Natural Band Alignments and Band Offsets of Sb$_2$Se$_3$ Solar Cells

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ABSTRACT: Sb$_2$Se$_3$ is a promising material for use in photovoltaics, but the optimum device structure has not yet been identified. This study provides band alignment measurements between Sb$_2$Se$_3$, identical to that used in high-efficiency photovoltaic devices, and its two most commonly used window layers, namely, CdS and TiO$_2$. Band alignments are measured via two different approaches: Anderson’s rule was used to predict an interface band alignment from measured natural band alignments, and the Kraut method was used in conjunction with hard X-ray photoemission spectroscopy to directly measure the band offsets at the interface. This allows examination of the effect of interface formation on the band alignments. The conduction band minimum (CBM) of TiO$_2$ is found by the Kraut method to lie 0.82 eV below that of Sb$_2$Se$_3$, whereas the CdS CBM is only 0.01 eV below that of Sb$_2$Se$_3$. Furthermore, a significant difference is observed between the natural alignment- and Kraut method-determined offsets for TiO$_2$/Sb$_2$Se$_3$, whereas there is little difference for CdS/Sb$_2$Se$_3$. Finally, these results are related to device performance, taking into consideration how these results may guide the future development of Sb$_2$Se$_3$ solar cells and providing a methodology that can be used to assess band alignments in device-relevant systems.

KEYWORDS: Sb$_2$Se$_3$, band alignments, window layer, photovoltaics, photoemission, HAXPES

INTRODUCTION

The field of solar energy has made great leaps forward in recent years, leading the charge for a switch from the unsustainable burning of fossil fuels to a green energy future. While technologies such as crystalline silicon and cadmium telluride (CdTe) thin films have achieved great success industrially, there is a need for additional technologies when striving to achieve terawatt scale. Antimony selenide (Sb$_2$Se$_3$) has all the desirable characteristics to be successful on an industrial level; it is a stable, binary compound made up of cheap and earth-abundant elements, has a direct band gap of 1.18 eV$^1$ and a very high absorption coefficient, $>10^4$ cm$^{-1}$. Its unusual 1D nanoribbon structure allows for very effective carrier transport if the correct orientation is achieved and has also been suggested to allow the formation of benign grain boundaries. $^2$−$^5$ Furthermore, the device performance has progressed rapidly since first being used in a solar cell, $^6$ $^7$ reaching nearly 10% in 2019. $^8$ $^9$

These qualities make Sb$_2$Se$_3$ a very promising material. However, Sb$_2$Se$_3$ photovoltaics (PV) remains an emerging technology, with a significant amount of fundamental understanding still missing from the literature. The impact of this is felt particularly in the design of various device structures utilizing different window layers (Figure 1). Cadmium sulphide (CdS) and titanium dioxide (TiO$_2$) are both used frequently, with some studies finding CdS to offer superior performance $^3$, $^10$, $^11$ and others finding the switch to TiO$_2$ extremely beneficial. $^4$, $^12$ There are many aspects of these alternative device structures that are not understood, particularly the role of band alignments in influencing the device performance.

Band alignment is a general term used to describe the way the valence and conduction bands of two materials line up to

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perform a certain function. The “natural” band alignment of
two materials describes the positions of the band extrema with
respect to the vacuum level when not in contact with each other.
The term band offset refers to the separation of the band
extrema between the two materials once contacted. A
“spikelike” band offset is defined as when the conduction
band minimum (CBM) of the window layer lies above the
CBM of the absorber and a “clifflike” offset as when the CBM
of the window layer lies below that of the absorber. With too
positive an offset (Figure 2a), electrons excited in the absorber
will face a potential barrier opposing their drift into the
window layer and lowering the short-circuit current (Jsc) (and
efficiency) of the cell. Too negative a CBO (Figure 2b) leads
to a recombination center and low built-in voltage.

Figure 2. Schematic diagram showing (a) a very positive CBO leading to a potential barrier in the conduction band and (b) a very negative CBO leading to a recombination center and low built-in voltage.

Methods

Film Deposition. CdS films were deposited onto TEC10 fluorne-
doped tin oxide (FTO)-coated glass substrates (supplied by NSG
Group) by RF-magnetron sputtering at 60 W, 5 mTorr of Ar gas and
a substrate temperature of 200 °C for 24 min. The CdS films were
~80 nm thick as determined by an Ambios Xp200 profilometer.
Anatase TiO2 films were deposited by a two-step process: first, an RF-
magnetron sputtered film was deposited at room temperature at 150
W and 5 mTorr for 30 min, and second an established spin-casting
process21 was carried out for a total film thickness of ~60 nm.
Sb2Se3 films were deposited by close-space sublimation (CSS) at a
source temperature of 390 °C with substrate heating at 330 °C and a
base pressure of ~0.05 Torr. Interfacial films for band alignment
measurements were deposited for only 30 s to achieve a film thin
eough to carry out the Kraut method (~20 nm). For the “bulk” samples, a thicker layer (~50 nm) was deposited so that the signal
from the layer beneath was not seen in the HAXPES measurements.
Detailed structural characterization (including cross-sectional trans-
mision electron microscopy and X-ray diffraction) of similar films can
be found in the work by Williams et al.13

Photoemission. HAXPES measurements were carried out at the
109 beamline at Diamond Light Source, Oxfordshire, UK. A double-
crystal Si(111) monochromator was used to select 5921 eV X-rays
followed by a Si(004) channel-cut crystal, resulting in energy
resolution of 0.25 eV (as determined by measuring the Fermi edge
of a polycrystalline gold reference sample at room temperature and
fitting a Gaussian-broadened Fermi–Dirac distribution to the data).
This allowed binding energy determination with a precision better
than ±0.1 eV. The spectra were acquired using a Scienta Omicron
EW4000 high-energy analyzer with an acceptance angle of ±28°.

Laboratory-based XPS data were collected using a monochromated
Al K\textsubscript{α} X-ray source (\(\lambda = 1486.6\ eV\)) operating at 250 W and a PSP
Vacuum Systems hemispherical electron energy analyzer with an
acceptance angle of ±3° operating with a constant pass energy of 10
eV. The energy resolution was determined to be 0.4 eV from fitting
a Gaussian-broadened Fermi–Dirac distribution to the Fermi edge of a
polycrystalline silver reference sample, allowing binding energy
determination with a precision of ±0.1 eV.

All samples exhibited a small C 1s contaminant peak (and O 1s for
the CdS sample) because of exposure to atmospheric conditions.
The films were sufficiently conducting and were grounded to the
spectrometer using a top electrical contact to avoid any surface-
charging effects.

Measuring Band Alignments by Photoemission. The
measurement of the natural band alignments via photoemission is a
commonly used procedure when screening materials for use as a
junction partner to an absorber in a PV device.13,23 While most
studies use ultraviolet photoemission spectroscopy (UPS), a highly
surface-sensitive technique for studying work functions, it is also
possible to use XPS, which is slightly less surface-sensitive (albeit
still limited to the top few nanometers). This method involves measuring
the ionization potential of a material, which describes the position of the valence band maximum relative to the vacuum level, and then using either a measured or literature-quoted band gap to determine the electron affinity, which describes the position of the conduction band relative to the vacuum level. When measuring the ionization potential, taking advantage of the fact that all XPS spectra are referenced to the Fermi level, one can also determine the position of the Fermi level in the band gap. Knowing that when two semiconductors are contacted, the Fermi levels of the two must be aligned, there is a need for a model of how this affects the alignments of the conduction and valence bands at the interface.

**Anderson’s Rule.** One widely used approach is known as Anderson’s rule or the electron affinity rule. This method states that the Fermi levels of the two materials align, while maintaining the difference in natural electron affinity at the interface (Figure 3). However, this method does not take into account the role of charge transfer, orientation, or interface-induced gap states upon contacting two materials. Therefore, if the two materials have significantly different electronegativities or lattice spacing, this approximation could differ significantly from the real band alignment. It also relies either on some assumptions or complex additional measurements to determine how the band bending is distributed across the two sides of the interface.

**The Kraut Method.** The alternative method used in this study, the Kraut method, uses a combination of measurements to take into account the charge transfer across the interface between two materials. First, the binding energy of high-intensity core (E_{CL}) levels and the VBM (E_{V}) are measured for both materials in vacuum. Then a film of one material is deposited onto the other, thin enough that photoelectrons from the lower layer can still escape and be detected during an XPS measurement. This allows an interface-sensitive measurement in which peaks from both materials are resolved. Then by measuring the separation between core levels in the two materials (ΔE_{CL}) and exploiting the fact that the core level shift upon interface formation is equal to the shift in the valence and conduction bands (|ΔE_{CL}| = |ΔE_{V}| = |ΔE_{C}|), the valence band offset between them can be directly determined, as shown in Figure 4 and eq 1:

\[
ΔE_V = (E_{CL}^B - E_{V}^B) - (E_{CL}^A - E_{V}^A) + ΔE_{CL}
\]

where A and B denote material A and material B and ΔE_{CL} = E_{CL}^A - E_{CL}^B, in the interfacial sample. The key difference between the Kraut method and Anderson’s rule, therefore, is that Anderson’s rule is a prediction of the band alignment based on measurements of the separate materials, whereas the Kraut method is a direct measurement of the band offset, albeit with some simplifications. The Kraut method approach is an abrupt interface approximation, meaning that a single measurement gives only a single offset between the bands and, though the effects of band bending are accounted for, the band bending itself is not measured. Multiple measurements carried out during interface formation can provide more detailed measurements of the band bending; however, this requires simultaneous in situ deposition and photoemission measurements, something that is not possible while using deposition techniques such as close space sublimation (CSS). A drawback to this method, however, is sample preparation. As shown in Figure 5, the inelastic mean free path (IMFP) of a photoelectron is dependent on its kinetic energy, and according to the Beer–Lambert rule:

\[
\text{IMFP} \propto \frac{1}{\text{energy}}
\]
law, 95% of the signal originates within three IMFPs of the surface. Accordingly, the sampling depth of XPS is then roughly 10 nm, and a film thinner than this is required to carry out any Kraut method studies using conventional laboratory-based XPS.

Many of the recent advances in Sb2Se3 device performance have come via the use of CSS or vapor transport deposition (VTD) of Sb2Se3.4,12,27,28 CSS allows for the formation of large grain sizes with good preferred orientation for carrier transport. This does, however, limit the thinness of films that can be deposited while still achieving good coverage, which is essential to the validity of the Kraut method measurements. At roughly 20 nm, good coverage is achievable by CSS and this falls well within the sampling depth (Figure 5) of HAXPES, a synchrotron-based technique that works by the same principle as conventional photoemission methods but with hard X-rays. With an excitation energy of 6000 eV, for example, the IMFP and effective probing depth of photoelectrons are greater than 9 and 27 nm respectively, for Sb2Se3 (as calculated using the TPP-2M equation29). With use of this method then, the band offset between a device-relevant layer of Sb2Se3, and a window layer can be directly measured. Combining this with natural alignments measurements can provide powerful insights into the formation of these interfaces simply by observing the differences between the two measurements.

Measurement of band alignments on material that was identical to that used in PV devices of good efficiency (>5%) was important to this study because the properties of Sb2Se3 are very sensitive to the deposition method and material quality.4,12,30 The following section includes results from natural band alignment measurements, Kraut method band offset measurements, and a comparison to device performance characteristics. The films used for all three aspects of these results are directly comparable because they are all deposited from the same source material via the same deposition method. This is, to the best of our knowledge, the most device-relevant measurement of band alignments in Sb2Se3 solar cells performed to date. Through direct comparison of films and devices, this work provides a method by which improved window layer partners for Sb2Se3 solar cells can be identified.

### RESULTS

**Natural Alignments.** Initially, we measured the ionization potential and work function of Sb2Se3, CdS, and TiO2 films that were deposited under the same conditions used for fabrication of devices.4,12 Figure 6 shows the secondary electron cutoff and valence band edge of TiO2, CdS, and Sb2Se3 that are used to measure the valence band and Fermi level positions of each material with respect to the vacuum level. Each cutoff was fitted with a linear fit. As can be seen in Figure 6, while the gradients naturally vary between the samples, there are no unusual shapes to any of the cutoffs.

![Figure 6](image-url)

**Figure 6.** Secondary electron cutoff (SEC) and valence band maximum (VBM) obtained by XPS for "bulk" samples of (a) TiO2, (b) CdS, and (c) Sb2Se3 with linear fits.
With use of the data from Figure 6 and the literature band gap values,\textsuperscript{1,31–33} the electron affinity of each material can be inferred and subsequently a band diagram drawn (Figure 7a). From Figure 7a it can be seen that all three materials are n-type. The n-type conductivity of Sb\(_2\)Se\(_3\) is a result of the presence of chlorine impurities in the purchased source material—a more detailed discussion of n-type Sb\(_2\)Se\(_3\) as well as the formation of an isotype heterojunction is provided by Hobson et al.\textsuperscript{34}

Figure 7b shows the alignment between Sb\(_2\)Se\(_3\) and TiO\(_2\) and between Sb\(_2\)Se\(_3\) and CdS if the Fermi levels are aligned according to Anderson’s rule. According to this rule, the difference in electron affinity is fixed at the interface, leading to a small spike of 0.36 eV between CdS and Sb\(_2\)Se\(_3\) and a smaller spike of 0.11 eV between TiO\(_2\) and Sb\(_2\)Se\(_3\). The bulk band positions of each material are determined from Figure 7a and are shifted up/down to align the Fermi levels. Band bending is then incorporated to resolve the discontinuity. An assumption has to be made regarding the distribution of the band bending—in this case it is almost entirely in the Sb\(_2\)Se\(_3\) given that the majority of the band bending will occur in the material with the lowest carrier density\textsuperscript{26} and that Sb\(_2\)Se\(_3\) is known to undergo significant band bending at the surface.\textsuperscript{34} From this it would appear that Sb\(_2\)Se\(_3\) and CdS have a good alignment for effective carrier transport in a PV device—a small spike up to 0.4 eV is widely considered to be conducive to achieving high efficiencies\textsuperscript{14,35,36} by maximizing available voltage and minimizing the chance of recombination while maintaining a CBO small enough for carriers to overcome. 

**Band Offset Measurements.** The Kraut method approach takes into account the charge transfer between the two materials by directly measuring the interface between them. In this study, HAXPES was used to enhance the inelastic mean free path of the photoemitted electrons, thereby allowing us to measure band alignments with a thicker layer of Sb\(_2\)Se\(_3\) (\textasciitilde20 nm). Figure 9 shows the photoemission data collected for the band alignment between Sb\(_2\)Se\(_3\) and either CdS or TiO\(_2\) (sample set shown in Figure 8). Figure 9a–c shows survey scans including insets of the detailed valence band scans used to determine VBM positions for each material. Figure 9d,e shows survey scans of the interfacial samples with insets showing the separately measured core levels from the window layers. Core level and VBM binding energies are included in Table S1 (Supporting Information). Detailed scans of the Ti, Cd, and Sb core levels used and the respective valence bands are included in the Supporting Information (Figures S1–S5).

Figure 8a shows the band offsets drawn from the VBOs measured by the Kraut method using HAXPES of Sb\(_2\)Se\(_3\) on both CdS and TiO\(_2\). In the Kraut method approach, no bulk band positions are measured and the offsets acquired are representative of the interface only. The VBOs were obtained using a number of characteristic Sb\(_2\)Se\(_3\) peaks (Sb 3d, Sb 4d, and Se 3d) but only one window layer peak was used as only the most intense one was resolvable (Cd 3d and Ti 2p) because of the attenuation of the window layer photoelectrons by the Sb\(_2\)Se\(_3\) overlayer. The values presented in this work are an average of the VBOs calculated from the different core levels—the full breakdown of values is included in Table S2. The Sb\(_2\)Se\(_3\)/CdS interface has a small CBO of \textasciitilde0.01 eV. The band alignment between Sb\(_2\)Se\(_3\) and TiO\(_2\) corresponds to a large clifflike CBO of \textasciitilde0.82 eV. These appear significantly different than the natural alignment results at first glance. However, before the two measurements can be compared, the impact of the assumptions and approximations involved in the two approaches must be considered.

**DISCUSSION**

The measurement of the band offsets via the Kraut method assumes flat bands and an abrupt junction. However, we must consider which regions of the interface contribute most strongly to the photoemission spectra. From the weakness of the Ti 2p signal from the TiO\(_2\) layer in Figure 9d (and similarly for Cd 3d from the CdS), it is clear that only a very thin part of...
the window layer would be detected, right at the interface with Sb₂Se₃ (red circles in Figure 10b). For the Sb₂Se₃, we can be sure that the bulk band position (green circles in Figure 10b) will dominate the signal considering that, as shown in Figure 5, the Beer–Lambert law dictates that 63% of the signal will originate from the top 9 nm. This leads us to assume that the most relevant comparison between the natural alignments and the Kraut method is as depicted in Figure 10b. Figure 10b shows the same data as presented in Figure 7b, with colored circles to indicate the equivalent regions that would be probed by the Kraut method. The predicted offsets (CBO° and VBO°) presented in Figure 10b show the energy separation between these circled regions of the Sb₂Se₃ and respective window layers, for easy comparison with Figure 10a. Therefore, the predicted band offsets quoted in Figure 10b are not measured, but are rather a projection of what the interface predicted by Anderson’s rule (Figure 7b), in the absence of interface charge transfer, would yield if measured via the Kraut method.

On the basis of this assumption, comparing parts (a) and (b) of Figure 10, we can see that for the CdS/Sb₂Se₃ interface there is very good agreement between the Kraut method and Anderson’s rule. This strengthens the conclusion that CdS and Sb₂Se₃ have excellent band alignments for good device performance in photovoltaics and suggests that the band alignment between CdS and Sb₂Se₃ predicted by Anderson’s rule is an accurate prediction of the true band alignment. However, for the TiO₂/Sb₂Se₃ interface, there is a significant difference between VBO and CBO given by the Kraut method and the modified Anderson’s rule results. Even when taking into account the differences between the two approaches regarding band bending (Figure 10b), the predicted offset (CBO°) between the flat band position in the Sb₂Se₃ and the edge of the TiO₂ band is only −0.18 eV in the modified Anderson model, compared to a CBO of −0.82 eV measured by the Kraut method. According to the Kraut method here, even with an equivalent amount of band bending as predicted
by Anderson’s rule, the CBO would actually be clifflike at the interface (Figure 10a), rather than the 0.11 eV spike predicted by Anderson’s rule (Figure 7b). This suggests that there is a large degree of charge transfer upon contact, which increases the VBO (and CBO) from the natural value. The existence of a clifflike offset is supported by the observation of a similar alignment for Sb$_2$S$_3$ and TiO$_2$ reported elsewhere.\textsuperscript{37}

There is a significant difference in how closely matched the natural alignment and Kraut method results are for Sb$_2$Se$_3$/CdS and Sb$_2$Se$_3$/TiO$_2$. For the Sb$_2$Se$_3$/CdS interface, the difference is minimal. The similitude of sulfur and selenium as anions in terms of both valency and electronegativity could play a part in this. While the electronegativity of all three cations (Ti, Cd, and Sb) are all reasonably similar (1.54, 1.69, and 2.05), the electronegativity of O (3.44) is far greater than those of S and Se (2.58 and 2.55), which are almost equal.\textsuperscript{38–40}

This means that CdS and Sb$_2$Se$_3$ are expected to have a similar overall electronegativity, while the electronegativity of TiO$_2$ is expected to be significantly greater (there being twice as many O atoms as Ti). A smaller electronegativity difference between the two contacted materials means less charge transfer upon contact and a smaller interface dipole.\textsuperscript{38,41}

From a device performance perspective, the results of the band alignment measurements show that the CdS/Sb$_2$Se$_3$ interface has a better alignment than TiO$_2$/Sb$_2$Se$_3$—according to the Kraut method, TiO$_2$ would form a large cliffike barrier at the interface with Sb$_2$Se$_3$, leading to a limited available voltage from these kinds of devices. CdS, however, has a conduction band that is perfectly aligned with the conduction band of Sb$_2$Se$_3$, showing that this would provide a near-perfect window layer partner, at least in terms of band alignment—a small interfacial spike between 0.3 and 0.4 eV has been shown to be ideal for PV devices with materials such as CZTS and CdTe.\textsuperscript{14,55,56} Additionally, the difference between the natural alignment and Kraut method offsets presents some interesting insights into the formation of these interfaces.

Interestingly, however, CdS-based devices do not necessarily perform better than TiO$_2$-based devices. It has been shown by our group previously that, for Sb$_2$Se$_3$ films grown by CSS, the devices utilizing a CdS window layer perform very poorly compared to those using TiO$_2$.\textsuperscript{12} Phillips et al. reported a power conversion efficiency of only 1.44% for a CdS-based device compared to 5.48% for a TiO$_2$-based device. While the $V_{oc}$ and FF were somewhat lower for CdS (0.42 V and 45.48%) than for TiO$_2$ (0.45 V and 48.96%), the most significant difference was in the $J_{sc}$: only 7.57 mA·cm$^{-2}$ for CdS compared to 25.44 mA·cm$^{-2}$ for TiO$_2$. This is the opposite of what would be expected from the band alignments measured in this study—the clifflike offset of the TiO$_2$/Sb$_2$Se$_3$ interface would be expected to cause a lower $V_{oc}$ than CdS/Sb$_2$Se$_3$, and the small CBO of the CdS/Sb$_2$Se$_3$ would lead to a very good current. This discrepancy is attributed to interdiffusion of the anions, S and Se, across the interface during the high-temperature growth stage of the Sb$_2$Se$_3$ devices, a process which leads to the formation of a CdSe layer between the Sb$_2$Se$_3$ and CdS.\textsuperscript{12} This is evidenced by time-of-flight secondary ion mass spectrometry and external quantum efficiency measurements by Phillips et al.\textsuperscript{12} and significantly reduces the efficiency of the carrier transport from the absorber to the window layer (the intermixing is not present in the samples used for the band alignments measurements as discussed below). This is further illustrated by Williams et al.\textsuperscript{12} where the overlapping presence of Cd, S, and Se at the interface as well as the possible presence of metallic Sb is shown with cross-sectional transmission electron microscopy with elemental mapping.\textsuperscript{12} The implication of this is that it may be possible to achieve a superior device performance if the interdiffusion can be prevented in such a way that the favorable band alignment between CdS and Sb$_2$Se$_3$ can be retained.

While the intermixed region is ever-present in the working devices, it is noted here that intermixing is not expected to occur in the samples presented here. Sb$_2$Se$_3$ films deposited by CSS for devices are made via a two-step process, an initial step at lower temperature to lay down a seed layer and then a longer, higher temperature deposition to achieve a good grain size/structure. Given that for the interfacial samples the deposition was only 30 s long and at the lower temperature used to deposit the seed layer, it is assumed that no significant intermixing was able to occur. Additionally, there is no evidence of any additional chemically shifted components in the photoemission spectra that could be attributed to CdSe or Sb$_2$S$_3$ in the interface region.

It is noteworthy here that the current record efficiency for any Sb$_2$Se$_3$ solar cell is held by Li et al.\textsuperscript{8} and that in their study...
a thin TiO2 interlayer deposited by atomic layer deposition was used between CdS and Sb2Se3 to block a similar interdiffusion process. While it must be acknowledged that the devices made by Li et al. contained a number of differences from the standard Sb2Se3 device structure considered in this work (the use of a substrate configuration and a nanorod structure among them), it is promising to the conclusions of this work that to the best of our knowledge the only study in which steps have been taken to prevent the interdiffusion between CdS and Sb2Se3 has achieved such outstanding performance. We postulate, therefore, that the band alignments between TiO2 and Sb2Se3 are a limit to the potential efficiency of Sb2Se3 devices that use TiO2 as a window layer. Furthermore, with use of CdS as a window layer (while blocking interdiffusion with an interlayer thin enough not to interfere significantly with the band alignments), the efficiencies of Sb2Se3 solar cells could be improved beyond 10%.

■ CONCLUSION
In this work we have used photoemission techniques to thoroughly study the band alignments between Sb2Se3 and two of its most commonly used window layers—CdS and TiO2. The results of natural alignment measurements showed CdS and Sb2Se3 to have a small CBO of 0.36 eV, while the offset between Sb2Se3 and TiO2 CBO was 0.11 eV. Kraut method measurements carried out using HAXPES revealed a similar result for Sb2Se3/CdS of −0.01 eV, while the offset for Sb2Se3/TiO2 was significantly different at −0.82 eV. The results suggest that CdS has an optimal band alignment with Sb2Se3, while TiO2-based devices are likely limited by a clifflike offset leading to recombination and a limited built-in voltage. This is especially relevant considering the evidence of detrimental intermixing at CdS/Sb2Se3 interfaces. This has led some groups to prefer the use of TiO2 as a window layer and has also inspired the use of an interdiffusion blocking interlayer in a recent record efficiency publication.8 The harnessing of advantageous band alignments while preventing interdiffusion could provide a platform for pushing the efficiencies of Sb2Se3 to the next level.

■ ASSOCIATED CONTENT

Supporting Information
The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsaem.0c01477.

Tables detailing the binding energies of all fitted core levels and valence bands and the calculated band offsets; graphs showing core level and band edge fits for all photoemission results (PDF)

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Notes
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