Energy Summer Program Report

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Project title: Optimization of BiOI Thick Films for X-ray Detection Applications

Introduction

Background on X-ray Detection

X-rays are high-energy electromagnetic waves capable of penetrating materials that are opaque to visible light. In X-ray imaging, a beam is directed through an object, and the transmitted intensity is recorded to form an image based on variations in attenuation. Dense tissues such as bone absorb more X-rays than soft tissues, creating contrast and enabling clear imaging.

X-ray detection systems

Accurate X-ray detection is crucial, especially in medical diagnostics where the aim is to achieve high-resolution imaging while minimizing radiation exposure. Detection systems typically follow two approaches: indirect detection and direct detection. In the indirect method, X-rays are absorbed by a scintillator that re-emits the energy as visible light, which is then detected by a photodiode. In contrast, the direct method eliminates this intermediate step, with X-rays absorbed directly by a photoconductive material that converts them into electrical signals. [1]

Direct conversion offers several advantages, including higher spatial resolution, reduced noise, and improved detection efficiency at lower radiation doses. These benefits are particularly important for medical applications, where patient safety is a priority. The BiOI devices discussed in this report operate via direct conversion, highlighting their importance as next-generation X-ray detectors.

The potential of BiOI as a detector

Traditional materials like a-Se, CZT, and lead halide perovskites face issues such as limited absorption, high cost, instability, or toxicity. However, BiOI combines high X-ray absorption due to Bismuth and Iodine which increases its ability to attenuate X-rays strongly and high sensitivity as well as low detectable dose rates. It is also easily scalable, highlighting BiOI as a compelling option for next-generation X-ray detectors. [2]

Aim and objectives of the research

The aim of this research is to investigate the potential of BiOI thin films as photoconductors for X-ray detection. To achieve this, BiOI films are compared and characterized on two different hole transport layers, NiO_x and Bi_2O_3 which are deposited on ITO substrates, to understand how the underlying layer influences film quality and device performance. Based on the optimized films, X-ray detection devices are then fabricated and systematically evaluated to assess their suitability for radiation detection applications and the difference between the films of the substrates.

Methodology

BiOI thin films were deposited using the Close Proximity Chemical Vapor Deposition (CPCVD) technique, which enables the growth of uniform, polycrystalline layers over large areas. The films were deposited onto ITO substrates coated with both NiO_x or Bi_2O_3, allowing a comparison of how different hole transport layers influence film morphology and optoelectronic properties. Deposition parameters such as source temperature, amount of substrate, gas flow during each deposition run were carefully optimized to achieve films of approximately 6 µm thickness. After deposition, gold electrodes (~80 nm) were evaporated on the substrates to complete the device structure.

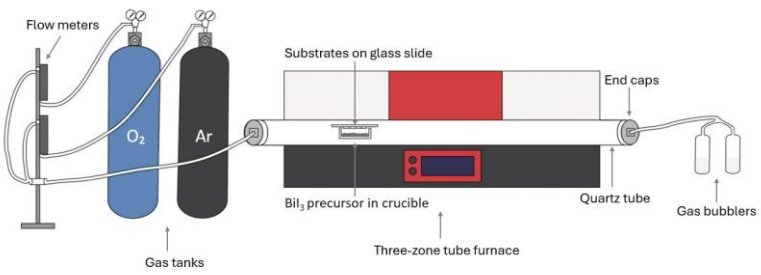


Figure 1. Illustration of the growth set up for BiOI

The crystallographic properties of the BiOI films were analyzed using X-ray diffraction (XRD), with patterns collected over a suitable 2θ range. The obtained data were further refined by Rietveld analysis to determine lattice parameters, phase purity, and preferred orientation. XRD data were plotted and processed using OriginLab software for visualization.

Film thickness was measured by profilometry, providing quantitative values for layer uniformity and growth optimization. Surface morphology and microstructure were examined by scanning electron microscopy (SEM), including both surface and cross-sectional imaging.

Electrical characterization of the fabricated devices was carried out through current–voltage (I–V) sweeps to evaluate charge transport behaviour, while current–time (I–t) measurements were performed under bias to assess device stability and the ON/OFF switching response under X-ray exposure.

Results and discussion

Film thickness measurement via profilometry

All four substrates exhibited an average thickness of approximately 6 µm, confirming consistent growth across the deposition runs. Representative profilometry results are shown in Figure 2 and 3.

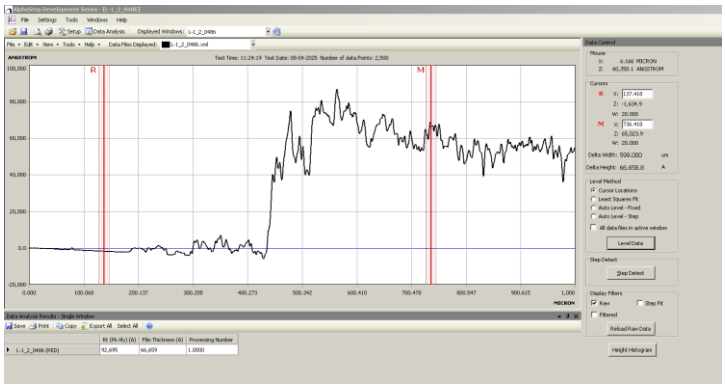


Figure 2. Profilometry of BiOI on Bi2O3/ITO

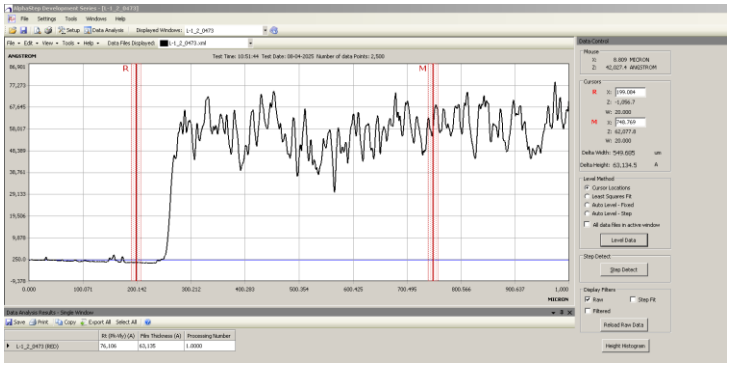


Figure 3. Profilometry of BiOI on NiOx/ITO

XRD and Structural Refinement

The crystalline structure of the BiOI films was analyzed using X-ray diffraction (XRD). Diffraction patterns were collected and subsequently refined using Rietveld analysis to evaluate phase composition, lattice parameters, and preferred orientation. The refinement results confirmed that the films achieved nearly 100% phase purity, with no detectable secondary phases.

A comparison of BiOI deposited on the two different hole transport layers revealed distinct structural characteristics. Films grown on Bi_2O_3-coated substrates exhibited a strong c-axis orientation, as evidenced by the enhanced intensity of the (001), (002), and (102) planes. In contrast, BiOI deposited on NiO_x substrates showed a more isotropic orientation, with broader diffraction peaks. This indicates that the choice of underlying layer significantly influences the crystallographic orientation of BiOI, which may in turn affect charge transport and device performance.

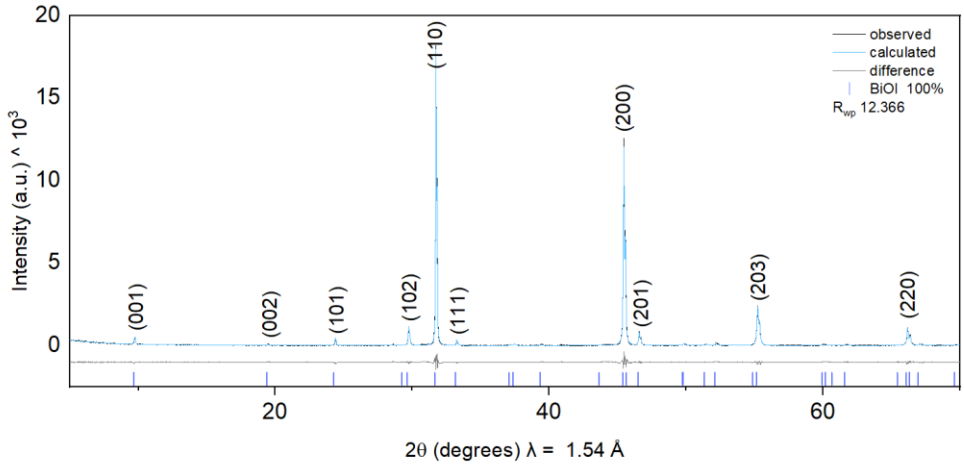


Figure 4. XRD refinement of BiOI grown on NiOx/ITO

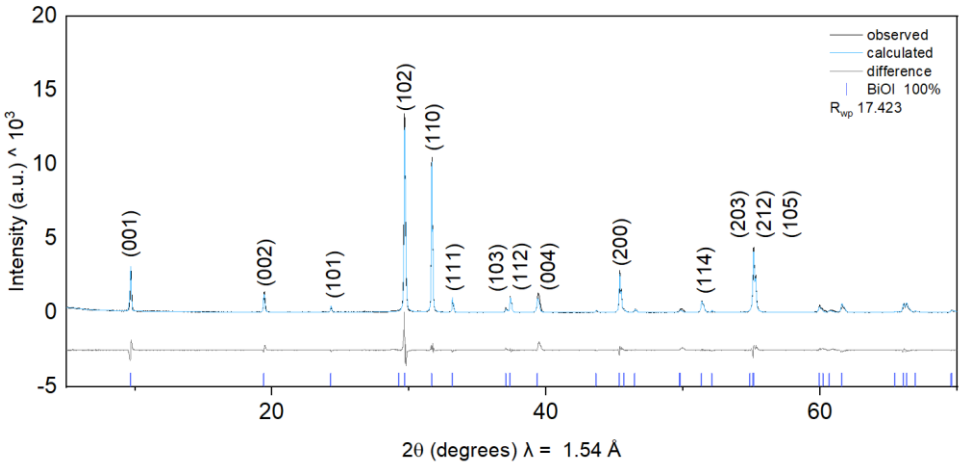


Figure 5. XRD refinement of BiOI on Bi2O3/ITO

SEM analysis

Depending on the film orientation, this structural anisotropy gives rise to distinct surface morphologies in SEM imaging. If the films are c-axis oriented, large platelet-like structures are observed lying flat. In contrast, a/b-axis oriented films exhibit vertically aligned nanosheets, exposing the edges of the layers and giving rise to sharp, needle-like features.

The first SEM image (Figure 6) shows a surface populated by vertical, needle-like nanosheets with sharp edges, which is characteristic of an a/b-axis orientation for the BiOI grown on NiOx/ITO. The second SEM image (Figure 7), however, reveals broad platelets stacked parallel to the substrate, consistent with a c-axis orientation for the BiOI film grown on Bi2O3/ITO.

These observations indicate that the BiOI films display different orientations depending on the underlying substrate type, with the second case suggesting a more favourable c-axis orientation that is often desirable for efficient charge transport in optoelectronic applications.

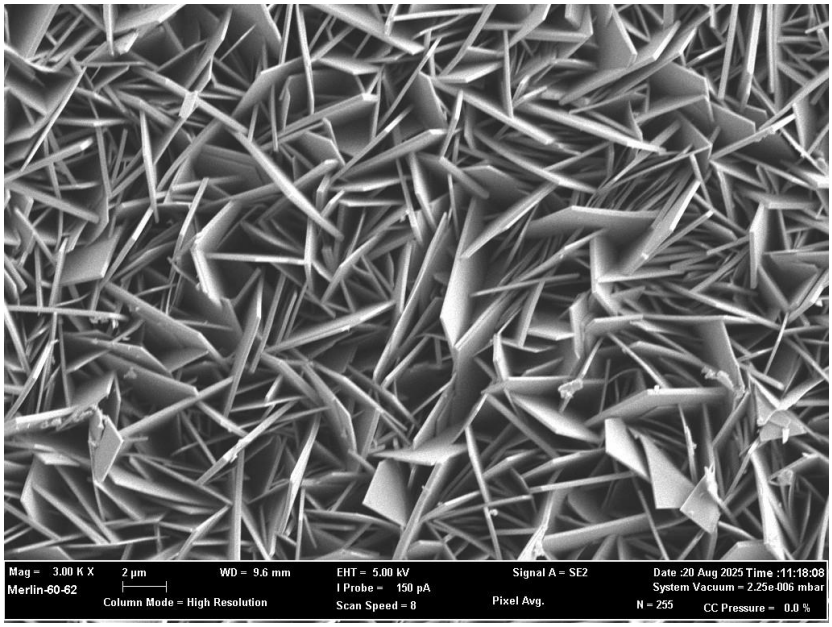


Figure 6. SEM morphology of BiOI on NiOx/ITO

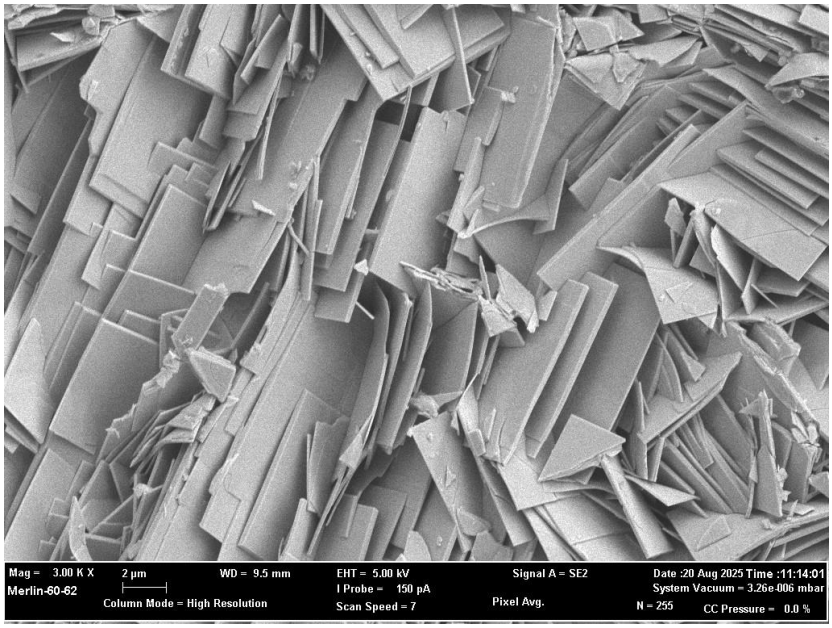


Figure 7. SEM morphology of BiOI on Bi2O3/ITO

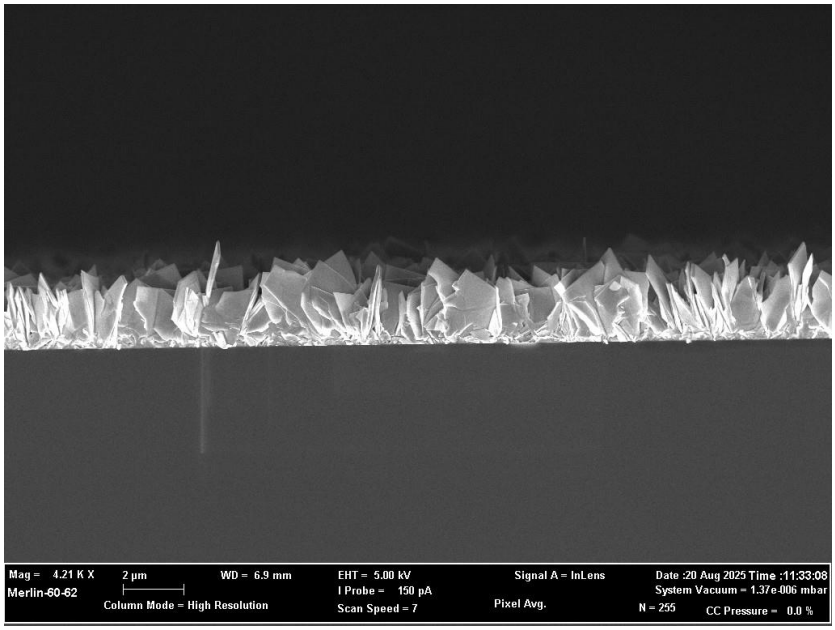


Figure 8. Cross sectional image of the BiOI film

Electrical Characterization

IV sweep and I-t measurements of NiOx device

The I–V curves demonstrate that P1 and P2 under illumination reach higher photocurrents (~6 × 10^{-7} A and ~3 × 10^{-7} A at +3 V), whereas P3 remains nearly flat with low conductivity. Dark currents are minimal, indicating a predominantly light-driven response. The I–t measurements show stable and reproducible current responses, with P2 exhibiting the highest photocurrent (~7.5 × 10^{-8} A at +1 V and −1.5 × 10^{-7} A at −1 V), while P3 shows weaker responses.

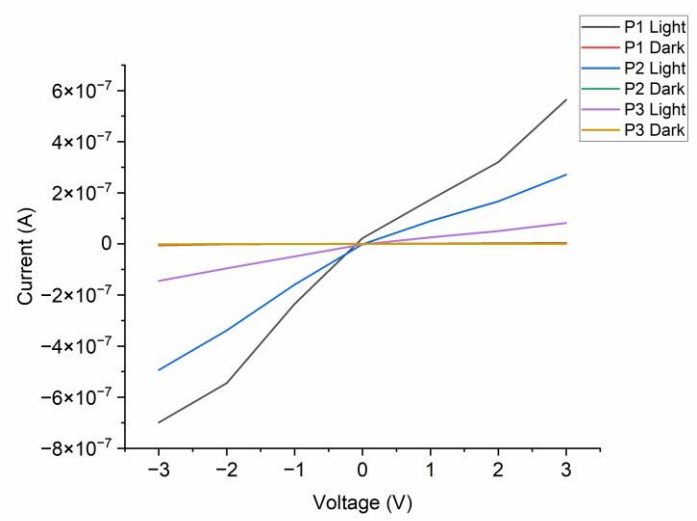


Figure 9. IV sweep of the NiOx device

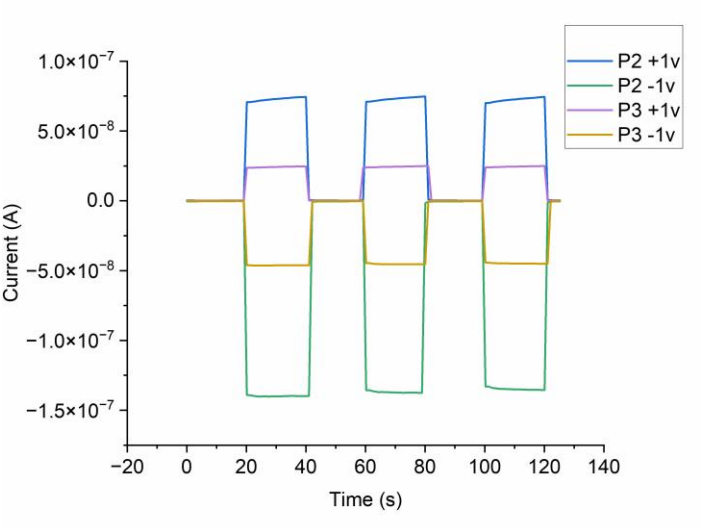


Figure 10. I-t stability measurement of the NiOx device

IV sweep and I-t measurements of Bi2O3 device

The I–V measurements of BiOI on Bi_2O_3 show strong photo response under illumination, with currents in the 10^{-6}–10^{-5} A range, while dark currents remain very low (10^{-9}–10^{-10} A), demonstrating excellent photo-to-dark contrast and efficient light-driven charge transport. Complementary I–t measurements confirm stable and reproducible photocurrent switching, with P2 and P3 reaching the highest positive responses (~4–4.5 × 10^{-6} A at +1 V), while P1 is slightly lower (3.5 × 10^{-6} A). Under reverse bias (−1 V), P2 exhibits the strongest negative current (−3 × 10^{-6} A).

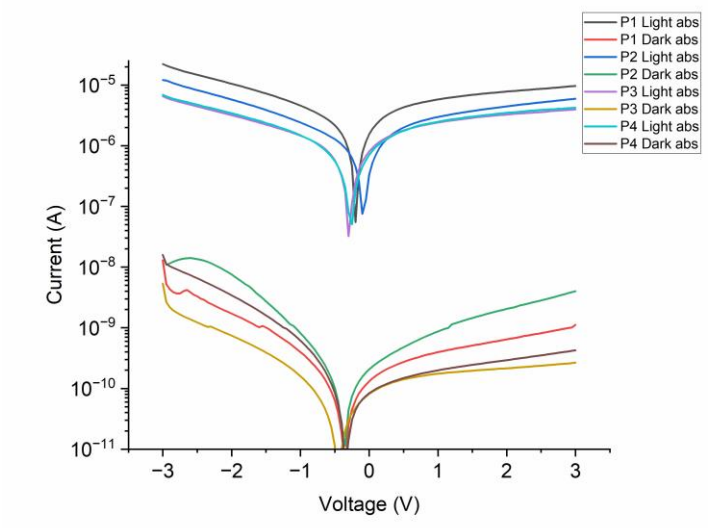


Figure 11. IV sweep of Bi2O3 device

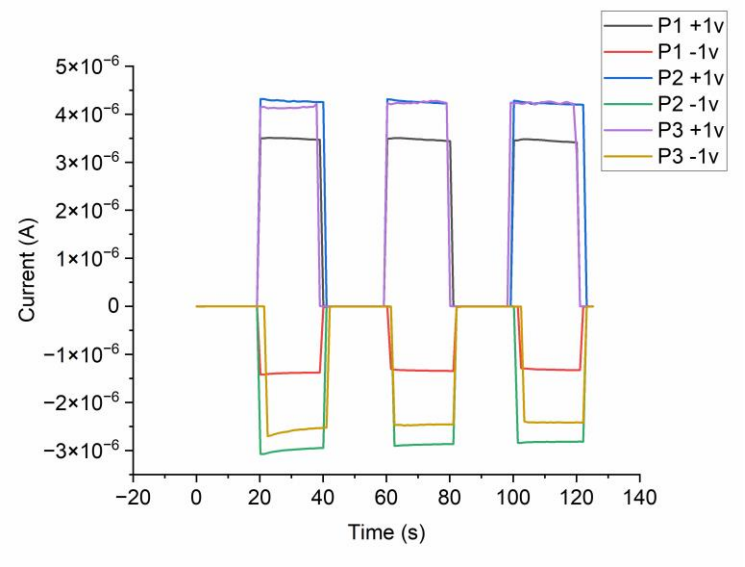


Figure 12. I-t measurement of the Bi2O3 device

On/Off ratio calculations

For BiOI on Bi_2O_3, ON/OFF ratios are very high, reaching 1422–9186 at +1 V and 544–2007 at −1 V, confirming efficient light-induced switching. In contrast, BiOI on NiOx shows much lower ratios (189–252 at +1 V and 333–347 at −1 V), indicating weaker photo-to-dark contrast and less effective charge separation.

Future work

Future studies will focus on further improving the performance and understanding of BiOI-based X-ray detectors. In particular, measuring the work function and energy level alignment via ultraviolet photoelectron spectroscopy (UPS) was planned, but time constraints did not allow this in the current work. Additionally, while the growth of BiOI films on NiO_x has been optimized, further optimization of thick-film deposition on Bi_2O_3 substrates is needed to evaluate how increased active layer thickness affects device efficiency, stability, and ON/OFF response. These studies would contribute to refining device design and unlocking the full potential of BiOI for high-performance direct X-ray detection.

Challenges and solutions

During device characterization, performing I–V and I–t measurements proved somewhat challenging due to the thin gold electrodes (~80 nm) deposited on the BiOI films. The delicate electrodes were easily scratched by measurement clips, leading to short-circuiting in some cases and rendering a few of the six pixels on each substrate unusable. To address these challenges, only the data from the 2–3 well-functioning pixels were used for analysis, ensuring that the reported results accurately reflected the device performance while minimizing the impact of these measurement artifacts.

Conclusion

BiOI films were successfully deposited on NiOx and Bi_2O_3-coated ITO substrates, yielding uniform ~6 µm thick layers with high phase purity. XRD and SEM confirmed that Bi_2O_3 promoted strong c-axis orientation with flat, plate-like nanosheets, while NiOx films showed more a/b-axis oriented growth.

Device testing revealed a trade-off: NiOx substrates enabled higher photocurrent, whereas Bi_2O_3 substrates achieved much higher ON/OFF ratios due to lower dark current. These results demonstrate that substrate choice strongly influences film orientation and device performance, highlighting BiOI's potential as a promising photoconductor for X-ray detection.

Acknowledgments

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References

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2. Dudipala, K. R., *et al.* (2023). *Halide perovskites and their derivatives for efficient, high-resolution direct radiation detection: Design strategies and applications*. Adv. Mater., 36, 2304523. https://doi.org/10.1002/adma.202304523