# MTTB: End-to-End Framework for Oxide TFT Channel Guidelines Beyond-IGZO

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## Abstract

As AMOLED displays move toward higher resolution and lower power operation, next-generation oxide semiconductors are needed to achieve high-performance, reliable backplane TFTs. However, existing ML-based screening has two limitations. It can distort design decisions by collapsing conflicts among multiple material descriptors into a single objective function. It also lacks an interpretable link between material-level predictions and device-level performance. To address these issues, we propose a four-stage hybrid framework, *MTTB* (Materials-to-TFT Bridge). (1) **AI-based property prediction**: rapidly infers material descriptors (band gap $G_x$, inverse spatial wavefunction overlaps $ISWO_C$ and $ISWO_V$, and formation energy $E_f$) from composition vectors. (2) **Pareto-based multi-objective composition search**: compresses promising candidates while preserving trade-offs among material descriptors. (3) **Candidate selection strategy**: selects final candidate compositions based on performance–stability trade-offs and target priorities. (4) **Physics-Inference Module (PIM)**: maps predicted properties to device-physics variables to efficiently infer TCAD-equivalent device metrics. Experimentally, global Pareto-knee candidates converge to Al–Mg-centered compositions under high-bandgap conditions. Composition-sensitivity analysis and PIM-based device simulations confirm the potential for balanced performance improvements over IGZO. Finally, we propose Al–Mg-based (beyond-IGZO) oxide archetypes and composition candidates that can replace IGZO.

## 1 Introduction

AMOLED (Active-Matrix Organic Light-Emitting Diode) displays offer high contrast and fast response. They are widely used as a core display technology in electronic devices, including smartphones (1). As demand increases for higher resolution and lower-power operation, requirements for the electrical performance and stability of AMOLED driving devices continue to intensify (2). Meeting these requirements requires thin-film transistors (TFTs) in the AMOLED backplane to provide both sufficient current-driving capability and long-term reliability (3).

Oxide TFTs exhibit higher carrier mobility and lower leakage current than amorphous silicon (a-Si) TFTs. Among them, indium–gallium–zinc oxide (IGZO) has been successfully commercialized and is now the most widely used representative material (4; 5). However, continued improvements in display performance require exploring multicomponent oxide materials beyond IGZO (5). The key challenge is the exponential growth of the design space as elemental combinations diversify. Conventional experiment-driven approaches alone are insufficient for identifying optimal compositions (6). Accordingly, high-speed screening frameworks that combine material-descriptor calculations (bandgap, ISWO, $E_f$) with machine learning (ML), such as the work of Kim *et al.* (2022) (14), have emerged as a key methodology for accelerating next-generation materials discovery.

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However, while these approaches help reduce the composition space, they have two fundamental limitations when linking predicted material properties to TFT device performance.

First, many ML-based screening methods integrate multiple material descriptors into a single objective function. This can fail to capture intrinsic physical trade-offs among bandgap, formation energy, and electronic localization (e.g., ISWO). For example, low formation energy suggests thermodynamic stability. However, if it accompanies excessive oxygen vacancies, it can reduce the bandgap and destabilize the threshold voltage (9). Collapsing multivariate trade-offs into a single scalar objective can prematurely exclude physically plausible compositions or yield unrealistic optima. Practical composition exploration therefore requires a multi-objective optimization framework that preserves balance among multiple material descriptors while refining the design space (10).

Second, many ML frameworks stop at composition or property prediction. Even when they predict device performance, they often rely on black-box models that do not explicitly reveal the underlying physical mechanisms (7). Commercial TCAD simulations can mitigate this issue, but their high computational cost limits repeated evaluation of large candidate sets (8). Some studies directly learn correlations between composition and device performance, but they do not sufficiently provide an interpretable link describing how changes in electronic structure map to device-physics variables (device parameters), such as carrier concentration or trap density (8).

The main contributions of this paper are summarized as follows.

- **MTTB framework**: We propose a four-stage hybrid framework, *MTTB* (Materials-to-TFT Bridge). It consists of (i) **AI-based material prediction**, (ii) Pareto-based multi-objective composition search, (iii) Candidate selection stratgey, and (iv) a Physics-inference module.
- **Addressing two fundamental limitations of prior ML-based approaches**: We address two limitations of prior ML-based screening studies. First, collapsing conflicting relationships among multiple material descriptors into a single objective can distort design decisions. We mitigate this using Pareto-based multi-objective optimization and decision rules. Second, many studies do not provide an explicit link between material-level predictions and device-level performance. We address this via the PIM.
- **Actionable beyond-IGZO candidates**: We apply MTTB to an Al–Mg-centered multi-component oxide composition space. We derive IGZO-replacement compositions that globally balance trade-offs among bandgap, mobility, and stability. We also provide specific next-generation (beyond-IGZO) compositions for follow-up experimental validation.

# 2 Related work

**ML-based discovery of amorphous oxide materials** van Setten *et al.* (14) proposed a framework that combines HT-DFT with support vector regression (SVR) models. It efficiently screens the composition space of amorphous multicomponent oxides. They learned composition–property relationships from computed data for primary and binary oxides. They then generalized the models to multicomponent (multinary) systems. This enabled prediction of key metrics such as bandgap and formation energy. They also prioritized promising composition regions to reduce search cost. They further demonstrated that the framework can propose new candidates. As an IGZO replacement candidate, they suggested Zn–Mg–Al–O (ZMAO). However, the approach has limitations. It is not an end-to-end workflow from material-property prediction to device-performance validation. It does not explicitly capture trade-offs among material descriptors because it relies on single-objective optimization. It also remains limited in scalability for large-batch parallel processing over large composition spaces.

# 3 Preliminary

## 3.1 Material Descriptors

To link atomic-scale electronic structure to device performance, we define four material descriptors, $\mathbf{x} = [G_x, ISWO_C, ISWO_V, E_f]$. The bandgap $G_x$ is defined as $G_x = E_{CBM} - E_{VBM}$ and is closely related to leakage current and charge-injection barriers; a larger $G_x$ is favorable for suppressing off-state leakage and improving visible-light transmittance.

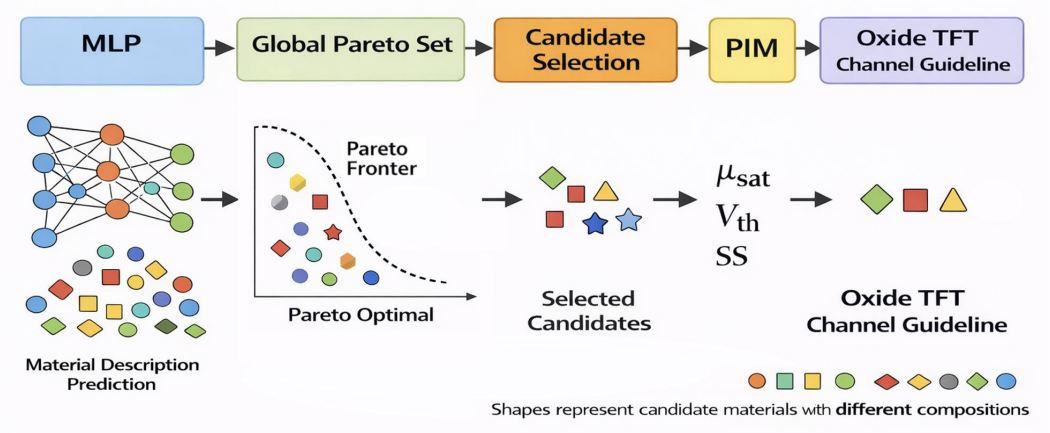



Figure 1: Overview of the MTTB framework.

Inverse Spatial Wavefunction Overlap (ISWO) is defined as the inverse of the orbital overlap integral $S$ ($ISWO \propto S^{-1}$). A smaller $ISWO_C$ indicates greater delocalization of conduction-band electron wavefunctions and thus higher electron mobility, whereas a larger $ISWO_V$ suppresses hole transport in the valence band and is favorable for n-type behavior.

The formation energy $E_f$ is defined as the total energy difference normalized by the number of oxygen atoms, $E_f = \Delta E_{tot}/N_O$, and reflects thermodynamic stability. Values lower than or comparable to IGZO indicate suppressed phase separation and reduced defect formation during processing.

To assess the de-mixing tendency of mixed amorphous oxides, we adopt the formation-energy-based stability metric $E_{\text{hull}}$ proposed by van Setten *et al.* (14). Here, $E_{\text{hull}} < 0$ indicates that the mixed state is thermodynamically more stable than separation into constituent single oxides. In this study, $E_{\text{hull}}$ is used only as a post hoc stability filter for Pareto-selected candidates.

### 3.2 TFT Performance Metrics

We summarize TFT electrical behavior using three metrics: mobility ($\mu_{sat}$), threshold voltage ($V_{th}$), and subthreshold swing ($SS$). $\mu_{sat}$ is the effective mobility extracted from the current characteristics in the saturation regime. It directly affects switching speed and on-current. $V_{th}$ is the gate voltage at which the channel forms and the drain current begins to increase substantially. It is a key parameter for low-power operation. $SS$ is the gate-voltage change required for the drain current to increase by one decade in the subthreshold regime. It is calculated as $SS = \partial V_{GS}/\partial(\log I_{DS})$.

## 4 Method

In this section, we present the MTTB framework, which integrates AI-based material property prediction, Pareto-based multi-objective screening, and physics-informed device-level inference. An overview of the framework is shown in Fig. 1.

### 4.1 AI-based Material Property Prediction

#### 4.1.1 Dataset Description

We used the amorphous oxide dataset reported in prior work (14), which comprises amorphous oxide properties computed using high-precision DFT. Amorphous structures were generated from local bonding motifs derived from unary ($X$–O) and binary ($X$–$Y$–O) crystalline structures in the Materials Project, with strictly stoichiometric compositions to exclude extrinsic n-type doping. Each unit cell contained approximately 200 atoms, and DFT calculations were performed on 10 independent amorphous configurations per composition to ensure statistical robustness. The dataset covers amorphous oxides composed of 12 metal elements (Ag, Al, Cd, Ga, In, Mg, Sb, Si, Sn, Ti, Zn, and Zr).

#### 4.1.2 MLP-based predictor

To address the limited expressiveness of the SVR model used in prior work, we adopt a two-layer multi-layer perceptron (MLP) to capture nonlinear relationships in high-dimensional composition space. The input is a normalized metal composition vector, and the model is designed for rapid inference without requiring explicit atomic-structure information.

Given the heterogeneous distributions and learning difficulties of different target properties, we trained independent MLPs for each property. The models predict four descriptors: bandgap ($E_g$), formation energy ($E_f$), $ISWO_C$, and $ISWO_V$. This design enables fast batch inference over large composition sets, significantly improving the efficiency of subsequent multi-objective screening.

### 4.2 Pareto-based Multi-objective Composition Optimization

#### 4.2.1 Rationale for Pareto Optimization in Materials Design

A weight-based single-objective function that compresses multiple properties into a single scalar can simplify the search. However, such an approach inherently fails to preserve explicit trade-offs between objectives (14). To address this, we treat each property as an independent objective and adopt a multi-objective optimization strategy to derive the Pareto-optimal set.

A Pareto-optimal set consists of solutions for which no objective can be improved without degrading at least one other. The resulting Pareto front delineates the boundary of potentially optimal candidate compositions while preserving the intrinsic trade-off structure among properties. This approach is particularly effective for materials design problems that must simultaneously consider competing requirements, such as electronic performance and stability (10; 23; 24).

#### 4.2.2 Search Space Definition and Composition Sampling

We defined the composition search space by generating all binary ($X$–$Y$–O) and ternary ($X$–$Y$–$Z$–O) oxide combinations that can be formed by selecting two or three elements from the 12-element set. Within each system, candidate compositions were generated via Dirichlet-distribution-based sampling. We used 30 compositions per ternary system and 15 compositions per binary system. To reflect practical controllability in deposition processes, we excluded trace components with an atomic fraction below 0.01% during sampling.

#### 4.2.3 Objective Function Formulation

ll objectives were formulated as minimization problems. For each candidate composition, we defined four objectives:

$$f_1 = (E_{gap} - (E_{gap,IGZO} + \Delta E_{target}))^2, \quad f_2 = ISWO_C, \quad f_3 = -ISWO_V, \quad f_4 = E_f.$$

We set $\Delta E_{target} \in \{0.0, 0.25, 0.50, 0.75, 1.00\}$. We considered $\Delta E_{target} \in \{0.0, 0.25, 0.50, 0.75, 1.00\}$. These objectives jointly capture electronic properties, carrier transport, and thermodynamic stability. The Pareto front of non-dominated solutions was then computed, enabling systematic selection of candidates that balance performance and stability beyond single-property criteria.

#### 4.2.4 Hierarchical Pareto Screening and Global Front Construction

We first computed local Pareto fronts independently for each binary and ternary composition system. System-level Pareto candidates were then aggregated across all binary systems and across all ternary systems to construct order-wise global Pareto fronts.

Next, a formation-energy-based de-mixing stability metric ($E_{hull}$) was applied to the binary and ternary Pareto candidate sets. Only compositions with no tendency toward phase separation in the mixed state ($Stability < 0$) were retained. Composition ratios were rounded to two decimal places to remove duplicates, and for identical chemical formulas, the candidate with the lowest de-mixing energy was kept. Finally, the filtered binary and ternary candidates were merged into a single set, and Pareto optimization was performed once more to obtain the final global Pareto set spanning the full composition space. From the global Pareto set (822 compositions), we formed candidate sets under three distinct criteria.

### 4.3 Candidate Selection Strategy from the Global Pareto Set

**Property-prioritized Candidate Buckets** Because industrial requirements do not reduce to a single property, we partitioned the merged global Pareto set into three candidate buckets reflecting different property priorities. The high-mobility bucket selects the top five compositions with the smallest $ISWO_C$ under target bandgap and stability constraints, whereas the high-stability bucket selects the top five compositions with the lowest formation energy $E_f$ while maintaining charge-transport properties. The balanced bucket applies a multi-criteria ranking that sequentially considers bandgap proximity, formation energy, and $ISWO_C$. This analysis serves as a supplementary tool for comparing candidate distributions under different property-driven design scenarios.

**Bandgap-conditioned Knee Point Selection** Next, for each target bandgap, we identified curvature-based knee points on the corresponding Pareto front to extract compromise candidates. Four objective functions—bandgap proximity, mobility, reliability, and formation energy—were normalized to the $[0, 1]$ range, and the sacrifice rate between adjacent candidates was computed. The knee point was defined as the candidate with the maximum sacrifice rate, characterizing locally optimal solutions for each bandgap condition.

**Global Knee-based Final Selection** Finally, in the normalized four-dimensional objective space that integrates all bandgap targets, we computed the Euclidean distance to the utopia point $(0, 0, 0, 0)$. We define the 20 compositions with the smallest global distances as the global-knee set. These candidates are considered to provide the most effective global compromise among bandgap, mobility, and stability. In this study, we propose the global-knee set as the primary target for subsequent device-physics simulations and experimental validation.

### 4.4 Physics-Inference Module (PIM)

We propose a Physics-Inference Module (PIM) that estimates device-level TCAD inputs and TFT electrical metrics from AI-predicted DFT material descriptors. Key features of the PIM include:

- **Relative anchor**: IGZO DFT predictions are used as a reference, and the target composition is interpreted through relative deviations, constraining inferred parameters to physically plausible ranges.
- **Physics-grounded linkage**: DFT descriptors are mapped to device parameters and subsequently to $I$–$V_g$ characteristics to extract $\mu_{sat}$, $V_{th}$, and $SS$.
- **Computational efficiency**: The physics-based mapping bypasses iterative TCAD simulations, enabling rapid evaluation of large candidate sets.

Specifically, based on semiconductor physics, the bandgap $G_x$ is mapped to a variable related to the intrinsic carrier concentration (16). The relative change in $ISWO_C$ is used as a proxy for changes in electron transport and mobility. Deviations in $ISWO_V$ and $E_f$ are converted into parameters that reflect changes in the distribution of defect/trap states. These parameters are reflected in the trap density and threshold-voltage variation. The estimated physical variables are then fed into an exponential model in the subthreshold regime and a gradual-channel-approximation model in strong inversion. This generates TFT transfer characteristics ($I$–$V_g$) (16; 17). Finally, we apply a parameter-extraction algorithm to the generated $I$–$V_g$ to extract $\mu_{sat}$, $V_{th}$, and $SS$ (22). Implementation details are provided in our released code.

**Scope and limitations of the PIM.** The PIM serves as a physics-informed surrogate for device-level evaluation, rather than a replacement for full TCAD simulations. Its mappings are based on simplified, relative, and IGZO-anchored relationships, and therefore do not capture detailed electrostatics, spatial defect distributions, or process-dependent variations. Accordingly, the PIM is intended for efficient comparative screening and trend analysis, while final quantitative validation requires rigorous TCAD or experimental verification.

## 5 Experiment

In this section, we evaluate the proposed framework by addressing the following research questions:
**RQ1.** Does the model accurately generalize across diverse oxide compositions?

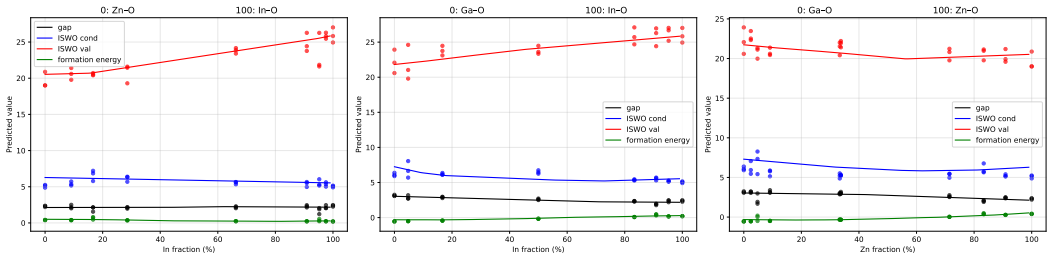



Figure 2: Validation of physical trends.Solid lines and scatter points denote MLP predictions and DFT calculations, respectively, for the In-Ga-Zn-O system.

Table 1: Comparison of property prediction performance across models.

| Target ($y$) | Gaussian | | | van Setten *et al.* (14) | | | Ours | | |
|---|---|---|---|---|---|---|---|---|---|
| | MAE | Corr | $R^2$ | MAE | Corr | $R^2$ | MAE | Corr | $R^2$ |
| $G_x$ | 0.216 | **0.962** | -0.214 | 0.256 | 0.369 | -0.594 | **0.186** | 0.379 | **-0.037** |
| $E_f$ | 0.944 | 0.351 | -16.326 | **0.019** | **0.995** | **0.986** | 0.026 | 0.994 | 0.976 |
| $ISWO_V$ | 2.599 | -0.143 | -14.712 | 1.160 | -0.134 | -2.295 | **1.132** | **0.462** | **0.183** |
| $ISWO_C$ | 1.130 | 0.455 | **0.201** | 1.184 | **0.457** | 0.056 | **0.966** | 0.137 | -0.969 |
| Avg. | 1.222 | 0.406 | -7.763 | 0.654 | 0.422 | -0.461 | **0.577** | **0.493** | **0.038** |

**RQ2.** How do optimal oxide systems shift across varying bandgap requirements?

**RQ3.** How can Pareto-optimal candidates be categorized for device requirements?

**RQ4.** What is the ultimate material archetype for high-performance oxide semiconductors?

**RQ5.** How robust is the Al–Mg archetype against composition variations?

**RQ6.** Do AI-designed oxide TFT channels deliver gains under TCAD validation?

### 5.1 Experimental Settings

The framework was implemented in Python 3.12 (18) using PyTorch 2.9 (19) and executed on Google Colab (20) with an NVIDIA T4 GPU (21). PIM-based TCAD-equivalent analyses (Section 4.4) were performed under the following device and operating conditions. All evaluations were conducted at room temperature ($T \approx 300\,\mathrm{K}$), consistent with standard oxide TFT characterization protocols (4; 5; 3). The channel geometry was set to $W = 50\,\mu\mathrm{m}$ and $L = 10\,\mu\mathrm{m}$, with a gate insulator thickness of $t_{ox} = 20\,\mathrm{nm}$. The relative permittivity of the gate insulator was fixed at $\varepsilon_{r,ox} = 10$, and the oxide capacitance was calculated using the standard MOS expression, $C_{ox} = \varepsilon_{r,ox}\varepsilon_0/t_{ox}$ (16; 17). The implementation of the proposed MTTB framework is available at `https://anonymous.4open.science/r/MTTB-228F/`.

### 5.2 Generalization Performance of the Prediction Model

We evaluated the model's generalization performance using quantitative metrics (Table 1) and physical consistency. On the unseen Mg–Zn–Al oxide dataset, the proposed model achieved the lowest error among the compared methods (mean MAE = 0.577) and attained positive values for $ISWO_V$ and the overall mean $R^2$, where prior models failed. This demonstrates reliable prediction performance for complex multicomponent systems. In a composition sweep of the In–Ga–Zn (IGZO) system (Fig. 2), the model accurately reproduced key physical trends: $ISWO_C$ improved with increasing In content, while the bandgap ($E_g$) widened with increasing Ga content. Smooth interpolation in data-sparse regions indicates that the model stably captures the underlying physical landscape shaped by inter-element correlations, supporting its qualitative reliability for multicomponent composition exploration.

Table 2: Summary of dominant systems and predicted property ranges by target $\Delta E_g$.

| Target $\Delta E_g$ (eV) | Representative Element | $E_g$ (eV) | $ISWO_C$ | Stability |
|---|---|---|---|---|
| 0.00 | `Ag, Zr, Ti` | 0.14–0.56 | 16.5–18.4 | $\approx -3.0$ |
| 0.25 | `Mg, Ti, Al` | 2.75–2.81 | 29.8–31.2 | $\approx -2.8$ |
| 0.50 | `Zr, Cd, In, Sn` | 2.96–3.03 | 21.1–24.5 | $\approx -3.4$ |
| 0.75 | `Al, Ga, Zn, Zr` | 3.26–3.30 | 17.1–21.3 | -1.8–2.8 |
| 1.00 | `Al, Mg, Sb` | 3.43–3.68 | 8.0–9.3 | $\approx -2.1$ |

Table 3: Statistical summary of material properties by performance bucket.

| Bucket | $\Delta E_g$ (eV) | | $ISWO_C$ | | $E_f$ | | Stability | |
|---|---|---|---|---|---|---|---|---|
| | Mean | Std | Mean | Std | Mean | Std | Mean | Std |
| `balanced` | 3.02 | 0.36 | 18.80 | 8.67 | -2.41 | 1.09 | -0.39 | 0.23 |
| `high_mobility` | 2.90 | 0.44 | 6.17 | 0.73 | -0.77 | 0.51 | -0.34 | 0.24 |
| `high_stability` | 3.03 | 0.28 | 27.88 | 1.81 | -3.99 | 0.19 | -0.24 | 0.10 |

### 5.3 System Transitions Across Bandgap Regimes

We identify distinct system transitions in which dominant elemental combinations shift abruptly at specific thresholds (Table 2).

**Low-bandgap regime ($\Delta E_g \approx 0.0$ eV).** Ag–Zr-based systems dominate, maintaining high conductivity while leveraging Zr to ensure minimal amorphous-structure stability.

**Intermediate transition regime ($\Delta E_g = 0.25$–$0.75$ eV).** Ag-based systems vanish near $\Delta E_g \approx 0.25$ eV, and the optimum shifts to Mg–Ti systems, reflecting a trade-off in which mobility ($ISWO_C$) is partially sacrificed to secure a wider bandgap via lightweight-metal-based stabilization. At higher targets, a Zr-based backbone re-emerges, combined with elements such as In, Sn, and Ga to restore the mobility–stability balance and maximize design flexibility.

**High-bandgap regime ($\Delta E_g \approx 1.0$ eV).** The strategy converges to an Al–Mg backbone, with strong gap openers such as Sb, signaling entry into a property regime suitable for dielectric or barrier layers beyond semiconductor channels.

### 5.4 Device-requirement-driven Candidate Categorization

To recommend optimal compositions aligned with user design objectives within the Pareto solution set, we analyzed candidates in three performance-oriented buckets (Table 3).

**High Mobility**: Dominated by the In–Ga–Zn family, this bucket maximizes $s$-orbital overlap and achieves the lowest $ISWO_C$ ($\approx 6.17$), at the cost of reduced bandgap and higher formation energy.

**High Stability**: Strong bonding driven primarily by Zr (63%) and Ti (23%) yields the lowest formation energy ($\approx -3.99$ eV). However, the increased ionicity limits conduction-band overlap, resulting in suppressed mobility.

**Balanced**: All property metrics converge to intermediate values. This regime reflects a cooperative design strategy, with Zr contributing stability, In/Ga/Zn enhancing transport, and Al/Mg enabling bandgap tuning.

### 5.5 Emergence of an Al–Mg Archetype in Global Pareto Optima

We analyzed the 20 global optima (Global Knee) obtained by integrating all bandgap targets. As shown in Fig. 4a, unlike bucket-based candidates biased toward either mobility or stability, the Global Knee candidates cluster at the optimal compromise between these properties, occupying a region with markedly lower formation energy and superior $ISWO_C$ relative to the IGZO baseline.

Notably, all 20 global optima emerge at the maximum bandgap requirement, $\Delta E_g = 1.0$ eV (i.e., $E_g \approx$ IGZO $+ 1.0$ eV; Fig. 3), indicating that high-bandgap conditions impose strong physical constraints to maintain charge transport and structural stability. These extreme constraints act as a physical filter that drives the Pareto knee to converge to a specific composition region.

Table 4: Statistical summary of Global Knee candidates ($n = 20$).

(a) System distribution and property ranges.

| System | Count | $\Delta E_{gap}$ | $ISWO_C$ | Stability |
|---|---|---|---|---|
| (Al, Mg) | 5 | 3.80–4.27 | 9.01–10.19 | $-2.64$–$-2.25$ |
| (Al, In, Mg) | 4 | 3.59–4.03 | 8.47–9.57 | $-2.52$–$-2.24$ |
| (Al, Ga, Mg) | 3 | 3.83–4.10 | 9.10–9.76 | $-2.53$–$-2.28$ |
| (Al, Mg, Si) | 3 | 3.82–4.04 | 9.03–9.45 | $-2.39$–$-2.26$ |
| (Al, Mg, Zr) | 2 | 3.79–3.83 | 9.50–12.86 | $-2.69$–$-2.29$ |

(b) Elemental composition statistics.

| Element | Mean | Std |
|---|---|---|
| Al | 0.5285 | 0.1254 |
| Mg | 0.4420 | 0.1204 |
| In | 0.0080 | 0.0217 |
| Zr | 0.0075 | 0.0217 |
| Si | 0.0075 | 0.0185 |

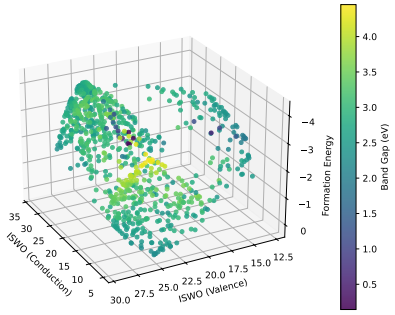



Figure 3: 3D global Pareto sets across all bandgap targets.

Consistently, the Global Knee systems share a common Al–Mg backbone (Table 4a), with Al and Mg accounting for approximately 97% of the total composition (Table 4b), suggesting convergence to a near-binary Al–Mg oxide archetype under the most stringent property requirements.

### 5.6 Composition Robustness of the Al–Mg Oxide Archetype

From the composition distributions of the global-knee optimal systems, we observe a flat region when the Al fraction exceeds 0.55, where material properties remain nearly invariant despite changes in the Mg:X ratio (Fig. 5). This indicates that the third element functions as a dopant, fine-tuning target properties without perturbing the underlying backbone.

As a result, the global optimum converges to a variable dopant configuration on a robust Al–Mg backbone. Higher Al content further suppresses sensitivity to composition variations, providing a practical materials design guideline for achieving high yield in large-area AMOLED manufacturing.

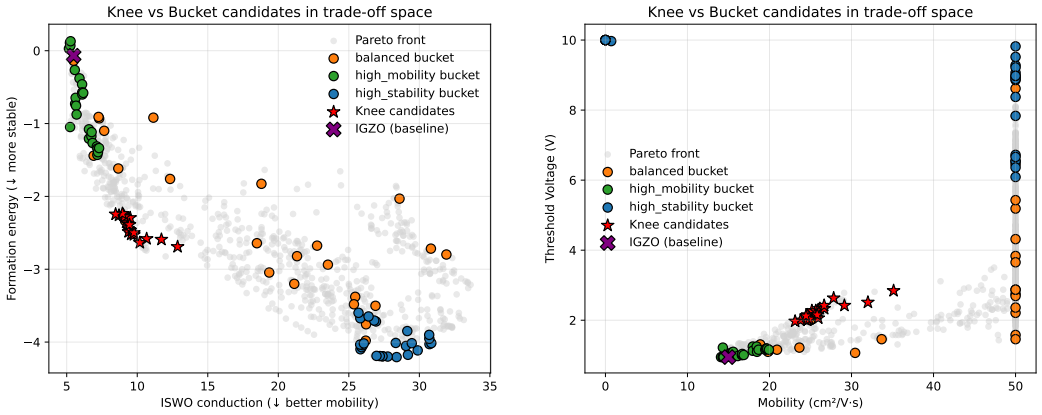
### 5.7 Device-level Validation of AI-designed Oxide TFT Channels

We performed PIM-based TCAD simulations to evaluate the practical utility of the AI-proposed compositions (Fig. 4b).

**IGZO baseline validation**: For commercial IGZO ($In_{50}Ga_{50}Zn_{50}$), we obtained $V_{th} = 0.95$ V and $\mu = 15.0$ cm$^2$/V $\cdot$ s. These values are consistent with typical experimental reports, supporting the reliability of the simulation setup.

**Device performance of Global Knee candidates**: The 20 global-optimal candidates showed strong statistical advantages over IGZO across all metrics. We obtained approximately 76% higher mobility ($\mu_{avg} \approx 26.4$) and excellent switching behavior ($SS_{avg} \approx 128.6$ mV/dec).

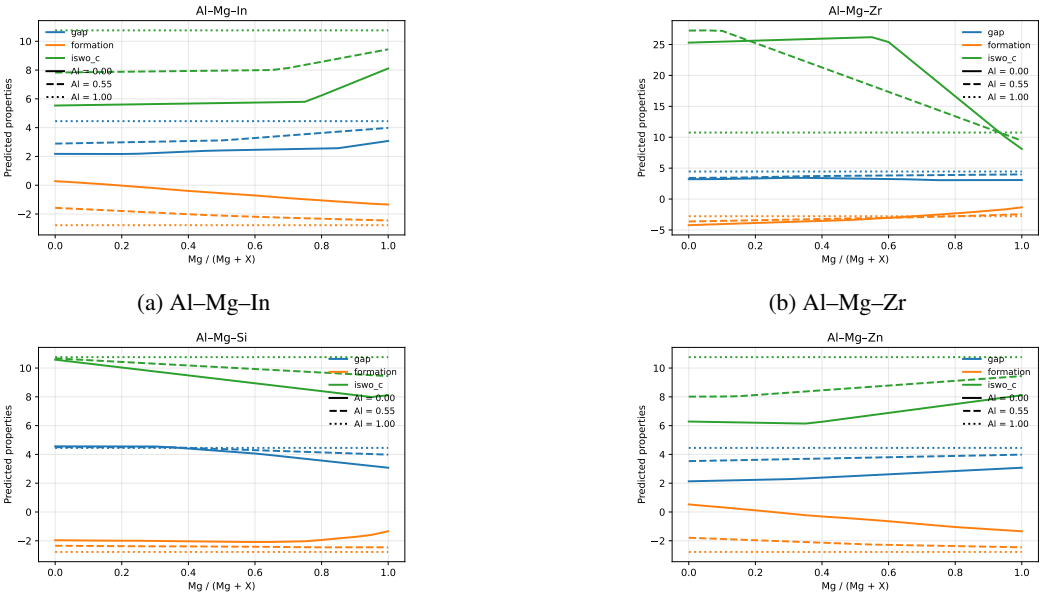
**Process reproducibility**: The threshold voltage is densely distributed within the operating window ($V_{th} = 2.26 \pm 0.23$ V), indicating high uniformity for large-area processing.




(a) $E_f$–$ISWO_C$ trade-off.

(b) TCAD performance validation.

Figure 4: Global distribution and performance of Pareto results.




(a) Al–Mg–In

(b) Al–Mg–Zr

(c) Al–Mg–Si

(d) Al–Mg–Zn

Figure 5: Fine-tuning effects of ternary elements (In, Zr, Si, Zn).

# 6 Conclusion

This study addresses the challenge of identifying oxide TFT channel materials that can replace IGZO to meet the high-performance and high-reliability demands of next-generation AMOLED backplanes. We propose the *MTTB* framework, which integrates composition-based property prediction, Pareto-based multi-objective screening, and TCAD-level device-performance inference via the Physics-Inference Module (PIM). Under stringent requirements such as a high bandgap, the design space is shown to converge to an Al–Mg binary archetype. We further demonstrate that Al–Mg–X systems exhibit low sensitivity to composition variations while enabling dopant-based fine-tuning, providing robust oxide TFT channel design guidelines for large-area AMOLED manufacturing. These systems also indicate improved device-performance potential compared with conventional IGZO.

The proposed framework supports physically consistent decision-making from material candidate discovery to device-performance validation and can be extended to incorporate process variables and device-stack-level co-design.

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# A Appendix / supplemental material

Optionally include supplemental material (complete proofs, additional experiments and plots) in appendix. All such materials **SHOULD be included in the main submission.**

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