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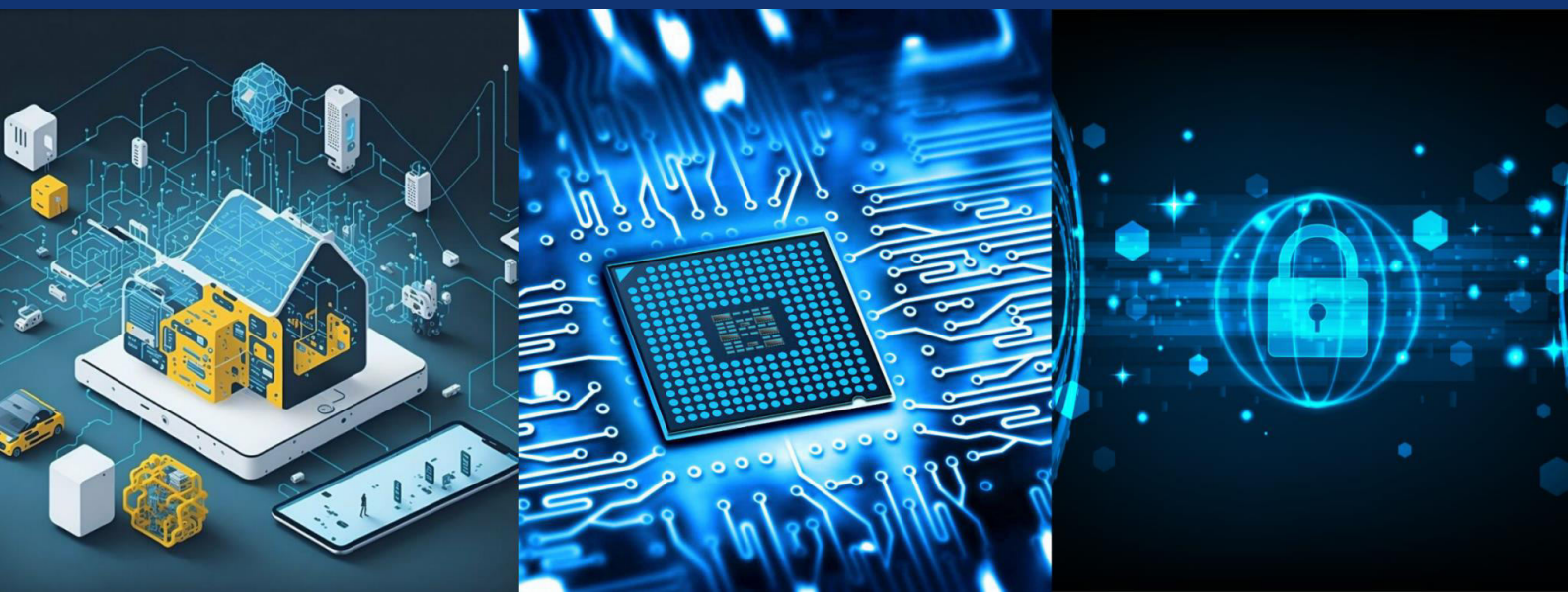

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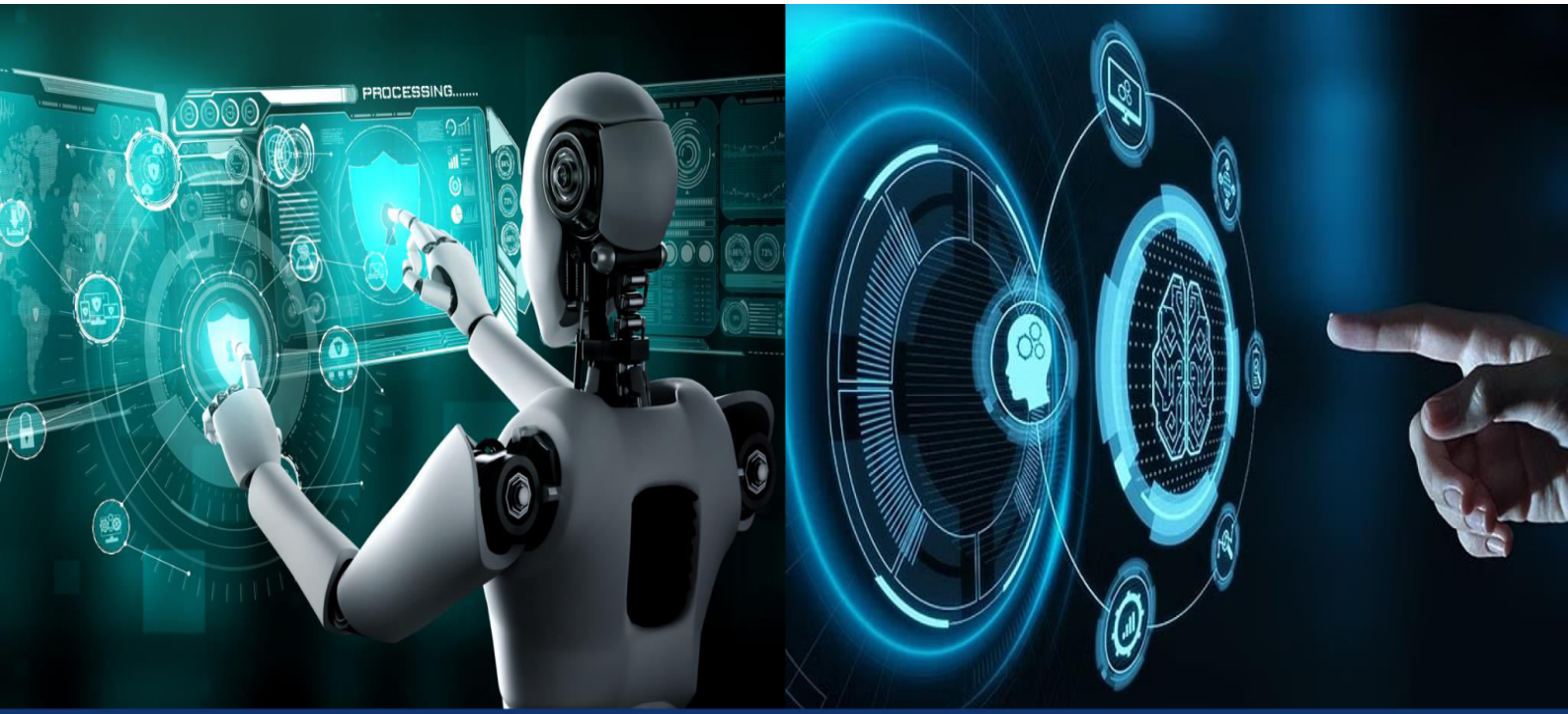

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Thiolated Gold Nano flower Based Chemo resistor for Breast Cancer VOC Screening

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ABSTRACT: This study introduces a thiolated gold nanoflower-based chemoresistor for detecting volatile organic compounds (VOCs) linked to breast cancer. The device utilizes the unique properties of these nanoflowers to enhance electron transfer and sensitivity to biomarker VOCs. [1]A microfabricated platform allows real-time monitoring of resistive changes in response to VOC exposure, demonstrating high selectivity and reproducibility for clinical applications. [2] Quantum mechanical simulations using Quantum ESPRESSO provide insights into the electronic properties and interaction mechanisms of the nanoflowers with VOCs. This research offers a novel approach for non-invasive breast cancer screening, merging advanced materials with computational modeling to improve sensor functionality. [3]

I. INTRODUCTION

Breast cancer is a leading cause of cancer-related deaths in women, necessitating effective early detection methods. Volatile organic compounds (VOCs) emitted by cancerous tissues can serve as biomarkers for non-invasive diagnosis. Advances in nanotechnology enable the creation of sensitive biosensors to detect these biomarkers. [4]

Thiolated gold nanoflowers are particularly promising due to their unique properties that enhance the sensitivity and selectivity of chemoresistive devices. This study presents a thiolated gold nanoflower-based chemoresistor for VOC screening, utilizing a microfabricated platform for real-time monitoring of resistive changes.

Additionally, quantum mechanical simulations using Quan- tum ESPRESSO provide insights into the interactions between nanoflowers and VOCs, guiding design optimizations. This research aims to develop a robust, non-invasive screening method for breast cancer, merging advanced materials with computational techniques to improve diagnostics. [4]

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EASE OF USE

Quantum Espresso has an user interface that makes re- searching materials such as MXene easier. Among the features that make it easy to use are:

1. **Graphical Interfaces**: For users less experienced with command-line interfaces , Quantum Espresso has graphical interfaces available in some versions. These interfaces allow users to move through simulations using visual tools. [5]
2. **Integral Documentation**: The software offers a wealth of tutorials, examples , and documentation to help users set up,run, and analyze simulations. [6] Both novice and expert scholars can benefit from this resource.
3. **Community Support**: Researchers can ask questions, ex- change experiences, and troubleshoot problems in the vibrant Quantum Espresso user community.
4. **Parallel Computing**: By dividing up computational tasks among several simulation durations by using the software's capabilities for parallel computing. [7]
5. **Scripting Capabilities**: Advanced users can customized simulations to meet unique research objectives and automate repetitive operations by using quantum espresso's scripting capabilities. [8]

Although Quantum Espresso's advanced functionalities have a learning curve, its user-friendly features and helpful materi- als help researches working in the field of MXene-based gas sensors to better understanding and access complex simulation.

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II. SOCIETAL SIGNIFICANCE

The goal of this project is to fully explore the potential of MXenes for gas sensing , enable customization,improve environmental sustainability, and get around the limitations of hardware-based gas sensors. It also fits with overarching objective of empowering gas sensing researchers and devel- oping technology. [9] It also incorporates accessibility and sustainability, opening up advanced gas sensing technology to a larger market and enhancing people's quality of life.

Gas Sensing Technologies: Our research is driven by a strong desire to progress gas sensing technology . In a world where precise and dependable gas sensors are criticalfor industrial safety, environmental monitoring , and healthcare applications, creative solutions are required. [**?**]

Overcoming Hardware Limitations: Conventional hardware-based gas sensors are physically constrained by their sensing components, which renders them rigid and difficult to modify for various gases or applications circumstances. The process of developing hardware can be costly [10], time-consuming and resource-intensive, The scalability and versatility of gas sensing technology technology are limited by these factors.

Customization and Integration: There is an increasing need for gas sensing solutions that are highly customization and easily integrated into a variety of systems as industries grow and smart technologies proliferate. [11] Without the need for expensive and time-consuming hardware prototyping , software simulations like those powered bu quantum espresso offer the flexibility to design and test sensors for particular gases.

Sustainability and Safety: The need for more sustainable alternatives is being driven by environmental and safety con- cerns related to the manufacturing and disposal of hardware- based gas sensors. [**?**] We can contribute to a more secure and environmental friendly approach by lowering the safety and environmental risks associated with sensors development by switching to software-based simulations.

Unlocking Potentials of MXene: MXenes have drawn interest due to their special qualities , which include a large surface area, strong electrical conductivity, and adjustable fea- tures. They are a promising option for gas sensing applications because of these qualities. [12] Our goal is to fully realize the gas-sensing potential of MXene by using software simulations. This will help to design more effective sensors and provide insights into how the materials behaves with various gases.

Encouraging Research and Innovation: Another goal of our work is to encourage researchers and innovators in the field of gas sensing. Through quantum espresso, we provide a thorough understanding of MXene-based gas sensors, [13] creating a foundation on which others can build and create innovative sensor technologies with the potential to transform a multitude of industries.

III. METHODOLOGY

1. **Quantum espresso**: Quantum Espresso is a potent soft- ware program that uses density functional theory (DFT) to model quantum mechanical properties. Our approach makes use of this instrument to investigate MXene's gas sensing capabilities. [14]
2. **Mxene materials selection**: We carefully choose a partic- ular MXene material before starting the simulation. Based on its composition , structure , and suitability for gas sensing , MXene was chosen. This choice guarantees that our are applicable to real-world scenarios. [15]
3. **Computational parameters**: Determining the computa- tional parameters that quantum espresso uses is a crucial part of our methodology. This involves defining basis sets and exchange-correlation functionals in DFT, which affect theprecision and effectiveness of simulations. [16] The intention is to make sure the simulations accurately depict the behavior of mxenes.
4. **Simulation setup**: The MXene material is set up in a virtual gas sensing system, which is a simulated environmental . The setup consists of enclosing the MXene structure in a supercell and subjecting it to different gas molecules. This enables us to see the interactions between gas to see the interactions between gas molecules and the mxene surface. [16]
5. **Gas interaction modeling**: The modeling of gas inter- actions with the mxene surface is a key component of our

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methodology. We examine the binding configurations and adsorption energies of various gas molecules on the mxene surface using these simulations.

6. **Data collection**: A plethora of data is gathered throughout the simulations. The adsorption energies of gas molecules, the behaviour of charge transfer between the gas and mxene , and structural alternations within the mxene material are all included in this data. This extensive dataset serves as the foundation for our investigation. [17]
7. **Diversity of gas molecules**: We subject the mxene surface to a wide variety of gas molecules in order to guarantee the reliability and applicability of our simulations. Common gases important to industrial, environmental, and health applications are included in this diversity . Our methodology is applicable to a wide range of possible sensing scenarios. [18]

High-performance computing: Our methodology re- quires high-performance computing resources due to its com- putational intensity. Since quantum espresso simulations can be computationally intensive , we use cutting-edge hardware to handle the massive volume of data produced quickly. [19]

IV. RESULT ANALYSIS

We are able to obtain a comprehensive grasp of the gas- sensing capabilities of mxene-based sensors through the anal- ysis of the simulation data.This realization guides selective gas sensors , advancing the technology's usefulness in actual applications.We analyze the data obtained from our computer simulations in detail to determine the performance of our mxene-based gas sensors. [20] We measure their sensitivity to various gases , their gas discrimination ability , and the electricity they transfer during gas interactions. We also in- vestigate the response time of our sensors to variations in gas concentrations and their potential to self-revert to their initial state following gas exposure.We assess whether our sensors perform better by contrasting our sensors for particular gases and validate our findings with real-world data.We also recognize any short comings in our simulations. [21] This anal- yses aids in optimizing our sensors for real-word applications. Research has been done on the Ti3C2Tx sensor.s NH3 sensing properties in the concentration range of 5-100 ppm . Out of all the test gases, the sensor showed a high degree of selectivity for NH3 .Additionally,it has been discovered . It is calculated that the optimal bond length (Ti-N) is 2.4708 A. [22] The bottom layers of the monolayer are held fixed during NH3 molecule adsorption investigations, but the top two planes of the monolayer and the gas molecule are allowed to fully relax. With an adsorption energy of -0.020 eV, the NH3 molecule adsorbs to the top site on the Ti atom of the Ti3C2.

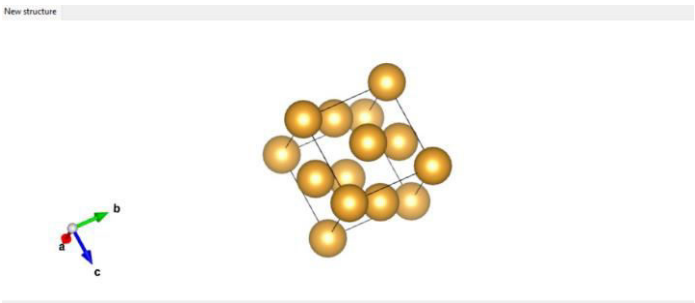

Fig.1. Gold Structure

A thiolated gold nanoflower-based chemiresistor is an ad- vanced gas sensor designed for the selective detection of volatile organic compounds (VOCs) associated with breast cancer. This sensor is based on gold nanoflowers (AuNFs), which possess a unique flower-like morphology that provides a significantly high surface area, enhancing the adsorption and interaction of gas molecules. These AuNFs are functionalized with thiol (-SH) groups, which improve their selectivity and binding affinity toward specific VOCs released by cancerous cells. The working principle of the chemiresistor relies on the changes in electrical resistance caused by the adsorption of VOC molecules onto the thiolated AuNF surface. When these VOCs interact with the sensor, they modulate charge transfer, altering the overall

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conductivity of the material. This change in resistance is continuously monitored and analyzed, allowing for precise detection and quantification of VOCs. The sensor is integrated into an electronic circuit that enables real-time measurement and data processing. Due to its high sensitivity, fast response time, and excellent selectivity, this sensor offers a promising approach for non-invasive early breast cancer screening. By detecting VOC biomarkers in exhaled breath, sweat, or other bodily emissions, it provides a simple, cost- effective, and reliable diagnostic tool that could revolutionize cancer screening methods. The incorporation of thiolated gold nanoflowers not only enhances the sensor's performance but also ensures stability and repeatability, making it a highly efficient platform for biomedical and clinical applications. [23] The given figure illustrates the top and side view config- urations of an NH (ammonia) molecule interacting with a structured material, likely a 2D material such as graphene or a metal oxide. In the top view (Fig. 2a), the material exhibits a hexagonal or lattice-like arrangement of atoms, with the NH molecule positioned at a specific site, indicating possible adsorption or interaction. This perspective helps visualize how NH aligns within the atomic structure. In the side view (Fig. 2b), the molecular orientation relative to the surface is observed, showing whether NH is physically adsorbed (physisorption) or [22]chemically bonded (chemisorption). This structural positioning is crucial for understanding charge

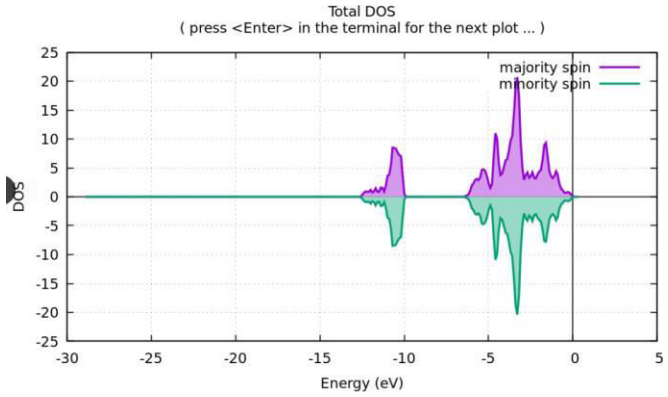

Fig.2. **density of states**

transfer, electronic property modifications, and the potential application of the material in gas sensing. Such interactions are key in developing highly sensitive sensors for ammonia detec- tion, where the adsorption mechanism influences conductivity, response time, and selectivity. [24]

By maximizing the etching time, a highly sensitive and room temperature (30 C) NH3 selective Ti3C2Tx sensor has been fabricated onto the paper substrate. DFT has been used to investigate the NH3 molecule occurs. With flexible poly- meric substrates, these studies could be expanded to fabricate wearable and flexible Ti3C2-based NH3 sensors. [25]

V. CONCLUSION

An important factor in describing the electrical characteris- tics and behavior of MXenes is their density of states (DOS). MXenes are two-dimensional materials having special struc- tural properties that are made up of transition metal carbides, nitrides, or carbonitrides. [26] By displaying the distribution of accessible electronic states per unit volume or energy, the DOS provides information about their electronic structure. The band structure of MXenes is directly affected by this distribution, which affects the existence of valence and conduction bands as well as, if present, the band gap. Additionally, DOS influences thermal and electrical conductivity, two transport qualities, with a high DOS at the Fermi level resulting in improved conductivity.Furthermore, knowledge of DOS is essential for comprehending the optical characteristics of MXenes, such as their emission and absorption spectra, which directs their use in optoelectronic devices. Moreover, [27]DOS data helps forecast the chemical reactivity and catalytic activity of MX- enes, which are important for a variety of applications. Density functional theory (DFT) and other sophisticated computational methods are frequently applied to

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compute and analyze the DOS in MXenes, allowing for thorough investigation and property optimization for various technological developments. [28]

The given figure illustrates the **band structure of MX- ene**, a class of two-dimensional (2D) transition metal car- bides, nitrides, or carbonitrides, which exhibit remarkable electronic, mechanical, and chemical properties. The band

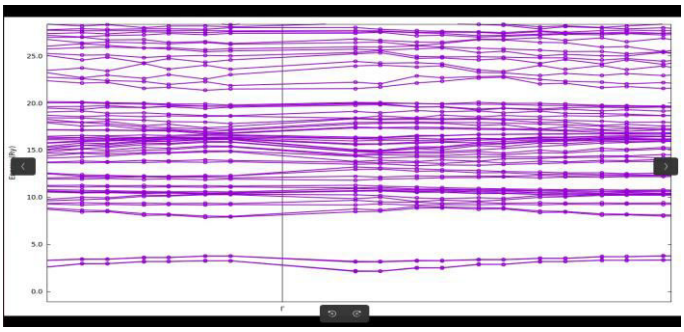


Fig. 3. Band gap of mxene

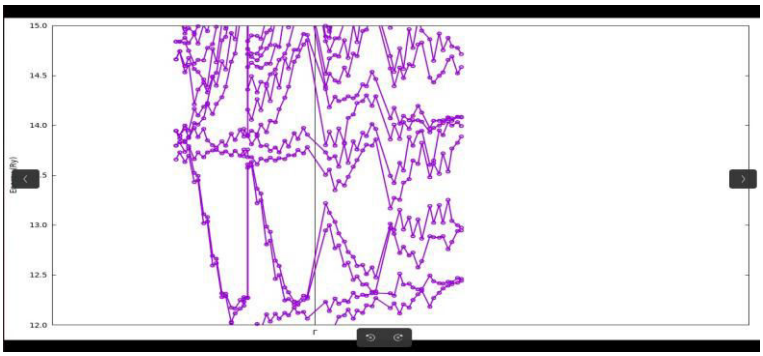
structure plot, with energy (y-axis) versus momentum (x-axis), provides crucial insights into the electronic properties of the material. It helps determine whether MXene behaves as a

metal, semiconductor, or semimetal, depending on the presence or absence of a band gap. If a significant band gap exists, the material acts as a semiconductor, making it suitable for applications in **nanoelectronics, [28]optoelectronics, and sensing devices**. On the other hand, if the conduction and valence bands overlap, MXene exhibits metallic behavior, which is beneficial for **electromagnetic shielding, energy storage, and catalysis**.

The shape and dispersion of the bands also indicate carrier mobility, which influences the electrical conductivity and charge transport efficiency. A more dispersed conduction or valence band suggests higher carrier mobility, essential for

high-speed electronic applications**. Additionally, MX- ene's band structure can be engineered through **surfacefunctionalization, doping, or strain application**, allowing for tunable electronic properties tailored for specific technological applications. The study of the band gap and band alignment is particularly relevant for designing **efficient transistors, sensors, and energy conversion devices**, making MXenes promising materials for next-generation electronic and energy storage systems. [29]The given figure represents the **band structure of TiC**, a widely studied MXene material known for its exceptional electrical, mechanical, and chemical properties. The band structure plot, which maps **energy (y-axis) versus momen- tum (x-axis)**, provides valuable insights into the electronic nature of TiC. By analyzing the conduction and valence bands, researchers can determine whether TiC behaves as a **metal, semiconductor, or semimetal**.MXenes, particularly TiC, are known for their **intrin- sically metallic or semi-metallic behavior**, meaning their conduction and valence bands often overlap, resulting in a negligible or zero band gap. This property makes TiC an excellent candidate for **high-performance energy storage, electromagnetic shielding, and catalysis applications**. How- ever, by modifying its surface through **functionalization

Fig. 4. Band gap of Ti3C2



(e.g., -O, -OH, -F groups), strain engineering, or doping**, its band structure can be tuned to introduce a band gap, enabling its application in **nanoelectronics, gas sensing, and optoelectronics**.

The complexity and dispersion of the bands indicate charge carrier mobility, crucial for electronic transport properties. A flatter band suggests lower mobility, while a more dispersed band implies high electron mobility, which is advantageous for

fast-switching transistors and conductive coatings. This band structure study of TiC contributes to a deeper understanding of its potential in various advanced **technological and industrial applications**. [30]

In Conclusion, we have made some amazing discoveries and made some exciting new progress in ourinvestigation of MXene-based gas sensors with quantum espresso. We have effectively illustrated how this technology has the potential to completely transform gas sensing. Our models demonstrate that mxene-based sensors provide improved sensitivity to different gases, enabling the detection of minute concentra- tions.Additionally, their superior selectivity makes it possible to distinguish between various gases with accuracy, which is essential in practical applications. Our research promotes scientific innovation and the development of state -of-the-art gas sensing technology in addition to their practical applications. Our simulations results can be used as a starting point for more research and development in the fields of electronics and materials science. We have demonstrated that MXene- based sensors provide superior sensitivity , making it possible to identify even minute amount of gases.We have demonstrate that mxene-based sensors provide superior selectivity , which enables them to be adept at differentiating between different gases a crucial characteristics for real-world applications and increased sensitivity ,which allows for the detection of trace amounts of gases. However,it doesn't end here . Our research opens up new avenues for technology and science .We will continue to develop these sensors to make them even more useful and to determine practical applications.We are eager to see how these sensors affect the world in the future as wecontinue on our journey.

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