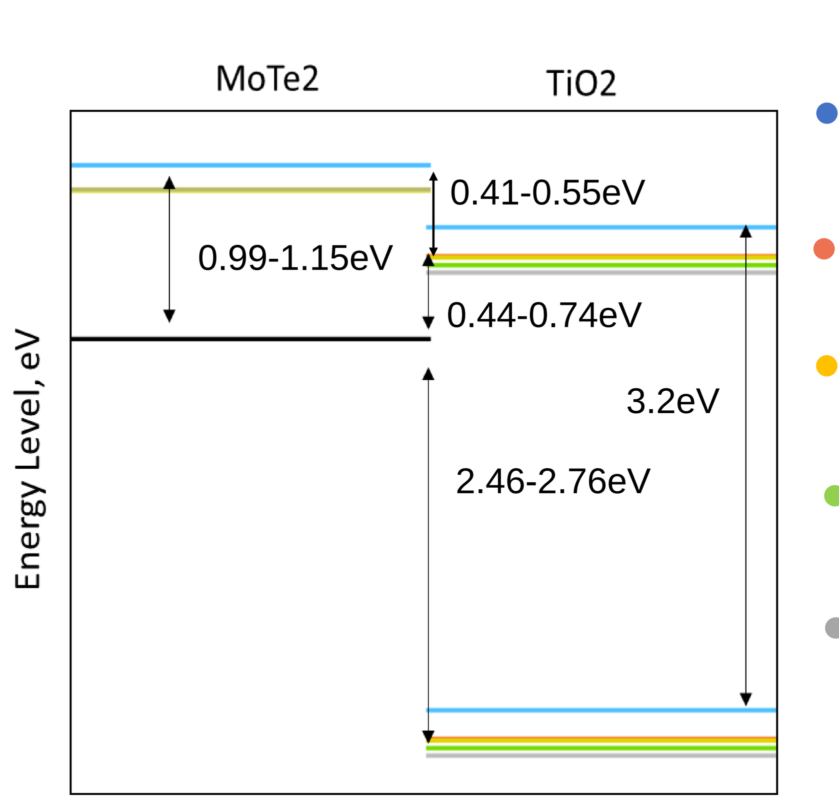
UV-Visible Spectroscopy (XPS)

- Measures absorption coefficient as function of wavelength
- Performed on all thicknesses of bare $MoTe_2$ samples

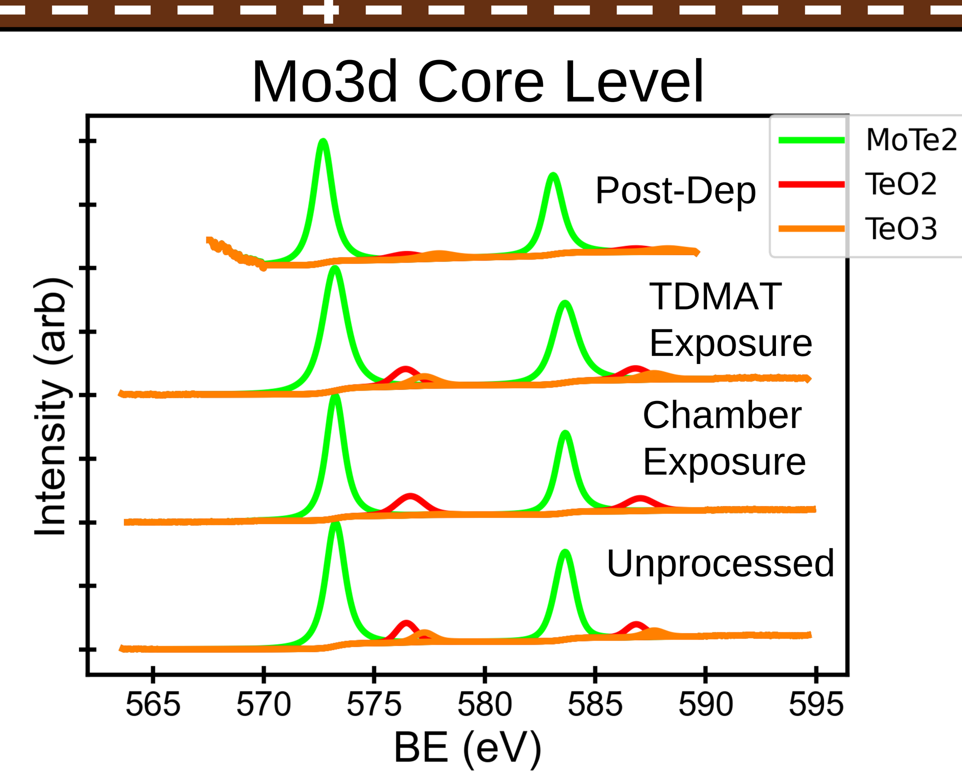


- Tauc Plots used to identify bandgap: characteristic linear features appear for hv vs different powers of αhv, extrapolating to y=0 gives bandgap
- Direct E_g= 1.15 eV seen for thinnest sample, indirect E_g= 0.99 eV for others
  - Consistent with typical behavior of $MoTe_2$ as a 2D material

Results



- Combined E_g and VBO data to determine alignment of E_C and E_V
- TiO_2 electron selective layer for all thicknesses
- VBO increases for thinner $MoTe_2$ samples



- Oxide forms on surface of $MoTe_2$
- Exposure to TiO_2 precursor found to reduce oxidation

References

1. Hyde, G. K., et al. (2011). Atomic layer deposition of titanium dioxide on cellulose acetate for enhanced hemostasis. *Biotechnology Journal*, *6*(2), 213–223. https://doi.org/10.1002/biot.201000342
2. Hynek, D. J. et al. (2020). CM²-Scale Synthesis of $MoTe_2$ Thin Films with Large Grains and Layer Control. *ACS Nano*, *15*(1), 410–418. https://doi.org/10.1021/acsnano.0c08069
3. Waldrop, J. R., Grant, R. W., Kowalczyk, S. P., & Kraut, E. A. (1985). Measurement of semiconductor heterojunction band discontinuities by x-ray photoemission spectroscopy. *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, *3*(3), 835–841. https://doi.org/10.1116/1.573326
4. Sivaramalingam, A., Thankaraj Salammal, S., Soosaimanickam, A., Sakthivel, T., Paul David, S., & Sambandam, B. (2021). Role of tio2 in highly efficient solar cells. *Metal, Metal-Oxides and Metal Sulfides for Batteries, Fuel Cells, Solar Cells, Photocatalysis and Health Sensors*, 147–168. https://doi.org/10.1007/978-3-030-63791-0_5

LEHIGH UNIVERSITY
P.C. Rossin College of Engineering and Applied Science