Towards Universal E-nose: Powering Chemical Sensing with Multimodal Sensing and Artificial Intelligence

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Abstract

Universal electronic nose (e-nose) is a type of advanced sensor that can analyze gases and provide odor descriptions in a manner akin to human olfaction. It is the ultimate goal of gas sensor research, but a challenge that is currently difficult to overcome. Here, we explore potential methods that could achieve this goal. We first introduce the current state of e-nose technology, including the electronic approach based on semiconductor materials, colorimetric approach based on color change of gas-sensitive colorants, and the biological approach based on biological macromolecules. Given the limitations of current technologies, we propose the key technologies needed to realize a universal e-nose. These encompass the development of multidimensional datasets, standardized processes for gas-sensitive material development, and the creation of complete and robust nose-on-chip systems. We also discuss the fundamental scientific research that may drive the development of these technologies, including cross-dimensional computational chemistry, non-equilibrium simulations of proteins, and large language models for label processing. Furthermore, we emphasize the importance of establishing unified standards for high-quality datasets. These perspectives will provide guidance for developing the next generation of gas sensing systems, as well as sensors and databases related.

Introduction

The five senses of humans include vision, hearing, touch, taste, and smell. Mimicking these senses acts as the basic motivation for sensor design[1]. Among these, visual sensors (cameras) and auditory sensors (microphones) have been extensively developed, significantly extending human sensory capabilities. Tactile sensors (force sensors) are also rapidly developing and have demonstrated superior performance in many scenarios[2–4]. Compared to others, the development of olfactory and gustatory sensors proves to be more challenging. The challenges faced by these two types of sensors are similar, as they both involve identifying chemical compounds or characterizing features of complex chemical mixtures in certain media (water or air). Gas sensors are harder to generate selectivity due to the weaker surface interaction[5,6], introducing additional difficulties in the development of e-noses.

Ray Bradbury, in his novel "Fahrenheit 451," describes an electronic hound with a powerful e-nose, capable of detecting even more scents than a real dog. Even 70 years later, such technology remains as remote to us as it is in science fiction. We need to rely on large-footprint instruments such as Gas Chromatography-Mass Spectrometry (GC-MS) to achieve accurate identification of the components in a gaseous mixture. Current portable e-noses' abilities of recognition of gas characteristics are limited to simple classifications included in the training set, such as air quality[7] and food freshness[8], unable to perform detailed analyses or extrapolations beyond the trained categories. This implies that the sensors and the underlying recognition algorithms can only learn the patterns present in the current scenario, rather than the intrinsic characteristics of the gases themselves.

The greatest challenge in current research stems from the complexity of chemical molecular information. Visual sensing fundamentally involves the detection of electromagnetic waves, while acoustic sensors merely need to detect vibrations in the air. In contrast to these two, gas sensing does not have a single, definitive physical quantity to target for detection. The olfactory system of mammals is based on the shape matching between olfactory receptors and gas molecules[9]. This recognition mechanism, combined with the hundreds of distinct olfactory receptors in mammals, ensures that biological olfactory systems maintain good specificity while also being able to produce consistent responses to previously unencountered gases. However, the fine-tuning of material structures, akin to olfactory receptors, significantly surpasses the current technical capabilities of material science. Currently, gas sensors for e-nose applications primarily operate based on redox reactions between gases and sensing materials (metal oxide sensors[10], electrochemical sensors[11]), or the selective adsorption of gas molecules on the sensor surface (Field Effect Transistor sensors[12]). The amount of information generated by these detection mechanisms is significantly less than that produced by biological olfactory systems. Due to the differences in sensing mechanisms, the information obtained from these detection methods cannot align with biological olfaction, making it difficult to accurately assess the characteristics of odors. Also, some studies attempt to create gas sensors based on olfactory receptors[13], engineered cells[14], or living organs[15]. Despite their superior selectivity, these biologically based sensors are costly, challenging to maintain, difficult to produce outside of a laboratory environment, and nearly impossible to fine-tune for customization, limiting their practical value for applications beyond the lab.

Universal e-nose is conceptualized as an advanced type of e-nose that is capable of consistently and accurately detecting and identifying a wide range of odorants, akin to the broad detection range of the human nose (Figure 1). This device would ideally have the capability to generalize across a wide spectrum of volatile organic compounds, providing a comprehensive analysis of an odor's profile, even if it is a new olfactory stimulus that has never been met before[16]. Recording smells in the same manner as using a handheld camera or sound recorder is the ultimate dream of researchers, although still appears to be far from reach. However, at the very least, we understand where the challenges lie.

In this perspective, we begin with the current state of e-nose technology and discuss the potential pathways toward achieving a universal e-nose. To align the readings of an e-nose with human sensory perceptions necessitates the coordinated development of sensor materials and artificial intelligence (AI) perception technologies. We discuss methods for expanding data dimensions, including the use of multisensory arrays, multivariable, multiparameter sensors, and virtual sensor arrays. We also discuss the challenges and potential approaches in standardizing the design of gas-sensitive materials. For sensors based on olfactory receptors, we explore potential methods to achieve robust receptor-based sensors, from receptor design to the engineering of interfaces. Finally, recognizing that the underlying technologies supporting a universal e-nose have not fully matured yet, we also discuss foundational scientific research that may present opportunities for advancements in this field.

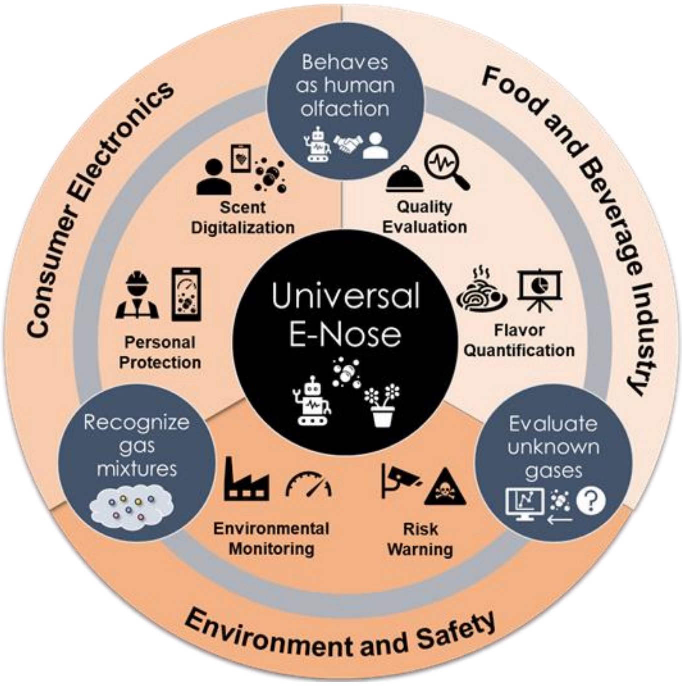

Figure 1| The basic concept of universal e-nose: a universal e-nose should be able to analyze gas mixtures, even if it contains some component outside of the training data, and output odor description in a similar way as human olfaction. Universal e-nose would have widespread applications, including but not limited to food science, environment, and consumer electronics markets.

1. Current Approaches to E-nose

1.1. Electronic Approach

In the electronic approach, sensor signals are generated on the surface of sensing electrodes. The types of sensors suitable for universal e-noses are relatively limited, typically utilizing redox reactions to achieve selectivity for gases. Based on the different initiation methods of redox reactions, sensors can be further divided into two categories: metal oxide gas sensors and electrochemical gas sensors.

Metal oxide (MOX) gas sensors are devices that detect gases through changes in the electrical conductivity of a metal oxide film (usually heated). When the sensor's surface, typically composed of transition metal oxide[17] like tin dioxide, titanium oxide or zinc oxide, is exposed to certain gases, the interaction between the target gas molecules and the adsorbed oxygen on the sensor's surface alters the concentration of charge carriers within the metal oxide. This change in carrier concentration affects the sensor's electrical resistance, which is measured and correlated to the gas concentration (Figure 2A). These sensors are widely appreciated for their sensitivity and relative low cost. Due to the varying properties of MOX sensors made from different materials, a common approach is to assemble an array of sensors made of different MOX materials. Since the sensors in the array exhibit differentiated responses to targets, functions such as gas identification[18] and health monitoring[19] can be achieved through machine learning or statistical methods.

Electrochemical gas sensors typically consist of a sensing electrode, a counter electrode, and a reference electrode, all immersed in an electrolyte solution (Figure 2B). When a target gas diffuses into the electrolyte, it undergoes either oxidation or reduction at the sensing electrode, generating a current proportional to its concentration. Measuring relative to the reference electrode, it can provide a quantitative analysis of the gas presence. The advantage of electrochemical gas sensors is that their output contains more information from different testing methods and the corresponding current-voltage features. Voltammetry is the most commonly used electrochemical sensing method, where a potential is applied to an electrode and the resulting current is recorded. During the measurement, the potential is swept across a range, either linearly in linear sweep voltammetry or cyclically in cyclic voltammetry, while the current response of the electroactive species in solution is monitored. The resulting plot of current versus potential provides valuable information about the electrochemical processes occurring on the electrode. This type of data exhibits greater tolerance to noise, and through machine learning algorithms such as Support Vector Machines (SVMs)[20] and Random Forests[21], both qualitative and quantitative detection of gases can be achieved. Electrochemical gas sensors' selectivity can also be achieved through the choice of electrode materials and the potential applied across the electrodes. The electrode material is chosen for its ability to catalyze the redox reaction of the specific target gas while minimizing reactions with other substances[22]. By controlling the potential, it is possible to set an electrochemical window within which only the desired gas is oxidized or reduced, while other gases remain electrochemically inactive.

Unfortunately, all gas sensors based on redox reactions inevitably encounter issues of cross-sensitivity. Cross-sensitivity refers to a sensor's similar responses to different gases, where the sensor cannot distinctly identify individual gases due to overlapping selectivity. Actually, the redox capacity is a general indicator of chemical reactivity rather than a specific marker for the molecular shape, which is more directly related to the perception of odors. Since the shape of a molecule determines how it fits into olfactory receptors, creating artificial sensors that can discern this shape is a complex challenge that goes beyond simple redox reactions. This disconnect means that while redox-based sensors can detect the presence of certain gases, they are less adept at differentiating complex odor profiles that would be readily distinguishable by biological olfactory systems.

1.2.Colorimetric Approach

Colorimetric approach utilizes color changes of chemically responsive colorants as they are exposed to gases[23], including pH responsive dyes, Lewis acid/base indicators, redox dyes, vapochromics, and surface-modified silver nanoparticles. These colorimetric sensors are often combined with optical sensors to digitally read out color changes. Colorimetric sensors have advantages in pattern recognition applications, as there is good orthogonality between different coloration mechanisms. Under the same mechanism, colorants with different properties can be designed, or the sensitivity of the color reaction can be altered by methods such as activation or passivation[24]. This type of sensor has already seen numerous applications in fields such as food safety (Figure 2D)[25], explosives detection (Figure 2C)[26], and medical diagnostics[27].

The potential drawback of colorimetric e-noses lies in their reusability. Due to the irreversibility of chemical reactions, most colorimetric sensors can only undergo color change once. This limitation hinders their application in long-term continues monitoring. For short time application scenarios like medical diagnostics, the development of low-cost disposable sensors can overcome the issue of limited reusability in colorimetric sensors. These disposable sensors can provide an effective solution for single-use applications, where the need for repeated use is not a primary concern. Balancing the stability, selectivity, and storage conditions of different chromogenic agents remains a significant challenge in the design of colorimetric e-noses. Designers need to ensure that these agents are stable enough to be stored and used effectively over time, while also maintaining their ability to selectively react to specific gases or odors. This requires careful consideration of chemical properties and environmental factors that could affect the performance of the chromogenic agents.

1.3.Biological Approach

To bridge the gap between the readings from e-noses and the perception of biological olfaction, a clever approach is to directly utilize biomolecules related to olfaction as the sensing materials. Including Olfactory Receptor (OR)[13], Odorant Binding Proteins (OBP)[28] and peptides[29]. Olfactory receptors are the molecular basis of mammalian olfaction. Olfactory receptors are a class of transmembrane proteins distributed on the cell membranes of olfactory-related cells[30]. Upon binding with odor molecules, olfactory receptors undergo a change in shape. This conformational shift leads to a change in the cell membrane potential, which triggers downstream signaling pathways. When exposed to a mixture of gases, a multitude of different olfactory receptors produce varied responses, collectively forming an olfactory map that the brain uses to identify odors[31]. When such receptor proteins are modified on the surface of a semiconductor (typically a carbon-based field-effect semiconductor), the binding of the receptor to odor molecules alters the distance between the surface charges of the receptor and the semiconductor surface, affecting the carrier density of the semiconductor and thereby inducing a change in resistance. The potential of this method lies in its ability to measure odors in the same manner as the biological olfactory system. The challenge lies in the fact that olfactory receptors are transmembrane proteins with a hydrophobic, lipid-soluble region in their structure. This means they cannot stably exist in aqueous environments and cannot be expressed using conventional bioengineering methods[32]. To modify wild-type receptors on the surface of sensors, artificial cell membranes (Figure 2E)[33–35] or living cells (Figure 2G)[14,36,37] need to be used as carriers, which severely limits the development and application of such sensors. There are protein engineering techniques that can modify the sequence of olfactory receptors to make them water-soluble[38,39]. Apart from the issue of the universality of these techniques, the function of the receptor binding region is thought to be related to cell membrane tension[40], and it is still unclear whether simply modifying water solubility will affect the receptor's function. In addition, the specific correlations between odors and olfactory receptors, that is, the detailed olfactory map, are not yet clear. The challenges in expressing and purifying receptor proteins further complicate the investigation into their functionality.

Olfactory receptors are not the only biomolecules that can be utilized for e-noses. Odorant Binding Proteins (OBPs) are small, soluble proteins that are secreted into the mucus of the nasal epithelium in vertebrates. They play an essential role in the olfactory system by transporting volatile odor molecules through the aqueous mucus layer to olfactory receptors, which are located on the cilia of olfactory sensory neurons[41]. Due to their solubility in water, OBPs can be readily modified on sensor surfaces, enabling highly sensitive gas sensing[42]. However, while OBPs function as universal carrier proteins, their specificity and diversity fall significantly short in comparison to olfactory receptors, which constrains their potential utility in e-nose applications. Utilizing peptide-modified sensors represents an alternative compromise solution. Based on wild-type receptor proteins, a peptide sequence can be designed to mimic the receptor's binding region while possessing improved stability and solubility in water (Figure 2F)[43,44]. However, there is currently no widely accepted method for designing receptor-like peptides, and the functional similarity between synthetic peptides and natural receptors remains questionable.

In summary, the common issue faced by the biological approach is that the biological olfactory system is a delicate and complex system that requires the close cooperation of multiple elements and artificial devices are far from achieving this level of complexity. Odor generation of neural signals requires a multi-tiered structure that includes mucus, odorant binding proteins, receptors, and the cell membrane. These structures support each other and together constitute the complete olfactory function. Even attempting to construct such a system in terms of its structure would result in an unacceptable engineering difficulty, and a simplified design that incorporates only some of the elements would not be able to capture the performance benefits of the biological approach.

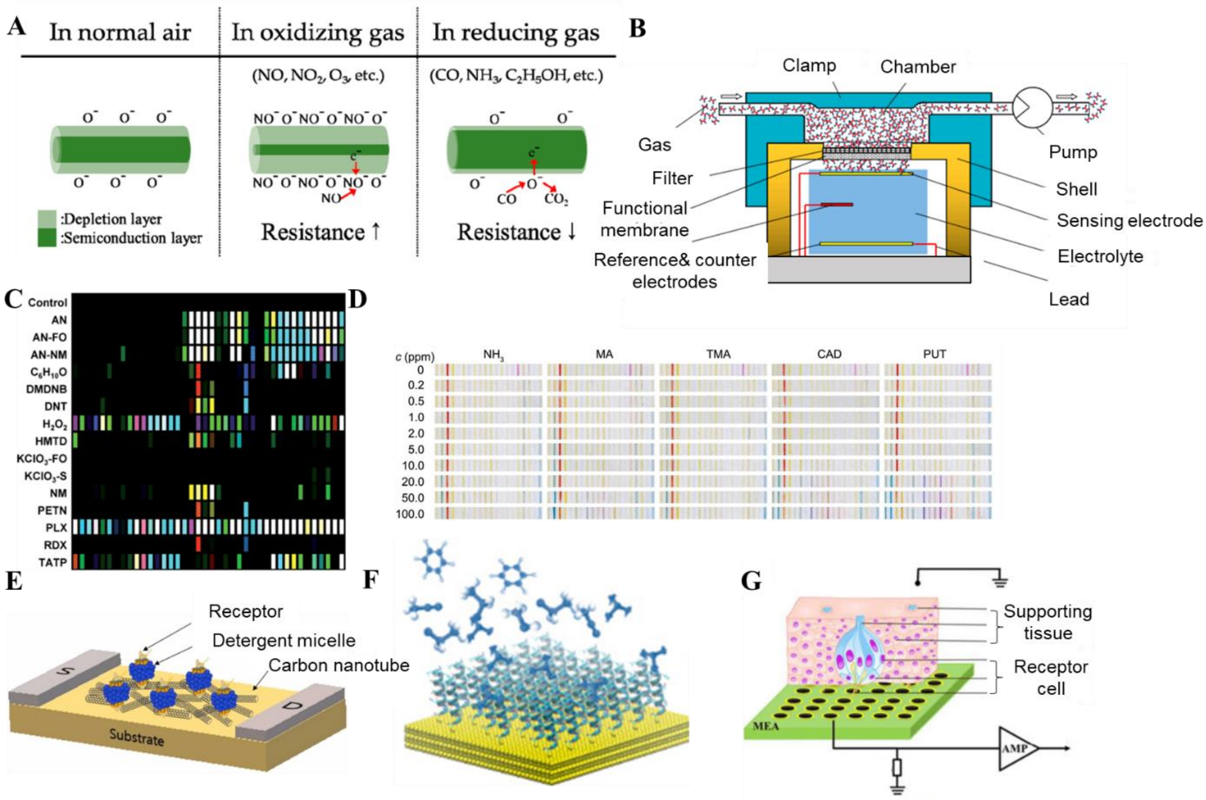

Figure 2| Current approaches to e-nose: Electronic approach (A, B), colorimetric approach (C, D) and biological approach (E-G). **A**, MOX sensor, reproduced under terms of the CC-BY license.[45] Copyright ©2015, The authors. Sensor resistance changes differently when exposed to different types of gases,. **B**, Structure and working way of electrochemical sensor, reproduced under terms of the CC-BY license.[46]Copyright ©2016, The authors.. **C**, Colorimetric sensor to detect explosives, Reproduced under terms of the CC-BY license.[26] copyright ©2019, The authors. Color combinations represent different chemicals. **D**, Colorimetric sensor for meat freshness monitoring indicating amines[25] copyright© 2020 Wiley-VCH GmbH. **E**, Gas sensor functionalized by olfactory receptor stabilized by detergent micelles, reproduced with permission[33], copyright © 2021 Elsevier B.V. **F**, Gas sensor functionalized by peptides. Peptides are modified on secondary transducers to generate signals, reproduced under terms of the CC-BY license[47]. Copyright ©2022, The authors. **G**, Gas sensor based on living cells expressing olfactory receptor. Changes in cell membrane potential are read out as signals, reproduced under terms of the CC-BY license[48]. Copyright ©2017, The authors.

2. Step Forward to Next-Generation E-nose

Current gas sensing solutions, whether based on electronic, colorimetric, or biological principles, still fall short of the performance of a universal e-nose. To identify multiple components or unfamiliar gases, a universal e-nose needs the capability to locate and navigate within the odor space. Given the complexity of the odor space, the e-nose is required to have an equal or higher data dimensionality. Therefore, the primary challenge on the path to a universal e-nose is to increase the data dimensionality of sensors, which includes the integration of multi-parametric and multimodal sensor data. In order to expand data dimension, it is also necessary to develop a more diverse range of sensors, which means creating various types of sensing materials. This requires the development of standardized material design methods to avoid the inefficiency of development based on experience. On this basis, it is also necessary to develop an artificial biological olfactory system in a laboratory environment to advance the alignment between e-nose data and human perception.

2.1.Expanding Data Dimension to Explore Odor Space

Although current e-nose technologies cannot perceive scents as living organisms do, progresses have been made in the research of predicting the olfactory characteristics of given molecules. One of the most notable recent studies in olfactory digitization is the measurement of the principal odor map[49]. Based on a dataset annotated by human volunteers that records gaseous molecules and their corresponding odor labels, the researchers implemented a graph neural network to achieve predictions of odor descriptions based on molecular structure. Compared with previous methods based on chemical descriptors, graph neural networks not only have better accuracy but also can provide relatively accurate predictions for new molecules[50]. This indicates that the model successfully encoded a generalized map of structure-odor relationships. This advancement presents an opportunity for e-nose research as it significantly reduces the dependency on human volunteers when investigating the relationship between e-nose readings and odor descriptions. Taking into account the capabilities of understanding and digitalizing nature language exhibited by large language models like Generative Pre-trained Transformer (GPT)(for example, to categorize 'raspberry flavor' and 'dark fruit flavor' as similar descriptions), we are witnessing the opportunity towards universal e-nose.

One of the most exciting prospects for a universal e-nose is the creation of an end-to-end AI model that can take readings from gas sensors and output a natural language description of the odors. AI is indeed adept at overcoming noise in data to learn underlying patterns. However, to achieve this, a sufficiently large and high-quality dataset is necessary. Particularly when we are uncertain which data are truly important, the dimensionality of the dataset should be as large as possible. This approach allows for the inclusion of a wide range of potentially relevant variables, offering a comprehensive set of features for the model to identify and learn from the underlying patterns that may be predictive of the phenomena of interest. Although sensor arrays have become a standard approach in e-nose research, these arrays often comprise only different variants of the same class of sensors[29,51,52]. In fact, beyond the properties of the gases themselves, the readings from gas sensors can be affected by multiple factors, including humidity[53,54], temperature[55,56], and even light exposure[57]. Therefore, to explore the olfactory space, the dataset to be established should not only include data from a variety of gas sensors with different types and mechanisms, but should also encompass data from other modalities such as temperature and humidity sensors, light sensors, etc. Performing such complex sampling on a large number of gases would take a considerable amount of time, but if the rate-determining step, human labeling of odors, could be replaced by AI, then it would be feasible to improve efficiency through scaled-up parallel sampling, much like Google's arm farm. Of course, this would necessitate close collaboration among academia, industry, and funding agency.

Based on a high-quality dataset, feature extraction and dimensionality expansion can be performed. This process is vital for enhancing the e-nose's ability to interpret complex odor data by translating raw sensor signals into a more interpretable and analyzable format. This often involves algorithms and techniques that can effectively reduce noise, extract relevant features, and expand the feature space to improve the e-nose's predictive performance and robustness, including Principal Component Analysis (PCA)[58], Independent Component Analysis (ICA)[59], t-Distributed Stochastic Neighbor Embedding (t-SNE)[60] or Generative Adversarial Networks (GANs)[61]. Through these processes, the model can learn which features are truly important, allowing for the final e-nose device to retain only the corresponding sensors that are relevant to target task, selected from a high-dimensional dataset.

2.2.Standardized Design Process for Gas-sensing Materials

To further the horizons of e-nose technology, tailoring the gas-sensitive materials to create more comprehensive datasets is pivotal. Gas sensors' diversity sets the bounds for the scope of detectable odorant features. Predominantly, the selectivity of these sensors relies on the characteristics of the gas-sensitive materials they incorporate. Current paradigm of material design often leans on labor-intensive experiments. While some techniques to tweak material properties exists—encompassing morphological engineering[62], chemical doping[63], and surface functionalization[64]—their application is largely experience-dependent. Outcomes are typically gauged in hindsight and post-fabrication, limiting our capacity to preemptively tailor materials for specific sensing roles.

The exigency of crafting gas-sensitive materials on a case-by-case basis poses significant demands in terms of resources and economic investment. Instituting a standardized methodology for gas-sensitive material design is essential for the progression of e-nose development. Crafting these materials involves intricate processes that require fine-tuning of multiple parameters and balancing several objectives concurrently. It would require the model to make comprehensive decision in extremely complex state space. Another similar scenario facing such challenge is drug design[65], which can give us some inspiration about how to model this problem. Although cannot replace human scientists yet, the integration of AI and machine learning into the design cycle is showing potential of transcending the traditional trial-and-error approach[66]. In the example of pharmaceuticals, AI-assisted frameworks have demonstrated their prowess in rationalizing the design process, predicting interactions, and streamlining the development of new compounds.

Leveraging similar AI-driven models in the development of gas-sensitive materials could dramatically enhance the predictability of material performance, leading to a more systematic exploration of the gas-sensing feature space[67,68]. A robust designing process should include the following structures (Figure 3): sensing material database as the foundation, multi-objective optimization and virtual screening algorism to design and select materials, and standardized testing method to evaluate it. Firstly, an open-source database for sensing materials, adhering to common standards, is required. This will provide a foundational data set for the development of subsequent algorithms. The design of new materials involves multi-objective optimization, implying that models need to balance between multiple, potentially conflicting properties. Predicting these coupled properties is a focal point in the design of related models. Some models are already capable of designing entirely new inorganic materials[69] or biomolecules[70], and can even be synthesized using fully automated methods[71]. However, the universality of these models still needs further development. Virtual screening can further enhance the efficiency of the design process. Independent computational methods, such as density functional theory or molecular dynamics simulations, can be utilized to cross-validate the designed sensor materials, thereby enhancing the reliability of the results. Finally, standardized testing methods need to be developed to validate the performance of the designed materials. It should include modular testing sets and standard model gases, to evaluate different materials under a common set of standards. The standardized design protocol for gas-sensitive materials is not only an academic endeavor but also a gateway to innovative industrial applications, enabling the e-nose to detect a broader spectrum of odors with greater precision and reliability.

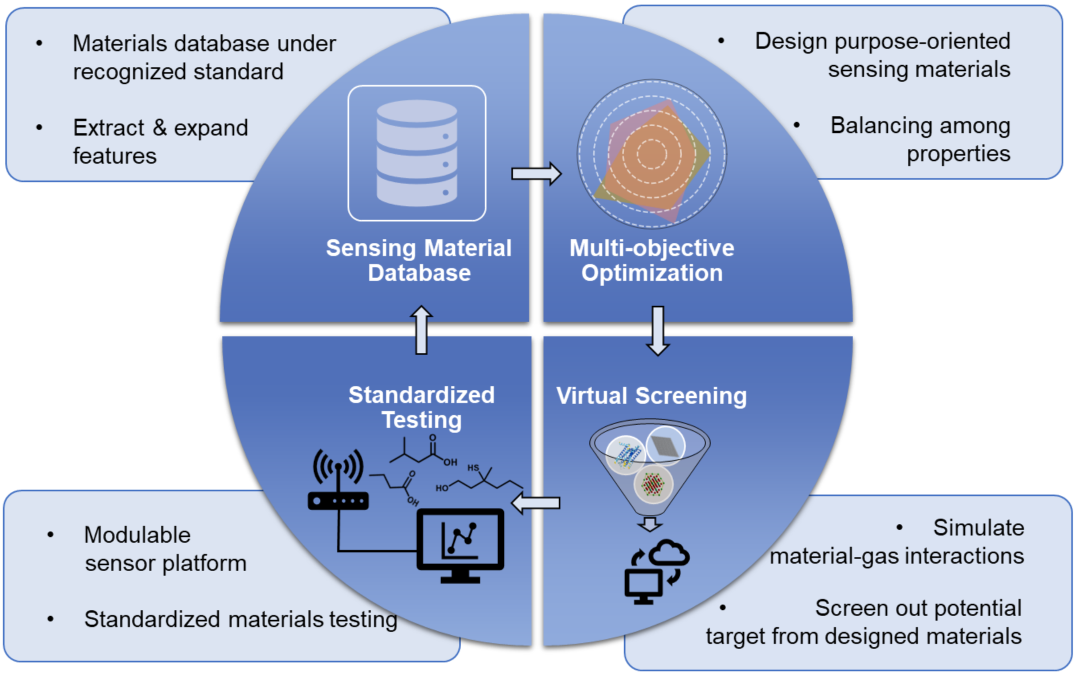

Figure 3| The workflow for standardized material design proceeds from the bottom up as follows: 1) Database and feature engineering, 2) Multi-objective optimization in material design, predicting various properties of the target materials and making reasonable optimizations, 3) Virtual screening based on computational chemistry to select candidate materials from the design results, 4) Standardized testing using modular gas sensors to evaluate the gas-sensitive materials.

2.3.Robust Artificial Bio-olfactory System

In the realm of odor sensing technology, electronic and biological approaches are not divergent paths operating in isolation, but rather parallel pipelines that mutually promotes each other. Biological e-noses based on receptors face significant limitations in terms of usability and lifespan. However, they inherently possess a natural advantage in aligning their readings with human perception. Although unable to replace conventional e-noses, biological e-noses still hold potential in niche areas such as medical diagnostics and fragrance evaluation. More importantly, a well-developed 'nose-on-chip' can aid in aligning the data from e-noses with human sensory perception and in quantifying the response patterns of olfactory receptors to gases, thereby advancing our understanding of mammalian olfaction[72].

The design of a nose-on-chip is not targeted at a single device; simulating the behavior of the olfactory system in a laboratory setting requires a comprehensive system design (Figure 4)[73], including sensing surfaces modified with various receptors, a liquid layer containing OBPs, and microfluidic devices to maintain the state of the liquid layer[74]. If the receptors themselves are not modified through protein engineering, an artificial phospholipid bilayer may be needed as a carrier. Since the actual structures of most olfactory receptors remain unclear, the prediction of protein structures[75] and the computation of receptor-ligand interactions (traditional[76] or AI[77] methods) would assist researchers in selecting appropriate receptors for the nose-on-chip.

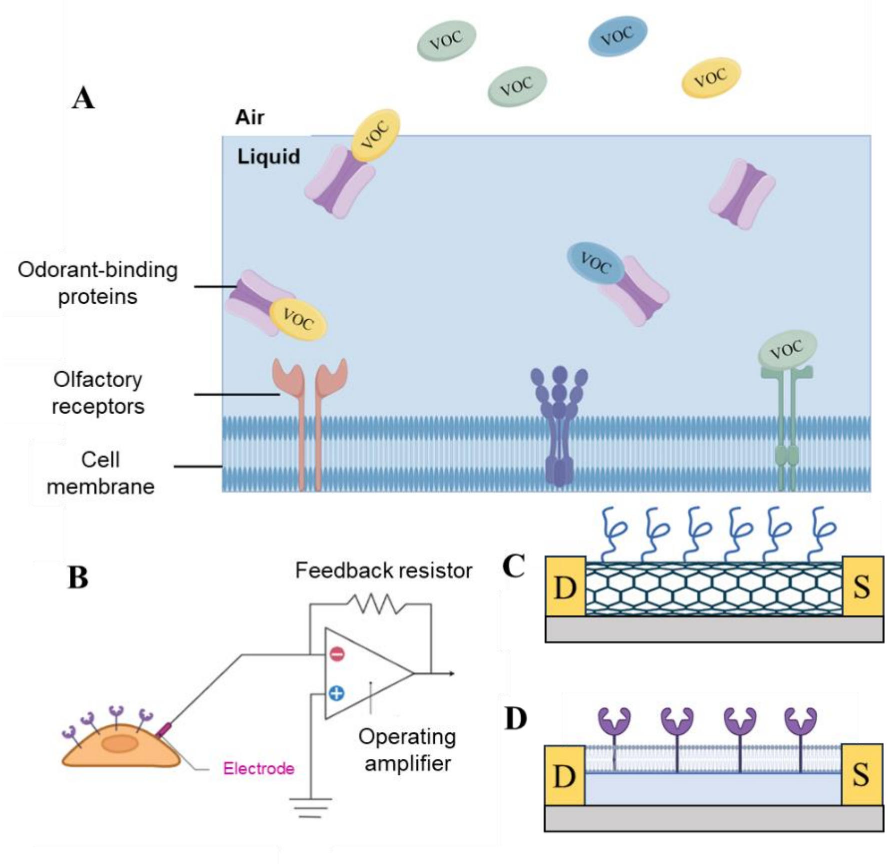

Figure 4| A: The complex structure of the mammalian olfactory system, including a variety of olfactory receptors on the cell membrane and OBPs that transport gas molecules within the liquid layer on the mucous membrane. Current biological gas sensing approach (B-D) cannot mimic this complex structure yet. VOC, volatile organic compounds. By Figdraw. **B**: Sensor based on living cells expressing olfactory receptors. By Biorender. **C**: Sensor based on peptides from receptors. By Biorender. **D**: Sensor based on olfactory receptors, supported by artificial lipid bilayer. By Biorender.

3. Fundamental Research That May Bring Opportunities

We have already discussed the potential pathways towards a universal e-nose. However, the development of engineering projects relies on the support of fundamental research, and breakthroughs in basic research can also bring new opportunities to engineering. The research on universal e-noses could benefit from advancements in material and computational sciences, including multi-scale computational chemistry, dynamic structural biology, and large language models tailored for scientific applications.

The design and selection of gas-sensitive materials require simulation of the interactions between the materials and gas molecules. With varying scales of simulation, different computational methods are applied. These include Density Functional Theory (DFT) for computing atomic-level interactions[78], molecular dynamics simulations for mesoscale interactions[79], and statistical mechanics for macroscopic interactions[80]. Each of these methods has its specific scale of applicability, encountering issues of inapplicability or inaccuracies when applied outside their optimal scales. However, the scenarios faced by gas-sensitive materials are multi-component and multi-scale challenges, requiring consideration of both the behavior of gas molecules on the material surface and the statistical behavior of a large number of molecules. Therefore, multi-scale computational chemistry simulations are extremely important, and they represent a focal point of research in this field (Figure 5)[81].

The 2013 Nobel Prize in Chemistry was awarded to scientists dedicated to the development of multiscale models for complex chemical systems. However, despite these achievements, numerous challenges and unresolved questions remain within this domain. One of the greatest challenges in multi-scale computational chemistry is effectively integrating these different scales into a coherent model. This integration requires not only advanced computational techniques but also a deep understanding of statistical physics and quantum mechanics. Successfully combining these scales can lead to breakthroughs in material design, offering new possibilities for more sensitive and selective gas detection.

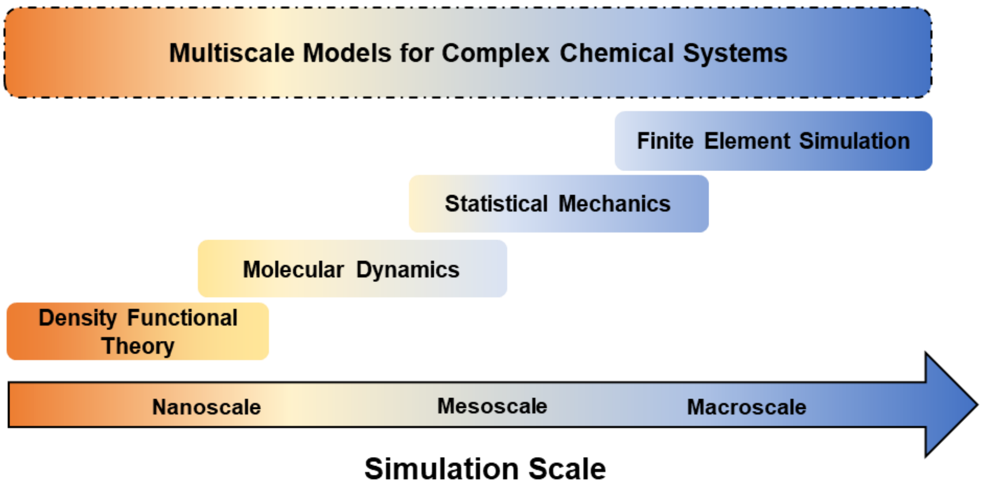

Figure 5| Computational chemistry at different scales requires the application of diverse methods[82] . To build up a universal model covering all scales presents a significant challenge.

For biological methods, the selection of olfactory receptors heavily relies on computational biology. At present, there are a number of methods for computing receptor-ligand interactions, collectively known as molecular docking[83]. However, these methods are not entirely suitable for calculating olfactory receptors. Their primary application scenarios involve drug interactions, where the binding between the ligand and receptor is often quite tight, resembling a key-lock situation in a stable state structure. For olfactory receptors, however, there is often no single ligand-receptor relationship (Figure 6)[84]. A single molecule can bind to multiple receptors, and a receptor can bind to various molecules. This multiplicity and the differences in signal strength among these many-to-many interactions are crucial components of the odor map[85]. Methods in dynamic structural biology[86] will play a vital role in olfactory research, addressing the dynamic and transient interactions characteristic of the olfactory system, which necessitates our algorithms to accurately capture the fine features of receptor conformational changes.

The objective of computing non-stationary, temporal conformations of proteins poses a significant challenge to traditional computational biology. This is primarily due to the extensive computational resources required to accurately model these dynamic structures. Such computations demand not only sophisticated algorithms but also substantial processing power, reflecting the complexity and fluid nature of protein conformations over time. The rapidly evolving field of AI-driven computational biology offers new avenues of hope in addressing these challenges. AlphaFold has achieved remarkable success in predicting the structures of protein complexes[87], showcasing the potential of machine learning in deciphering complex biological puzzles. However, to enable AI to effectively comprehend the complex states of non-stationary proteins, there is a critical need for more high-quality datasets, which may include high-resolution data obtained from cryo-electron microscopy, stopped-flow spectroscopy, and other transient observation techniques.

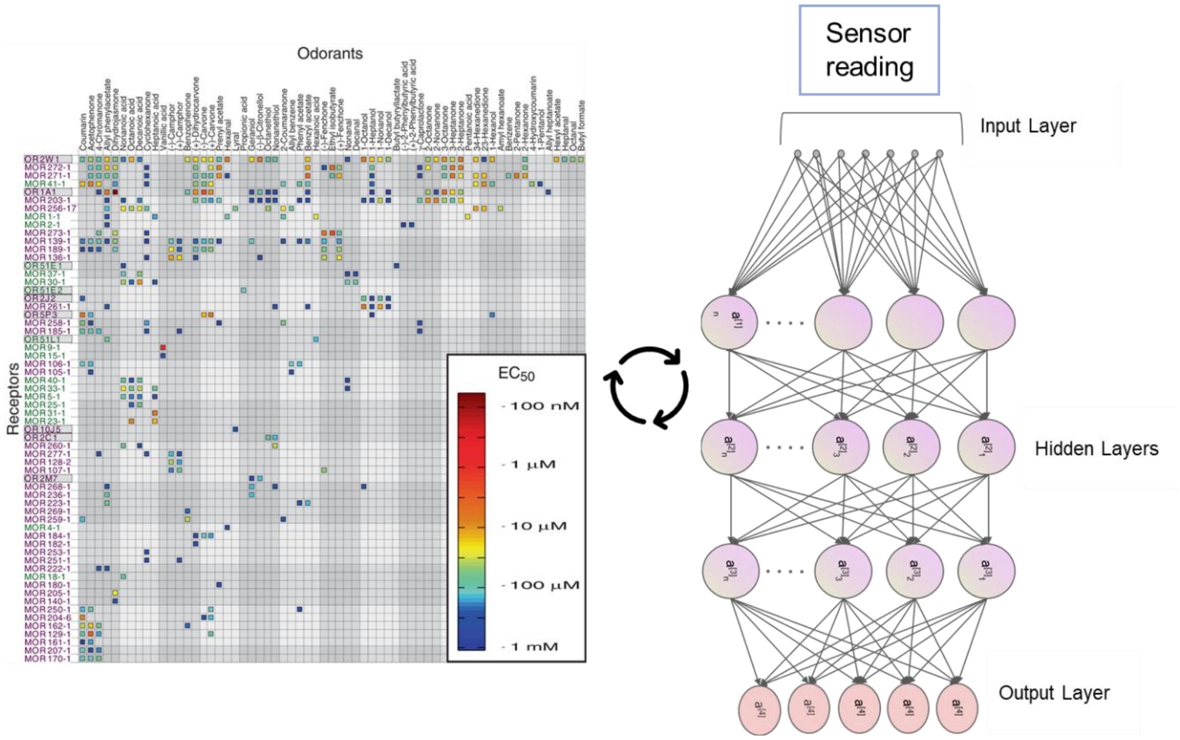

Figure 6 | The response patterns of olfactory receptors to odor molecules form the basis of mammalian olfaction, reproduced with permission.[31] Copyright © 2009, American Association for the Advancement of Science. Correlating such response patterns with artificial sensor reading is an important pursuit in artificial olfactory systems.

Finally, another challenge in olfactory research lies in the subjectivity of olfactory perception. For the same scent, different volunteers may provide varying descriptions based on their own experiences, particularly for more complex mixed odors. For instance, in the case of a certain wine, descriptions like 'blackcurrant' or 'blueberry' may refer to the same characteristic. To explore the complex space of odors, we require natural language processing (NLP) methods capable of digitizing these subjective labels[88]. Recent advancements in natural language processing, particularly through large language models, offer promising solutions[89]. These models can process and analyze vast amounts of descriptive data, helping to identify common patterns in how scents are perceived and described. Moreover, coupling these language models with sensor data from e-noses could enable a more nuanced interpretation of scents, closely mirroring human perception.

4. Conclusion

In this perspective, we focus on the future approach to universal e-nose, a kind of device that can analyze gas capable as human olfactory. We first reviewed current approaches, including electronic, colorimetric, and biological methods. Based on different sensing mechanisms, these approaches can perform specific sensing tasks but fail in universal olfactory recognition. We propose that the key point of developing universal e-nose is to generate high dimensional data from sensors, in order to fit the complex chemical space of odors. The fundament of this is standardized designing of sensing materials, supporting the diversity and orthogonality of gas sensors. Also, the robust biological nose-on-chip system is essential to establish alignment between sensor reading and mammal olfaction. Based on the challenges we proposed, we encourage researchers to focus on some fundamental research that may bring opportunities to this field. Related topics include multiscale simulation for complex chemical systems, dynamic structural biology computing for non-stationary receptor conformations, and new language models to digitalize nature language description of odors.

The path towards a universal e-nose is undoubtedly one intelligent integration. Just as with all AI-for-science endeavors, its development is fundamentally driven by data. The collective efforts in this domain should pivot around the meticulous construction and augmentation of datasets. It involves both enriching data dimensions and formulating unified data standards. These standards are imperative to boost the interoperability and reusability of data sourced from varied origins. The ambition of achieving these goals surpasses the capacities of individual researchers or singular institutions, but mandates a synergistic collaboration between academic, industry stakeholders and funding agencies.

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((**For Reviews and Perspectives,** please insert author biographies and photographs here for those authors who should be highlighted, max. 100 words each))

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