

MOF-based memristors for in-sensor computing: Materials, devices, and integration

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Based on the in-sensor computing strategy, integrating sensing and computing in memristors offers a promising solution to the limitations (excessive power consumption, high latency, poor compatibility) of traditional "sensing-computing separation" sensory recognition systems. However, mainstream memristive materials like metal oxides lack reliable multimodal sensing and information fusion capabilities, hindering their effectiveness. Honored by the 2025 Nobel Prize in Chemistry for their customizable structure and function, metal-organic frameworks (MOFs) uniquely address this by unifying multimodal sensing and on-site memristive computing. This perspective adopts a "materials-device-integration" framework to elaborate MOFs' foundational role, reveal cross-scale mechanism bottlenecks (e.g., material instability, device crosstalk, integration incompatibility) and targeted solutions (e.g., ligand engineering, frequency-dependent operation, technology optimization), and outline future directions (e.g., bio-integrated systems, adaptive edge networks, AI-driven MOF design). It highlights MOFs' potential to overcome traditional limitations and advance "material-centric computing" for next-generation intelligent systems.

INTRODUCTION

For decades, traditional computing and sensing systems have adhered to a "sensing-computing separation" paradigm, where raw sensor data is transmitted to dedicated processing units. This architecture suffers from inherent drawbacks: high power consumption, large latency, security risks, and poor compatibility between organic sensors and silicon processors. Such incompatibility arises from mechanical and integration mismatches: flexible, low-modulus organic sensors induce interface stress and high contact resistance with rigid silicon chips, hindering reliable monolithic integration. All drawbacks mentioned above have become increasingly severe in the IoT and AI eras,¹ driving the development of in-sensor computing that integrates perception and processing into a single hardware platform to minimize redundant data movement.²

Memristors, with a typically metal-insulator-metal (MIM) sandwich structure, rely on resistive switching (RS) mechanisms including charge trapping and ion migration. By rationally designing the resistive layer and optimizing switching dynamics, memristors can leverage their nonlinear electrical characteristics to simultaneously realize sensory information perception and processing, thereby enabling in-sensor computing.

The evolution of sensing-computing systems has primarily passed through 4 key milestones: First stage: before 2000, a traditional von Neumann architecture-based sensing-computing separation architecture, with centralized processing as the main approach; Second stage: from 2001 to 2015, the initial collaboration between sensing and computing, and the nascent development of distributed edge preprocessing; Third stage: the deep integration of sensing and computing, and the popularization of distributed edge computing; Fourth stage: since 2021, integrated sensing and computing, with the implementation of neuromorphic computing. Therefore, the memristor with the ability of in-sensor computing that emerges in the third stage will shine brightly in the fourth stage. The inherent characteristics and performance of RS materials are crucial for simultaneously achieving sensing and computing functions. However, conventional materials such as metal oxides still suffer from poor structural designability, stochastic RS behavior, and limited multimodal sensing-computing integration. For instance, in the aspect of multimodal perception, oxide-based photo-memristors can process opti-

cal signals but cannot detect gases, while hybrid discrete systems introduce extra interfaces that increase power loss and degrade reliability. Ideal in-sensor computing materials should simultaneously support sensitive responsiveness (e.g., analyte adsorption, photoresponse) and programmable electrical properties (e.g., synaptic plasticity), with good fabrication compatibility.³

Metal-organic frameworks (MOFs), recognized by the 2025 Nobel Prize in Chemistry, uniquely satisfy these demands. As porous crystalline materials formed by metal nodes and organic linkers, MOFs exhibit exceptional structural/functional tunability: pore sizes can be tailored for specific analytes, ligand modification enables customized sensing, and high surface areas provide abundant adsorption sites.^{4,5} Moreover, their intrinsic memristive behavior (driven by ion migration or charge trapping) enables on-site data processing. Unlike metal oxides, MOFs integrate multimodal sensing and computing in one material, addressing the "multifunctionality gap" plaguing current solutions.⁶

This perspective adopts a "materials-device-integration" framework to explore MOF-based memristors for in-sensor computing. It details MOFs' multimodal sensing and memristive computing capabilities, summarizes device optimization advances, analyzes cross-scale challenges (synthesis to integration), and proposes targeted solutions. Distinct from traditional reviews, this perspective systematically reveals MOFs' "mechanism bottlenecks" and provides synergistic solutions—offering a clear roadmap to translate these Nobel-recognized materials into practical in-sensor computing systems.

MOF: MULTIFUNCTIONAL FOUNDATIONS FOR IN-SENSOR COMPUTING

MOFs meet in-sensor computing's multifunctional demands via unique, customizable structural and functional properties—distinct from conventional materials—manifested in pore structure, functional groups, and fabrication technology.

Based on ligand design, MOF pore sizes can be precisely tuned from sub-nanometer to 50 nm.⁷ For instance, the IRMOF series achieves continuous aperture adjustment (e.g., 7.5 Å in MOF-5 to 15.4 Å in IRMOF-10) via organic linker extension, enabling size-based discrimination of dye molecules through molecular sieving. Other typical MOFs also enable efficient sensing-computing integration: ZIFs provide stable porous frameworks for gas sensing and low-power memristive systems; UiO series exhibit excellent stability with tunable conductivity through defect engineering; HKUST-1 offers high surface area and active sites for analyte adsorption and synaptic modulation. Additionally, 2D MOFs with layered structures favor fast charge transport for high-performance devices. These features establish a "structure-tunability-function-customization" paradigm. Moreover, the high specific surface area of MOFs acts as a buffer layer to reduce interfacial thermal/mechanical stress, showing superior stability over brittle metal oxides during complementary metal-oxide-semiconductor (CMOS) processing.⁸

Ligand modification introduces functional groups that link sensing, memory, and processing: azobenzene-functionalized MOFs act as optical transducers via light-triggered isomerization; sulfonic acid-modified MOFs enable proton-conductive, pH-responsive ion-based memristors. MOFs also reduce interface complexity in multi-component systems by integrating sensing, synaptic memory, and signal amplification in a single stack. Tunable pore structures enhance sensing selectivity and reliability (especially for ion migration-based memristors); tailored functional groups boost sensitivity for specialized needs; optimized fabrication technologies narrow the gap with

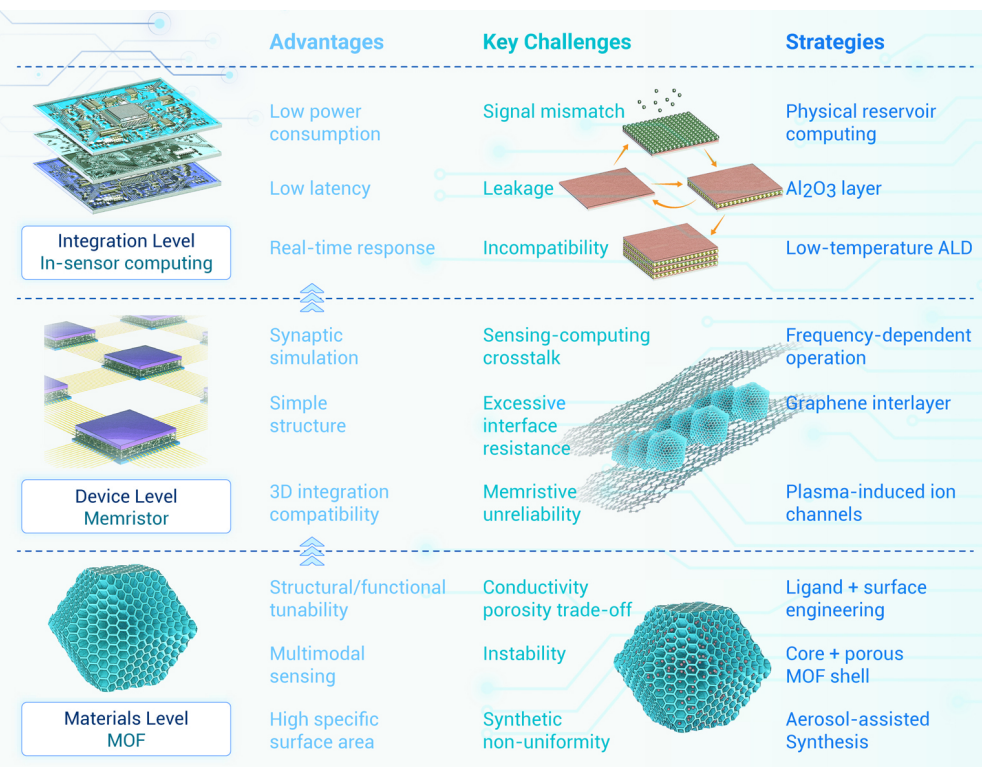


Figure 1. Illustration of the advantages, challenges, and strategies of MOFs for applications in in-sensor computing systems from the perspectives of materials, devices, and integrations.

disrupt timing. Ion diffusion between adjacent memristors raises leakage currents and degrades signal transmission accuracy. Moreover, MOF sensing/computing operates at millisecond scales, far slower than CMOS nanosecond operation, creating latency penalties that offset the advantages of in-sensor computing.

These challenges form a "mechanism bottleneck": material instability undermines device reliability, device inefficiencies reduce data accuracy, and integration mismatches prevent scaling. Addressing them requires cross-disciplinary solutions grounded in understanding MOFs' unique transport and structural mechanisms.

ADDRESSING CROSS-SCALE CHALLENGES: MATERIALS TO INTEGRATION

To resolve these challenges, targeted solutions across materials, devices, and integration are required—all leveraging MOFs' intrinsic

CMOS processes. Together, these features position MOFs as emerging foundational materials for heterogeneous in-sensor computing.

CRITICAL CHALLENGES: FROM MATERIALS TO INTEGRATION

Translating MOF-based memristors into practical in-sensor computing systems is hindered by interconnected challenges across materials, devices, and integration.

Material level

Intrinsic tradeoffs compromise reliability and further restrict device and system performance, with three core issues: environmental instability, conductivity-porosity tradeoffs, and synthetic non-uniformity. MOFs' coordination-bonded crystalline frameworks are vulnerable to humid or aqueous conditions. For instance, common Co-based MOFs suffer structural collapse under high humidity, as water molecules displace organic linkers and destroy ion migration pathways vital for memristive behavior. Intrinsically insulating MOFs require conductive dopants, yet high loading blocks sensing pores while low loading fails to form continuous transport channels, raising operating voltages. Uncontrolled nucleation in synthesis also causes inconsistent crystal size and defect density, leading to unstable memristive performance that limits array-scale integration.

Device level

Three critical issues persist: sensing-computing crosstalk, excessive interface resistance, and memristive unreliability behavior. Crosstalk arises as analyte adsorption modifies MOF electronic/structural properties and disturbs RS process. For example, gas molecules adsorbed at defect sites slow ion migration and induce errors in synaptic weight updates. Schottky barriers formed at MOF-electrode interfaces raise resistance due to surface dipoles, increasing power consumption and degrading signal quality. Random ion transport pathways in porous MOF networks also cause uneven ion hopping, resulting in asymmetric synaptic plasticity and reduced neural network accuracy.

Integration level

Three urgent challenges remain: CMOS incompatibility, uncontrolled leakage currents, and signal mismatch. MOF synthesis conditions often damage CMOS components (e.g., etching interconnects or degrading dielectrics), while even low-temperature processes may react with passivation layers and

features to address the mechanism roots of the "bottlenecks".

Materials-level solutions

To tackle environmental instability, ligand engineering and surface modification create a hydrophobic protective layer (e.g., long alkyl chain-functionalized ZIF-8 reduces water adsorption, preserving pore structure and sensing capability at high humidity). For the conductivity-porosity tradeoff, core-shell architectures decouple conductive pathways from porous sensing regions: a conductive core (e.g., polypyrrole nanowires) provides continuous electron transport for memristive switching, while a thin MOF shell preserves porosity for analyte adsorption.⁹ Aerosol-assisted synthesis controls nucleation *via* microdroplet confinement, reducing crystal size variation to <10% for batch consistency.

Device-level solutions

Frequency-dependent operation mitigates sensing-computing crosstalk: mid-high-frequency pulses (> 1 kHz) for computing (short duration << 1 ms minimizes ion migration interference) and < 10 Hz sampling for sensing (sufficient time for analyte adsorption), with time division preventing signal interference. Notably, trap and defect effects remain non-negligible in this mid-high-frequency regime and are addressed via targeted strategies (e.g. MOF ligand functionalization and interface passivation). Graphene interlayers match metal electrode work functions (e.g., Au), reducing Schottky barrier height from ~0.5 to ~0.1 eV, cutting power consumption threefold and enhancing signal-to-noise ratio. Defect engineering (e.g., Ar plasma treatment of UiO-66) creates directional ion channels by introducing linear oxygen vacancy chains, reducing ion hopping distance variation by 60%, and improving synaptic long-term potentiation/long-term depression symmetry.

Integration-level solutions

Low-temperature atomic layer deposition (ALD) with non-reactive precursors (e.g., Zr(OtBu)₄ instead of ZrCl₄) ensures CMOS compatibility, avoiding corrosion of Cu interconnects and reaction with SiO₂ passivation layers, yielding MOF-CMOS hybrids with > 90% manufacturing yield. Thin ion-blocking layers (e.g., dense Al₂O₃) between memristor cells suppress ion diffusion, reducing leakage currents from > 1 μA to < 100 nA per device (meeting wearable power limits < 500 μW). Physical reservoir computing addresses the MOF/CMOS temporal mismatch by using nonlinear ion-transport dynamics within the MOF porous framework: ions undergo field-driven capture-release

cycles to form a dynamic physical reservoir, which nonlinearly maps slow millisecond-scale sensing signals into fast 10 μ s spikes. This time-compression mechanism directly matches the nanosecond operation speed of CMOS, eliminating buffering delays.¹⁰

Collectively, these solutions form a hierarchical framework: material engineering stabilizes MOFs and optimizes functional balance; device design eliminates transport inefficiencies; integration co-design bridges MOFs with hardware. A fully integrated wearable system, combining humidity-stable MOFs, low-resistance graphene interfaces, and CMOS-compatible ALD-validates this framework, enabling continuous environmental and physiological monitoring. MOFs' tunability thus overcomes traditional sensing-computing separation limitations.

CONCLUSION AND OUTLOOK

To date, cross-scale challenges in developing high-performance MOF-based memristors for sensing-computing integration have been initially resolved: material-level advances (ligand engineering, core-shell designs) resolve stability and conductivity-porosity tradeoffs; device innovations (frequency-dependent operation, defect-engineered ion channels) match oxide-based memristors performance; integration solutions (low-temperature ALD, ion-blocking layers) enable CMOS and flexible platforms compatibility. These advances confirm MOFs as enablers of a new in-sensor computing paradigm, unifying multimodal perception and *in-situ* processing in a single material system.

Looking forward, three transformative directions emerge: bio-integrated systems, adaptive edge networks, and cross-scale sensing-computing fusion. Bio-integrated MOF memristors could integrate with neural interfaces to create closed-loop implantable systems, leveraging MOFs' biocompatibility (e.g., low cytotoxicity of HKUST-1) and tunable pores to target specific neurotransmitters (e.g., dopamine), enabling real time sensing and local modulation of neural activity. Adaptive edge nodes based on MOF composites could act as distributed "intelligent filters" in smart cities: they process environmental data (gas, temperature, light) in real time, use memristive synaptic plasticity to identify critical events (e.g., pollution hotspots), and transmit only actionable insights to the cloud, reducing power use by more than half compared to silicon-based edge nodes. Cross-scale fusion, merging MOFs with quantum technologies, could unlock unprecedented sensing precision: MOFs' porous frameworks can host quantum dots or single-atom catalysts to enhance single-molecule detection, while their memristive behavior interfaces with quantum processors for hybrid classical-quantum in-sensor tasks (e.g., ultra-weak magnetic field monitoring).

AI-driven MOF design accelerates these visions: generative AI models trained on structure-property datasets create custom ligand-metal combinations *via* target parameters. For real-time volatile organic compounds (VOC) sensing-computing, specifying ≈ 0.5 nm pores, photo-responsive groups, and CMOS-compatible metal nodes yields a "Zr⁴⁺-azobenzene-modified terephthalic acid" MOF-Zr⁴⁺ ensures stability/CMOS compatibility, azobenzene enables light-triggered computing, and 0.5 nm pores match VOC sizes-shortening the R&D cycle from 2-3 years to 3-6 months.¹¹ Addressing remaining challenges (e.g., long-term biological fluid stability, large-scale array unifor-

mity) requires interdisciplinary collaboration.

In computing evolution, MOF-based memristors offer a promising pathway to advance "material-centric computing"—an emerging paradigm where intrinsic material properties, alongside circuit design, define core capabilities. MOFs' revolutionary tunability redefines functional material design; promising a more efficient, intelligent future where sensing and computing unify in materials' molecular fabric.

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AUTHOR CONTRIBUTIONS

All authors contributed to and approved the manuscript.

DECLARATION OF INTERESTS

The authors declare no competing interests.