Accelerated *in-situ* Photo-Electron Spectroscopy for Materials by Design

Scientific Achievement

Characterized the interfacial electronic band alignment using new high-throughput measurements by coupling spatially resolved photoelectron spectroscopy (PES) mapping with combinatorially deposited crossed-gradient thin-film samples.

Significance and Impact

Rapid measurements of energy band alignments at material interfaces are essential to enable a feedback loop for computationally designing materials to tailor functional interface properties for technologies such as thin-film photovoltaics. The technique developed here accelerates interface characterization, allowing rapid Materials Genome Initiative materials development for applications where band alignment is important.

Research Details

Synthesis: The 1-D thickness gradient enables high-throughput band alignment determination from mapping PES. Additional orthogonal gradients (e.g., temperature, composition) facilitate band alignment engineering.

Under Vacuum Transfer: Mobile high-vacuum chambers or vacuum cluster tools preserve clean interfaces.

Characterization: Automated spatially resolved PES measurements.

S. Siol, A. Zakutayev *et al.*, *Advanced Materials Interfaces*, **in-press** (2016).

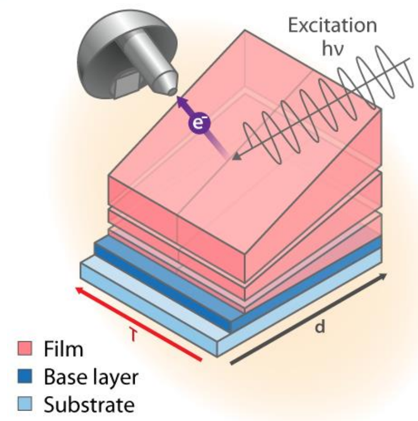

Fig. 1: Schematic illustration of spatially resolved mapping PES measurements of sample with orthogonal thickness and temperature gradients.

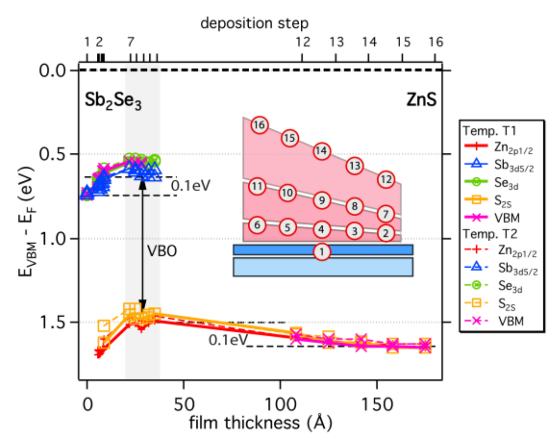

Fig. 2: Measured thickness dependence of valence-band maximum (VBM) and core-level (CL) binding energies.

U.S. DEPARTMENT OF ENERGY | Office of Science | NREL NATIONAL RENEWABLE ENERGY LABORATORY | Massachusetts Institute of Technology | HARVARD UNIVERSITY | SLAC NATIONAL ACCELERATOR LABORATORY | OSU Oregon State University | MINES | BERKELEY LAB | CNGMD Incorporating Metastability