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Overview of Recent Research on Novel Materials for Sensor Applications

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ABSTRACT: Recent advances in nanotechnology, artificial intelligence (AI), the Internet of Things (IoT), and smart electronics have significantly increased the demand for high-performance sensors with high sensitivity, fast response, low power consumption, and miniaturized dimensions. This review presents an overview of recent research progress on novel materials for sensing applications, focusing on their structural characteristics, sensing mechanisms, and potential applications in gas sensors, biosensors, optical sensors, and wearable electronics. Various advanced nanomaterials, including Graphene, Carbon Nanotubes, Silicene, Germanene, Stanene, Transition Metal Dichalcogenides, MXenes, metal-oxide nanomaterials, Perovskite materials, conducting polymers, and plasmonic nanostructures are discussed in detail. These materials exhibit remarkable sensing performance because of their large specific surface area, tunable electronic properties, strong adsorption capability, and excellent charge-transfer efficiency. In particular, low-dimensional materials have demonstrated outstanding sensitivity toward toxic gases, biomolecules, and optical signals, even at room temperature. The review also highlights the important role of Density Functional Theory (DFT) in predicting adsorption mechanisms, electronic structures, and sensing behavior before experimental fabrication. In addition, emerging trends such as nano-heterostructures, flexible and wearable sensors, self-powered devices, and AI- integrated sensing systems are summarized. Furthermore, recent developments in hybrid nanocomposites and multifunctional sensing platforms have opened new opportunities for next- generation healthcare monitoring, environmental protection, industrial safety, and smart-city technologies. The integration of machine learning techniques with sensor systems has also improved signal processing, real-time detection, and data analysis accuracy. Finally, current challenges and future perspectives toward sustainable, intelligent, low-cost, and high-performance sensor technologies are discussed, emphasizing the importance of interdisciplinary research in advancing practical sensing applications for future electronic and biomedical systems.

KEYWORDS: MXenes; gas sensors; biosensors; smart sensors.

1. INTRODUCTION

Recent advances in artificial intelligence (AI), the Internet of Things (IoT), Industry 4.0, biomedicine, and smart electronics have significantly increased the demand for highly sensitive and low-power sensors. Modern sensors are widely applied in environmental monitoring, healthcare, smart agriculture, and intelligent transportation systems [1–3]. Gas sensors are used for detecting toxic gases such as NO_2, NH_3, CO, and VOCs, while biosensors enable sensitive detection of biomolecules and viruses [4].

Sensor performance strongly depends on material properties including electronic structure, carrier mobility, surface area, and adsorption capability [5]. Conventional materials such as silicon, metal oxides, and polymers often suffer from limited sensitivity and high operating temperatures [6,7]. Therefore, low-dimensional nanomaterials have attracted considerable attention for next- generation sensing applications. Graphene and other two-dimensional materials, including silicene, germanene, stanene, MoS_2, and MXenes, exhibit excellent sensing performance because of their tunable electronic properties and large surface areas [8]. Graphene can detect individual gas molecules through conductivity changes [9], while MXenes and TMDs such as MoS_2 and WS_2 demonstrate high

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sensitivity and stable room-temperature operation [10,11]. In addition, plasmonic nanoparticles, perovskites, and nanocomposites have been extensively investigated for optical and biosensing applications [12]. Alongside experimental studies, Density Functional Theory (DFT) has become an important computational approach for predicting adsorption behavior, charge transfer, and electronic properties of sensing materials, thereby accelerating the development of high-performance sensors [13].

2. CARBON NANOMATERIALS IN SENSORS

Carbon nanomaterials are among the earliest and most extensively studied materials in sensor technology, including Graphene, carbon nanotubes (CNTs), fullerene, and graphene oxide.

2.1. Graphene

Graphene is one of the most extensively studied nanomaterials for sensing applications because of its excellent electrical conductivity, high carrier mobility, and large surface area [14,15]. Since all carbon atoms are exposed on the surface, adsorption of gas molecules or biomolecules can strongly modify its electrical properties, leading to high sensing sensitivity. Graphene-based sensors can detect gases such as NO_2, NH_3, H_2O, and CO through charge-transfer-induced conductivity changes and can operate efficiently at room temperature with low power consumption [16,17]. In addition, graphene has shown strong potential in biosensing because biomolecules such as DNA and proteins can be immobilized on its surface [18]. However, pristine graphene suffers from zero band gap and limited selectivity [19]. Therefore, doping, defect engineering, and hybrid structures such as graphene/SnO_2, graphene/ZnO, and graphene/PANI are widely used to improve sensing performance, flexibility, and suitability for wearable devices [20,21].

2.2. Carbon Nanotubes

Carbon Nanotubes (CNTs), including SWCNTs and MWCNTs, are promising sensing materials because of their high electrical conductivity, large surface area, and excellent mechanical properties [22–24]. Their sensing mechanism mainly relies on charge transfer between adsorbed molecules and the CNT surface, enabling sensitive detection of gases such as NH_3, NO_2, CO, and H_2 [25,26]. CNT-based sensors can operate at room temperature with fast response and low power consumption, making them suitable for flexible and wearable devices [27]. CNTs are also widely used in biosensing because of their efficient electron transfer and easy surface functionalization, with applications in glucose, DNA, and immunosensors [28,29]. To improve sensitivity and selectivity, CNTs are often combined with metal nanoparticles, metal oxides, and conducting polymers such as CNTs/SnO_2 and CNTs/PANI [30,31]. Despite fabrication challenges, CNTs remain highly promising for next-generation sensing technologies.

3. TWO-DIMENSIONAL (2D) MATERIALS

Following the success of Graphene, many other two-dimensional materials have been intensively investigated for sensing applications.

3.1. Silicene, Germanene, and Stanene

After the discovery of graphene, silicene, germanene, and stanene have attracted considerable interest for sensing applications because of their tunable electronic properties, buckled structures, and strong chemical activity [32,33]. These materials exhibit high sensitivity toward gases such as NO_2, NH_3, CO, SO_2, and H_2S through charge-transfer interactions that modify their electronic structures and conductivity [34–40]. Among them, stanene nanoribbons are particularly promising because of their strong spin–orbit coupling, tunable band gap, and high adsorption capability [38– 40]. Transition-metal doping (Fe, Co, Ni) and halogen functionalization (F, Cl, Br) are widely used to improve adsorption strength, charge transfer, and gas selectivity [41–43]. DFT studies have shown that doped systems generally exhibit stronger adsorption energies and more stable sensing performance than pristine materials [44]. Therefore, silicene, germanene, and stanene are considered promising materials for next-generation nanosensors.

3.2. Transition Metal Dichalcogenides (TMDs)

Transition Metal Dichalcogenides (TMDs) such as MoS_2, WS_2, $MoSe_2$, and WSe_2 are promising sensing materials because of their layered two-dimensional structures and intrinsic semiconducting band gaps of 1–2 eV [45,46]. Among them, MoS_2 is the most extensively studied due to its excellent chemical stability and room-temperature sensing capability. Monolayer MoS_2 possesses a direct band gap of about 1.8 eV, enabling high sensitivity and efficient current modulation [47]. Its large surface area and Mo d orbitals promote strong interactions with gas molecules through charge transfer [48,49]. MoS_2-based sensors exhibit high sensitivity toward gases such as NO_2, NH_3, CO, SO_2, and H_2S [50]. In particular, NO_2 strongly modifies conductivity because it acts as an electron acceptor [51]. Defect engineering and transition-metal doping can further enhance sensing performance [52]. MoS_2 is also widely used in biosensors for glucose, protein, and DNA detection because of its good biocompatibility and efficient electron transfer [53]. Other TMDs such as WS_2 and $MoSe_2$ also demonstrate promising sensing properties [54]. Furthermore, heterostructures combining TMDs with graphene, CNTs, or MXenes can improve charge transfer and sensing efficiency, making TMDs attractive candidates for next-generation nanosensors.

4. MXene MATERIALS

MXenes are a new family of two-dimensional materials with the general formula $M_{n+1}X_nT_x$, distinguished by their high electrical conductivity, abundant surface functional groups (–O, –OH, –F), excellent hydrophilicity, and strong adsorption capability. These characteristics make MXenes highly promising for gas sensors, biosensors, and flexible sensing devices. Among them, $Ti_3C_2T_x$ is the most extensively studied because of its excellent conductivity and strong interaction with gas molecules such as NH_3, ethanol, and acetone. Previous studies have shown that $Ti_3C_2T_x$- based sensors can operate effectively at room temperature with high sensitivity and rapid response [55–56]. In addition, MXenes exhibit excellent mechanical flexibility, making them suitable for wearable sensors and flexible electronic devices [57]. Current research trends focus on fabricating MXene composites with Graphene or conducting polymers such as PANI and PEDOT:PSS to improve stability, charge-transfer efficiency, and sensing selectivity [58]. However, MXenes still face challenges related to oxidation and conductivity degradation in ambient environments.

Therefore, surface functionalization and hybrid-structure engineering are being intensively explored to improve their long-term stability.

5. METAL OXIDE NANOMATERIALS

Semiconducting metal oxides such as ZnO, SnO_2, TiO_2, WO_3, and In_2O_3 remain important materials in sensor technology because of their low cost, high stability, and good sensing performance. ZnO is widely studied for gas sensing owing to its wide band gap (~3.37 eV), high chemical stability, and diverse nanostructures including nanowires, nanorods, and nanosheets [59]. Its sensing mechanism is mainly based on resistance changes caused by oxygen adsorption and interactions with gas molecules [60,61]. ZnO exhibits high sensitivity toward gases such as ethanol, H_2, and NO_2, while one-dimensional nanostructures provide enhanced electron transport and sensing performance [62]. In addition, doping and hybridization with graphene, CNTs, and conducting polymers can improve selectivity and reduce operating temperature. SnO_2 is another widely used metal oxide in commercial gas sensors because of its high sensitivity toward gases such as CO, H_2, NO_2, NH_3, and ethanol [63]. However, pristine SnO_2 sensors often require high operating temperatures, resulting in high power consumption [64]. To improve performance, transition-metal doping and heterostructure engineering with ZnO, TiO_2, and MoS_2 have been widely explored [65,66]. Furthermore, combining SnO_2 with graphene or CNTs can enhance charge transport, increase surface area, and enable lower-temperature sensing operation [67].

6. PEROVSKITE MATERIALS

Perovskite materials have attracted significant attention in optoelectronic and sensing applications because of their excellent optical and electronic properties. Organic–inorganic halide perovskites generally possess the formula ABX_3, where A is an organic or inorganic cation, B is a metal such as Pb or Sn, and X is a halogen atom [68]. Their tunable band gaps, high carrier mobility, and strong light absorption make them promising for photodetectors, UV sensors, and optical sensing devices [69–71]. Perovskites also show strong potential in biosensing and humidity sensing because of their efficient photoelectric conversion and sensitivity to water-vapor adsorption [72,73]. However, poor environmental stability under moisture, oxygen, heat, and strong illumination remains a major challenge [74]. Therefore, current research focuses on improving stability through doping, encapsulation, hybrid structures, and lead-free perovskite systems.

7. CONDUCTING POLYMER MATERIALS

Conducting polymers such as Polyaniline (PANI), Polypyrrole (PPy), and PEDOT:PSS are promising sensing materials because they combine electrical conductivity with excellent mechanical flexibility and room-temperature operation [75]. They can also be synthesized through simple and low-cost methods [76]. Among them, PANI is the most widely studied due to its good stability and high conductivity after proton doping [77]. PANI exhibits strong sensitivity toward NH_3 through a deprotonation mechanism that reduces conductivity during gas adsorption [78]. Conducting polymers are also widely used in biosensors because of their efficient electron transfer and easy functionalization with biomolecules [79]. To overcome limitations in conductivity and selectivity, conducting polymers are often combined with graphene or Carbon Nanotubes [80]. Composites such as PANI/graphene and PANI/CNTs show enhanced sensitivity toward NH_3, NO_2, and VOCs, together with faster response and improved recovery behavior [81].

8. PLASMONIC MATERIALS AND OPTICAL SENSORS

Noble metal nanoparticles such as Au and Ag are widely used in plasmonic sensing because they support Surface Plasmon Resonance (SPR), which enhances local electromagnetic fields and enables highly sensitive optical detection [82,83]. Ag nanoparticles provide stronger plasmon intensity, while Au nanoparticles offer better chemical stability and biocompatibility for biomedical applications [84]. SPR sensors are extensively applied in biosensing and medical diagnostics for detecting proteins, DNA, viruses, and antigen–antibody interactions with very high sensitivity [85]. They have also been used for rapid detection of influenza, HIV, and SARS-CoV-2, as well as real-time DNA hybridization monitoring [86,87]. Recently, hybrid plasmonic systems combined with graphene, MoS_2, and MXenes have attracted strong interest because they enhance adsorption and optical signals [88]. These systems can also generate surface-enhanced Raman scattering (SERS), enabling ultralow-concentration molecular detection [89]. Therefore, plasmonic sensors are considered highly promising for future optical and biosensing technologies.

9. ROLE OF MATERIAL SIMULATION IN SENSOR RESEARCH

Material simulation methods play an important role in designing and optimizing nanosensors, especially for low-dimensional materials such as graphene, TMDs, MXenes, and nanoribbons. Among them, Density Functional Theory (DFT) is one of the most widely used computational approaches because it can accurately describe electronic structures and atomic interactions with reasonable computational cost [90]. DFT is widely applied to study interactions between sensing materials and adsorbed molecules through structural optimization, enabling determination of stable adsorption sites, bond lengths, and lattice reconstruction after adsorption [91]. These analyses are essential for evaluating sensing performance in gas and biosensor applications.

DFT is also widely used to calculate adsorption energies, which characterize the interaction strength between gas molecules and sensing materials.

$$E\_ads = E\_total - E\_material - E\_gas$$

where E_total is the total energy of the adsorbed system, E_material the energy of the pristine material, and E_gas is the energy of the isolated gas molecule. Adsorption energy values help distinguish physisorption from chemisorption and predict sensor recovery behavior [92]. Moderate adsorption energies are generally ideal for gas sensing because they balance sensitivity and sensor recovery. DFT can analyze electronic band structures, where changes in band gap or electronic states near the Fermi level are closely related to sensing signals [93]. In materials such as silicene, stanene, and MoS_2, gas adsorption can strongly modify conductivity or even induce semiconductor-to-metal transitions. Density of states (DOS) and partial density of states (PDOS) analyses are widely used to study orbital hybridization and charge-transfer mechanisms [94]. For transition-metal-doped systems, spin-polarized DFT calculations can also predict magnetic properties and spin polarization changes caused by gas adsorption [95]. Several DFT packages are commonly used in sensor research, including VASP, Quantum ESPRESSO, and NanoDCAL [96– 98]. Recently, combining DFT with AI and machine learning has become an important trend for rapidly predicting adsorption energies, electronic structures, and material stability, thereby reducing computational cost and accelerating material discovery [99].

10. FUTURE DEVELOPMENT TRENDS

Future research on sensing materials will focus on miniaturization, higher sensitivity, low power consumption, and multifunctional integration. Emerging two-dimensional materials such as MXenes, phosphorene, borophene, silicene, germanene, stanene, and Janus 2D materials are attracting strong interest because of their tunable electronic properties and high surface activity [100]. Nano-heterostructures including graphene/MoS_2, MXene/ZnO, and CNTs/SnO_2 can enhance charge transfer, sensitivity, selectivity, and device stability [101]. In addition, flexible and wearable sensors based on conducting polymers, graphene, MXenes, and nanowires are being developed for real-time healthcare and biomedical monitoring [102]. Self-powered sensors based on piezoelectric, triboelectric, and thermoelectric effects are also promising, with materials such as ZnO nanowires, MoS_2, and perovskites showing strong potential [103]. Meanwhile, integrating Artificial Intelligence (AI) and the Internet of Things (IoT) is enabling intelligent sensing systems capable of real-time data processing and large-scale monitoring applications [104]. Sustainable and environmentally friendly sensor materials are also gaining attention, with efforts to reduce toxic elements and develop recyclable or biodegradable materials [105]. In addition, combining experimental studies with Density Functional Theory (DFT) and machine learning can accelerate the discovery of high-performance sensing materials by rapidly predicting adsorption behavior and electronic properties [106]. Overall, the convergence of nanotechnology, AI, and advanced simulations is expected to drive the development of ultrahigh-performance and intelligent sensing systems in the future.

11. CONCLUSION

Research on novel sensing materials has become an important field in modern materials science. Nanomaterials such as graphene, MXenes, TMDs, stanene, perovskites, and conducting polymers have shown strong potential for improving sensor sensitivity, selectivity, and room-temperature operation because of their large surface areas and tunable electronic properties. Density Functional Theory (DFT) also plays a key role in predicting adsorption mechanisms and electronic-structure changes, helping accelerate material discovery while reducing experimental cost and development time. In the future, combining nanomaterials with Artificial Intelligence (AI), machine learning, and IoT technologies is expected to enable intelligent, low-power, flexible, and ultraminiaturized sensing systems. Environmentally friendly materials and self-powered sensors will also become increasingly important for sustainable technological development.

REFERENCES

1. Nguyen, D. C., Ding, M., Pathirana, P. N., & Seneviratne, A. (2021). Blockchain and AI-based solutions to combat coronavirus (COVID-19)-like epidemics: A survey. *IEEE Access*, *9*, 95730– 95753. https://doi.org/10.1109/ACCESS.2021.3093633
2. Lee, J., Bagheri, B., & Kao, H.-A. (2015). A cyber-physical systems architecture for Industry 4.0-based manufacturing systems. *Manufacturing Letters*, *3*, 18–23. https://doi.org/10.1016/j.mfglet.2014.12.001
3. Atzori, L., Iera, A., & Morabito, G. (2010). The Internet of Things: A survey. *Computer Networks*, *54*, 2787–2805. https://doi.org/10.1016/j.comnet.2010.05.010
4. Turner, A. P. F. (2013). Biosensors: Sense and sensibility. *Chemical Society Reviews*, *42*, 3184–3196. https://doi.org/10.1039/C3CS35528D
5. Yamazoe, N. (2005). Toward innovations of gas sensor technology. *Sensors and Actuators B: Chemical*, *108*, 2–14. https://doi.org/10.1016/j.snb.2004.12.075
6. Korotcenkov, G. (2007). Metal oxides for solid-state gas sensors: What determines our choice? *Materials Science and Engineering B*, *139*, 1–23. https://doi.org/10.1016/j.mseb.2007.01.044
7. Wang, C., Yin, L., Zhang, L., Xiang, D., & Gao, R. (2010). Metal oxide gas sensors: Sensitivity and influencing factors. *Sensors*, *10*, 2088–2106. https://doi.org/10.3390/s100302088
8. Novoselov, K. S., et al. (2004). Electric field effect in atomically thin carbon films. *Science*, *306*, 666–669. https://doi.org/10.1126/science.1102896
9. Schedin, F., et al. (2007). Detection of individual gas molecules adsorbed on graphene. *Nature Materials*, *6*, 652–655. https://doi.org/10.1038/nmat1967
10. Naguib, M., et al. (2011). Two-dimensional nanocrystals produced by exfoliation of Ti_3AlC_2. *Advanced Materials*, *23*, 4248–4253. https://doi.org/10.1002/adma.201102306
11. Radisavljevic, B., et al. (2011). Single-layer MoS_2 transistors. *Nature Nanotechnology*, *6*, 147–150. https://doi.org/10.1038/nnano.2010.279
12. Homola, J., Yee, S. S., & Gauglitz, G. (1999). Surface plasmon resonance sensors: Review. *Sensors and Actuators B: Chemical*, *54*, 3–15. https://doi.org/10.1016/S0925-4005(98)00321-9
13. Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*, A1133–A1138. https://doi.org/10.1103/PhysRev.140.A1133
14. Novoselov, K. S., et al. (2004). Electric field effect in atomically thin carbon films. *Science*, *306*, 666–669. https://doi.org/10.1126/science.1102896
15. Geim, A. K., & Novoselov, K. S. (2007). The rise of graphene. *Nature Materials*, *6*, 183–191. https://doi.org/10.1038/nmat1849
16. Schedin, F., et al. (2007). Detection of individual gas molecules adsorbed on graphene. *Nature Materials*, *6*, 652–655. https://doi.org/10.1038/nmat1967
17. Korotcenkov, G. (2007). Metal oxides for solid-state gas sensors: What determines our choice? *Materials Science and Engineering B*, *139*, 1–23. https://doi.org/10.1016/j.mseb.2007.01.044
18. Shao, Y., et al. (2010). Graphene based electrochemical sensors and biosensors: A review. *Electroanalysis*, *22*, 1027–1036. https://doi.org/10.1002/elan.200900571
19. Schwierz, F. (2010). Graphene transistors. *Nature Nanotechnology*, *5*, 487–496. https://doi.org/10.1038/nnano.2010.89
20. Wei, D., et al. (2009). Synthesis of N-doped graphene by chemical vapor deposition and its electrical properties. *Nano Letters*, *9*, 1752–1758. https://doi.org/10.1021/nl803279t

21. Wang, C., Yin, L., Zhang, L., Xiang, D., & Gao, R. (2010). Metal oxide gas sensors: Sensitivity and influencing factors. *Sensors, 10*, 2088–2106. https://doi.org/10.3390/s100302088
22. Iijima, S. (1991). Helical microtubules of graphitic carbon. *Nature*, *354*, 56–58. https://doi.org/10.1038/354056a0
23. Saito, R., Dresselhaus, G., & Dresselhaus, M. S. (1998). *Physical properties of carbon nanotubes*. Imperial College Press. https://doi.org/10.1142/9781848162572
24. Treacy, M. M. J., Ebbesen, T. W., & Gibson, J. M. (1996). Exceptionally high Young's modulus observed for individual carbon nanotubes. *Nature, 381*, 678–680. https://doi.org/10.1038/381678a0
25. Collins, P. G., et al. (2000). Extreme oxygen sensitivity of electronic properties of carbon nanotubes. *Science, 287*, 1801–1804. https://doi.org/10.1126/science.287.5459.1801
26. Kong, J., et al. (2000). Nanotube molecular wires as chemical sensors. *Science, 287*, 622– 625. https://doi.org/10.1126/science.287.5453.622
27. Snow, E. S., et al. (2005). Chemical detection with a single-walled carbon nanotube capacitor. *Science, 307*, 1942–1945. https://doi.org/10.1126/science.1109128
28. Wang, J. (2005). Carbon-nanotube based electrochemical biosensors: A review. *Electroanalysis, 17*, 7–14. https://doi.org/10.1002/elan.200403113
29. Liu, Y., et al. (2008). Carbon nanotube based biosensors. *Sensors, 8*, 398–418. https://doi.org/10.3390/s8010398
30. Zhang, C., et al. (2013). Hydrogen sensors based on palladium decorated carbon nanotubes. *Sensors and Actuators B: Chemical, 181*, 395–401. https://doi.org/10.1016/j.snb.2013.01.080
31. Wang, C., Yin, L., Zhang, L., Xiang, D., & Gao, R. (2010). Metal oxide gas sensors: Sensitivity and influencing factors. *Sensors, 10*, 2088–2106. https://doi.org/10.3390/s100302088
32. Cahangirov, S., Topsakal, M., Aktürk, E., Şahin, H., & Ciraci, S. (2009). Two- and one- dimensional honeycomb structures of silicon and germanium. *Physical Review Letters*, *102*, 236804. https://doi.org/10.1103/PhysRevLett.102.236804
33. Kara, A., et al. (2012). A review on silicene—New candidate for electronics. *Surface Science Reports, 67*, 1–18. https://doi.org/10.1016/j.surfrep.2011.10.001
34. Guo, Z. X., Furuya, S., Iwata, J., & Oshiyama, A. (2013). Absorption of gas molecules on silicone and germanene. *Physical Review B, 87,* 235435. https://doi.org/10.1103/PhysRevB.87.235435
35. Ding, Y., & Wang, Y. (2014). Electronic structures of silicene gas sensor. *Applied Surface Science*, *307*, 477–482. https://doi.org/10.1016/j.apsusc.2014.04.066
36. Dávila, M. E., Xian, L., Cahangirov, S., Rubio, A., & Le Lay, G. (2014). Germanene: A novel two-dimensional germanium allotrope akin to graphene and silicene. *New Journal of Physics*, *16*, 095002. https://doi.org/10.1088/1367-2630/16/9/095002
37. Hussain, T., De Sarkar, A., & Ahuja, R. (2015). Strain tuned gas sensing properties of germanene. *Applied Physics Letters, 107*, 253103. https://doi.org/10.1063/1.4938125
38. Xu, Y., et al. (2013). Large-gap quantum spin Hall insulators in tin films. *Physical Review Letters*, *111*, 136804. https://doi.org/10.1103/PhysRevLett.111.136804
39. Wu, F., Yu, W., & Song, Q. (2017). Adsorption of gas molecules on stanene: A first-principles study. *Superlattices and Microstructures*, *112, 235–242.* https://doi.org/10.1016/j.spmi.2017.09.033
40. Ezawa, M. (2012). Topological origin of quasi-flat edge bands in silicene nanoribbons. *New Journal of Physics*, *14*, 033003. https://doi.org/10.1088/1367-2630/14/3/033003
41. Sahin, H., & Peeters, F. M. (2013). Adsorption of alkali, alkaline-earth, and 3d transition metal atoms on silicene. *Physical Review B*, *87*, 085423.https://doi.org/10.1103/PhysRevB.87.085423
42. Shukla, A., & Bhamu, R. (2019). Electronic and magnetic properties of Fe-doped stanene nanoribbons: A DFT study. *Physica E*, *108*, 160–166. https://doi.org/10.1016/j.physe.2018.12.019
43. Lin, X., Yang, W., Liao, K., & Yang, J. (2016). Tunable electronic and magnetic properties of halogenated stanene. *RSC Advances*, *6*, 41212–41218. https://doi.org/10.1039/C6RA04966K
44. Hussain, T., Chakraborty, S., & Ahuja, R. (2020). Gas sensing with 2D materials: A DFT perspective. *Applied Materials Today*, *20*, 100674. https://doi.org/10.1016/j.apmt.2020.100674
45. Wang, Q. H., Kalantar-Zadeh, K., Kis, A., Coleman, J. N., & Strano, M. S. (2012). Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nature Nanotechnology*, *7*, 699–712. https://doi.org/10.1038/nnano.2012.193
46. Mak, K. F., Lee, C., Hone, J., Shan, J., & Heinz, T. F. (2010). Atomically thin MoS_2: A new direct-gap semiconductor. *Physical Review Letters*, *105*, 136805. https://doi.org/10.1103/PhysRevLett.105.136805

47. Splendiani, A., et al. (2010). Emerging photoluminescence in monolayer MoS_2. *Nano Letters*, *10*, 1271–1275. https://doi.org/10.1021/nl903868w
48. Jariwala, D., Sangwan, V. K., Lauhon, L. J., Marks, T. J., & Hersam, M. C. (2014). Emerging device applications for semiconducting two-dimensional transition metal dichalcogenides. *ACS Nano*, *8*, 1102–1120. https://doi.org/10.1021/nn500064s
49. Radisavljevic, B., et al. (2011). Single-layer MoS_2 transistors. *Nature Nanotechnology*, *6*, 147–150. https://doi.org/10.1038/nnano.2010.279
50. Li, H., et al. (2012). Fabrication of single- and multilayer MoS_2 film-based field-effect transistors for sensing NO at room temperature. *Small*, *8*, 63–67. https://doi.org/10.1002/smll.201101016
51. Late, D. J., et al. (2012). Hysteresis in single-layer MoS_2 field effect transistors. *ACS Nano*, *6*, 5635–5641. https://doi.org/10.1021/nn301572c
52. Pham, T., Li, G., Bekyarova, E., Itkis, M. E., & Mulchandani, A. (2019). MoS_2-based optoelectronic gas sensor with sub-parts-per-billion limit of NO_2 gas detection. *ACS Nano*, *13*, 3196–3205. https://doi.org/10.1021/acsnano.8b08199
53. Yao, Y., et al. (2020). MoS_2 based nanomaterials for biosensors. *Materials Today Chemistry*, *16*, 100259. https://doi.org/10.1016/j.mtchem.2020.100259
54. Chhowalla, M.~~, et al. (2013). The chemistry of two-dimensional layer~~ed transition metal dichalcogenide nanosheets. *Nature Chemistry*, *5*, 263–275. https://doi.org/10.1038/nchem.1589
55. Naguib, M., et al. (2011). Two-dimensional nanocrystals produced by ~~exfoliation of Ti_3AlC_2.*Advanced Materials*~~, *23*, 4248–4253. https://doi.org/10.1002/adma.201102306
56. Lee, J., et al. (2017). Titanium carbide MXene gas sensors for room-temperature NH_3 detection. *ACS Applied Materials & Interfaces*, *9*, 37184–37190. https://doi.org/10.1021/acsami.7b11055
57. Ma, Y., et al. (2020). Flexible MXene-based pressure sensors. *Advanced Functional Materials*, *30*, 2003015. https://doi.org/10.1002/adfm.202003015
58. Xu, Y., et al. (2020). MXene/graphene hybrid materials for advanced sensing applications. *Advanced Functional Materials*, *30*, 1907377. https://doi.org/10.1002/adfm.201907377
59. Özgür, Ü., et al. (2005). A comprehensive review of ZnO materials and devices. *Journal of Applied Physics*, *98*, 041301. https://doi.org/10.1063/1.1992666
60. Yamazoe, N., & Shimanoe, K. (2008). Theory of power laws for semiconductor gas sensors. *Sensors and Actuators B: Chemical*, *128*, 566–573. https://doi.org/10.1016/j.snb.2007.07.036
61. Wang, Z. L. (2004). Zinc oxide nanostructures: Growth, properties and applications. *Journal of Physics: Condensed Matter*, *16*, R829–R858. https://doi.org/10.1088/0953-8984/16/25/R01
62. Comini, E., et al. (2010). Metal oxide nanowire chemical sensors: Innovation and quality of life. *Materials Today*, *13*, 36–44. https://doi.org/10.1016/S1369-7021(10)70158-7
63. Korotcenkov, G. (2007). Metal oxides for solid-state gas sensors: What determines our choice? *Materials Science and Engineering B*, *139*, 1–23. https://doi.org/10.1016/j.mseb.2007.01.044
64. Yamazoe, N. (2005). Toward innovations of gas sensor technology. *Sensors and Actuators B: Chemical*, *108*, 2–14. https://doi.org/10.1016/j.snb.2004.12.075
65. Comini, E., Faglia, G., & Sberveglieri, G. (2002). Stable and highly sensitive gas sensors based on semiconducting oxide nanobelts. *Applied Physics Letters*, *81*, 1869–1871. https://doi.org/10.1063/1.1504867
66. Wang, C., Yin, L., Zhang, L., Xiang, D., & Gao, R. (2010). Metal oxide gas sensors: Sensitivity and influencing factors. *Sensors*, *10*, 2088–2106. https://doi.org/10.3390/s100302088
67. Kauffman, D. R., & Star, A. (2008). Carbon nanotube gas and vapor sensors. *Angewandte Chemie International Edition*, *47*, 6550–6570. https://doi.org/10.1002/anie.200704488
68. Green, M. A., Ho-Baillie, A., & Snaith, H. J. (2014). The emergence of perovskite solar cells. *Nature Photonics*, *8*, 506–514. https://doi.org/10.1038/nphoton.2014.134
69. Kim, H. S., et al. (2012). Lead iodide perovskite sensitized all-solid-state submicron thin film mesoscopic solar cell. *Scientific Reports*, *2*, 591. https://doi.org/10.1038/srep00591
70. Stranks, S. D., et al. (2013). Electron-hole diffusion lengths exceeding 1 micrometer in an organometal trihalide perovskite absorber. *Science*, *342*, 341–344. https://doi.org/10.1126/science.1243982

71. Fang, Y., Dong, Q., Shao, Y., Yuan, Y., & Huang, J. (2015). Highly narrowband perovskite single-crystal photodetectors enabled by surface-charge recombination. *Nature Photonics*, *9*, 679– 686. https://doi.org/10.1038/nphoton.2015.156
72. Lin, Q., et al. (2018). Perovskite-based biosensors. *Advanced Materials*, *30*, 1705176. https://doi.org/10.1002/adma.201705176
73. Yuan, Z., et al. (2019). Perovskite humidity sensors with high sensitivity and fast response. *Sensors and Actuators B: Chemical*, *296*, 126660. https://doi.org/10.1016/j.snb.2019.126660
74. Park, N.-G. (2015). Perovskite solar cells: An emerging photovoltaic technology. *Materials Today*, *18*, 65–72. https://doi.org/10.1016/j.mattod.2014.07.007
75. Skotheim, T. A., & Reynolds, J. R. (2007). *Handbook of conducting polymers*. CRC Press. https://doi.org/10.1201/9781420046177
76. Janata, J., & Josowicz, M. (2003). Conducting polymers in electronic chemical sensors. *Nature Materials*, *2*, 19–24. https://doi.org/10.1038/nmat768
77. MacDiarmid, A. G. (2001). "Synthetic metals": A novel role for organic polymers. *Synthetic Metals*, *125*, 11–22. https://doi.org/10.1016/S0379-6779(01)00508-0
78. Virji, S., et al. (2004). Polyaniline nanofiber gas sensors: Examination of response mechanisms. *Nano Letters*, *4*, 491–496. https://doi.org/10.1021/nl035122e
79. Gangopadhyay, R., & De, A. (2000). Conducting polymer nanocomposites: A brief overview. *Chemistry of Materials*, *12*, 608–622. https://doi.org/10.1021/cm990537m
80. Dan, Y., Lu, Y., Kybert, N. J., Luo, Z., & Johnson, A. T. C. (2009). Intrinsic response of graphene vapor sensors. *Nano Letters*, *9*, 1472–1475. https://doi.org/10.1021/nl8033637
81. Kauffman, D. R., & Star, A. (2008). Carbon nanotube gas and vapor sensors. *Angewandte Chemie International Edition*, *47*, 6550–6570. https://doi.org/10.1002/anie.200704488
82. Raether, H. (1988). *Surface plasmons on smooth and rough surfaces and on gratings*. Springer. https://doi.org/10.1007/BFb0048317
83. Homola, J., Yee, S. S., & Gauglitz, G. (1999). Surface plasmon resonance sensors: Review. *Sensors and Actuators B: Chemical*, *54*, 3–15. https://doi.org/10.1016/S0925-4005(98)00321-9
84. Maier, S. A. (2007). *Plasmonics: Fundamentals and applications*. Springer. https://doi.org/10.1007/0-387-37825-1
85. Homola, J. (2003). Present and future of surface plasmon resonance biosensors. *Analytical and Bioanalytical Chemistry*, *377*, 528–539. https://doi.org/10.1007/s00216-003-2101-0
86. Ahmadivand, A., et al. (2021). Rapid detection of infectious viruses using surface plasmon resonance. *ACS Sensors*, *6*, 423–433. https://doi.org/10.1021/acssensors.0c01922
87. Mayer, K. M., & Hafner, J. H. (2011). Localized surface plasmon resonance sensors. *Chemical Reviews*, *111*, 3828–3857. https://doi.org/10.1021/cr100313v
88. Bonaccorso, F., et al. (2010). Graphene photonics and optoelectronics. *Nature Photonics*, *4*, 611–622. https://doi.org/10.1038/nphoton.2010.186
89. Kneipp, K., et al. (1997). Single molecule detection using surface-enhanced Raman scattering (SERS). *Physical Review Letters*, *78*, 1667–1670. https://doi.org/10.1103/PhysRevLett.78.1667
90. Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*, A1133–A1138. https://doi.org/10.1103/PhysRev.140.A1133
91. Martin, R. M. (2004). *Electronic structure: Basic theory and practical methods*. Cambridge University Press. https://doi.org/10.1017/CBO9780511805761
92. Hussain, T., Chakraborty, S., & Ahuja, R. (2020). Gas sensing with 2D materials: A DFT perspective. *Applied Materials Today*, *20*, 100674. https://doi.org/10.1016/j.apmt.2020.100674
93. Singh, D. J., & Nordström, L. (2006). *Planewaves, pseudopotentials and the LAPW method*. Springer. https://doi.org/10.1007/0-387-29684-8
94. Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. *Physical Review*, *136*, B864–B871. https://doi.org/10.1103/PhysRev.136.B864
95. Kübler, J. (2000). *Theory of itinerant electron magnetism*. Oxford University Press. https://doi.org/10.1093/acprof:oso/9780198508023.001.0001

96. Kresse, G., & Furthmüller, J. (1996). Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set. *Physical Review B, 54*, 11169–11186. https://doi.org/10.1103/PhysRevB.54.11169
97. Giannozzi, P., et al. (2009). QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials. *Journal of Physics: Condensed Matter*, *21*, 395502. https://doi.org/10.1088/0953-8984/21/39/395502
98. Taylor, J., Guo, H., & Wang, J. (2001). *Ab initio* modeling of quantum transport properties of molecular electronic devices. *Physical Review B*, *63*, 245407. https://doi.org/10.1103/PhysRevB.63.245407
99. Butler, K. T., et al. (2018). Machine learning for molecular and materials science. *Nature*, *559*, 547–555. https://doi.org/10.1038/s41586-018-0337-2
100. Geim, A. K., & Grigorieva, I. V. (2013). Van der Waals heterostructures. *Nature*, *499*, 419–425. https://doi.org/10.1038/nature12385
101. Wang, Q. H., et al. (2012). Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nature Nanotechnology*, *7*, 699–712. https://doi.org/10.1038/nnano.2012.193
102. Kim, D.-H., et al. (2011). Epidermal electronics. *Science*, *333*, 838–843. https://doi.org/10.1126/science.1206157
103. Wang, Z. L. (2012). Self-powered nanosensors and nanosystems. *Advanced Materials, 24,* 280–285. https://doi.org/10.1002/adma.201104365
104. Butler, K. T., et al. (2018). Machine learning for molecular and materials science. *Nature*, *559*, 547–555. https://doi.org/10.1038/s41586-018-0337-2
105. McKone, J. R., Lewis, N. S., & Gray, H. B. (2014). Will solar-driven water-splitting devices see the light of day? *Chemistry of Materials*, *26*, 407–414. https://doi.org/10.1021/cm4021518
106. Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*, A1133–A1138. https://doi.org/10.1103/PhysRev.140.A1133