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REVIEW ARTICLE

2D Materials for Environment, Energy, and Biomedical Applications

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ABSTRACT

Recently 2D materials are booming in the field of energy, environment, and biomedical application. Incorporation of metal/non-metal within 2D materials significantly influences the physical and chemical properties, making them intriguing materials for various applications. The advancement of 2D material requires strategic modification by manipulating the electronic structure, which remains a challenge. Herein, we describe 2D materials for the environment, energy, and biomedical application. A predominant aim of this short communication is to summarize the literature on the advanced 2D materials for environment, energy, and biomedical application (especially COVID-19).

INTRODUCTION

Two Dimensional (2D) materials have appeared as a novel material platform due to their unique properties such as high surface area, large reactive sites, flexibility, tunable configuration to change the band gap, thickness at the atomic level, high conductivity, magnetic and fluorescence. These unique characteristic of the 2D materials make them an exceptional candidate for various end application mainly environmental remediation, energy, and biomedical application. Since, the discovery of single-layer graphene using mechanical exfoliation method by Andre Geim and Kostya Novoselov [1-3], a new era of 2D materials has lead that aided advantages in developing a next-generation innovative device with miniaturization and flexibility by assembling a single nanosheet. Moreover, high surface area with enormous active sites to move electrons, and mechanical stability are incorporated advantage of 2D materials. Numerous 2D materials such as Transition Metal Chalcogenides (TMDs), MXene, WS₂, silicene, germanene, and phosphorene are another class of 2D materials having a surge of scientific and engineering interest as these materials are fulfilling the demand of advanced materials for energy, environmental, and biomedical application [4-6]. Additionally, their cutting edge properties such as reduction/oxidation ability in-plane electric conductivity, high reactivity, and high biocompatibility significantly aided advantages for energy and biomedical applications [7-10]. In this concern, electronic structure modulation with changes in the design and synthesis process of 2D materials to create feature-rich functional micro-architectures for sustainable energy, clean technologies, and biomedical applications remain a challenge. In this context, researchers continue to develop newer strategies to synthesize 2D materials that efficiently improve applicability in end applications.

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Various synthesis methods such as mechanical/liquid exfoliation, microwave synthesis, Chemical Vapor Deposition (CVD), hydrothermal, and self-assembly etc., have been used for the development of 2D materials. CVD is the most widely used method to synthesize the high-quality 2D material without defects or vacancy in the electronic structure. Moreover, the self-assembly method has attracted other methods for the synthesis of 2D materials because 2D-nano-architecture lacks intermolecular interaction such as hydrogen bonding or hydrophobic interaction during layer assembly that reduces agglomeration and restacking, thereby well-defined nano-architecture [11,12]. The process of self-assembling is different in the case of 2D material as this material exhibits wide distributed in-plane shape, and size. However, the other process is limited by their severe restacking and irreversible aggregation [13-16]. In this regard, tailoring the geometry of nano-architecture with exploiting the material properties is one of the significant tasks to design several nano-composite materials for next-generation materials for energy, environment, and biomedical application.

Recently, several researchers focusing synthesizing 2D materials mainly AgBiP₂Se₆ monolayer, BiOCl based nanosheet, Cu nanosheets, 2D-NiO, 2D/2D Z-scheme SnNb₂O₆/Bi₂WO₆ system, MOS₂, MOSe₂, WS₂, WO₃, graphene, and Graphene Oxide (GO) for various end applications such as environment, energy, and biomedical

[17-28]. These studies are in good agreement with the use of 2D materials as an effective charge transport layer to apply as environment, energy, and biomedical application. Figure 1 shows the schematic representation of different 2D materials and their application. In this context, we devote attention towards various end application of 2D materials.

PROPERTIES OF 2D MATERIALS

The interaction of the analyte with 2D materials is essential in removing several contaminants from water, subsequently environmental protection. The most common properties of 2D material to deal with the environment is their large surface-to-volume ratio compared to other nanomaterials. A large surface-to-volume ratio creates a large interaction site, which subsequently helps create a strong force for removing analytes from contaminated water. Next, 2D materials are flexible to configurationally tuning, which supports modulating the band gap of these materials by playing in their electronic structure. These modifications require simple metal or non-metal doping or creating defects in their structure. The lower the band gap of 2D materials, the higher is the probability of oxidation and reduction reaction within the water to degrade contaminants. Further, these layered materials' atomic thickness significantly contributes to various inherent properties, mainly conductivity, reactivity, fluorescence, and magnetic permeability [29-35]. Such unique characteristic of the 2D materials makes

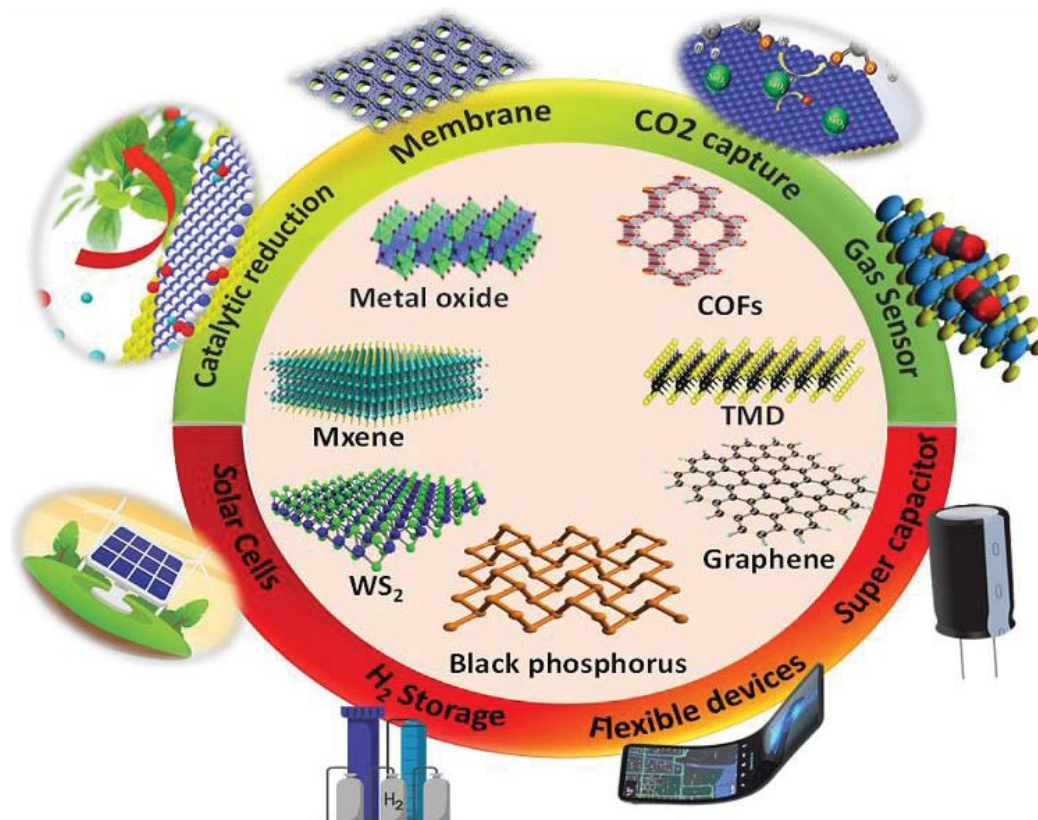


Figure 1 A schematically representation of different 2D materials and their applications.

them exceptional candidate for environmental remediation, energy, and biomedical applications.

APPLICATION OF 2D MATERIALS

2D materials for environmental remediation

2D materials offer a new avenue to explore high-performance filtration materials with high permeability and selectivity compared to other nanomaterials. Controlled pore size distribution, functional sites, and creation of heterojunction to lower the band gap can be utilized in separation process using 2D materials. Numerous studies focused on synthesizing several 2D materials for environmental remediation application; for example, Ikram, et al. [36] synthesized MoS₂ nano petals for dye degradation. Iqbal, et al. [37] synthesized La and Mn-co-doped Bismuth Ferrite/Ti₃C₂ based composites for photodegradation of congo red dye. Another study by Zhu, et al. [38] synthesized MOF on BiOBr based 2D-nanosheet to degrade rhodamine, methylene blue, and methyl orange dye. These studies are based on 2D-nanosheet, and their composite for efficient degradation of various organic contaminants attributed active sites of the 2D materials binds with analyte and also create heterojunction. The heterojunction reduce the band gap position of CB and VB that improve photoelectron adsorption in visible range and degrade organic contaminants by taking part in redox reactions, subsequently support in the removal of contaminants from water.

Additionally, band gap modulation depends on various doping element as geometry and crystal shape efficiently helps to tune the chemical potential results in band gap modulation of 2D-2D heterojunction. Doping and organic functionalization introduce new density of state near fermi level leads to affect carrier density and new lattice constants, which are fundamental properties of 2D materials. The mechanical properties including high in plane stiffness and tensile strength with low flexible rigidity makes 2D materials an impressive candidate in various advance devices. These properties can also be modulated by incorporating various heteroatom doping as modification in these properties alter bond strength and geometry, subsequently lattice constant. Several examples of these modifications are Liu, et al. [39] synthesized 2D-ZnO based single-crystal nanosheets consist of mesoporous structure synthesized using an intriguing colloidal templating approach. The single synthesized crystal shows exposed polar facets, supporting selective adsorption and rhodamine B photodegradation. Another study by Monga, et al. [40] synthesized single-crystalline 2D-BiOCl nanorods decorated with 2D-MoS₂ nanosheets. Incorporating MoS₂ in BiOCl nanorods modulates the band gap supporting MB degradation and Cr(VI). The GO incorporated ZnO-based photocatalyst materials efficiently degrade dye molecules [41] (Figure 2). The photocatalytic activity of GO incorporated ZnO-based photocatalyst material. This literature shows that tuning

and crystal modification provide high degradation efficiency for photodegradation of various pollutants due to change in their electronic structure followed by bandgap lowering so that it can absorb visible light radiation and work under the normal environmental condition reduce contaminants from environments.

2D materials for energy applications

2D materials possess several unique properties such as mechanical robustness, high surface area, functional sites, and mass transport in advanced electronic devices. The working mechanism behind the success of 2D material in energy storage is based on their ability to capture charge and effectively transport or store it inside the structure or migrate through the ions on the surface [42-45]. Researchers found several ways, such as doping, intercalation, altering the chemical composition, etc., to enhance the spacing of the layers of 2D materials to store or transport charge to control charge effectively. To synthesize a promising electrode material, foreign ions can be intercalated between the layers of 2D materials as the layers are stacked together through weak interactions, which allow ions or molecules to pass through them or store inside them to form active sites [46,47]. The particle size and morphology are also significant to enhance charge storage performance. For example, Feng et al. synthesize MoS₂ nanoflake having curves to form nanotube-like morphology. This morphology allows Li⁺ to intercalate easily and increase the battery performance compared to MoS₂ nanosheets [48]. Another study by Teng, et al. [49] synthesized MoS₂ nanosheet grown over graphene. The MoS₂ is grown vertically over graphene using the hydrothermal method. This creates an enormous oxygen functional group on the surface result in enhance charge transport, subsequent high-rate performance, and cycling stability as lithium-ion battery electrodes. Liu synthesized V₂C MXene by self-discharge method for hybrid batteries that allows Li ions to pass through the interlayer space and increase the spacing between the layers, which provides ample space for ion diffusion [50]. These studies suggest that the intercalation of foreign ions enhances battery performance by increasing the gap between layers to facilitate ions' transport in advance battery performance.

Similarly, 2D material has an advantage when combined with other nanomaterials as interfacial transfer significantly affects the performance of 2D materials. For example, Wen, et al. [51] synthesized nitrogen (N)-doped MXene (N-MXene). N-MXene increases the c-lattice parameters of MXene. Post etching annealing method with ammonia was used to synthesize MXene. The N-MXene increased gravimetric capacitance performance and is considered a promising candidate in supercapacitor application. Similarly, pseudo-capacitance can be improved by incorporating oxygen functional group in MXene surface to initiate redox reaction over the surface of MXene subsequently increase performance. For example, Zhang, et al. [52] synthesized

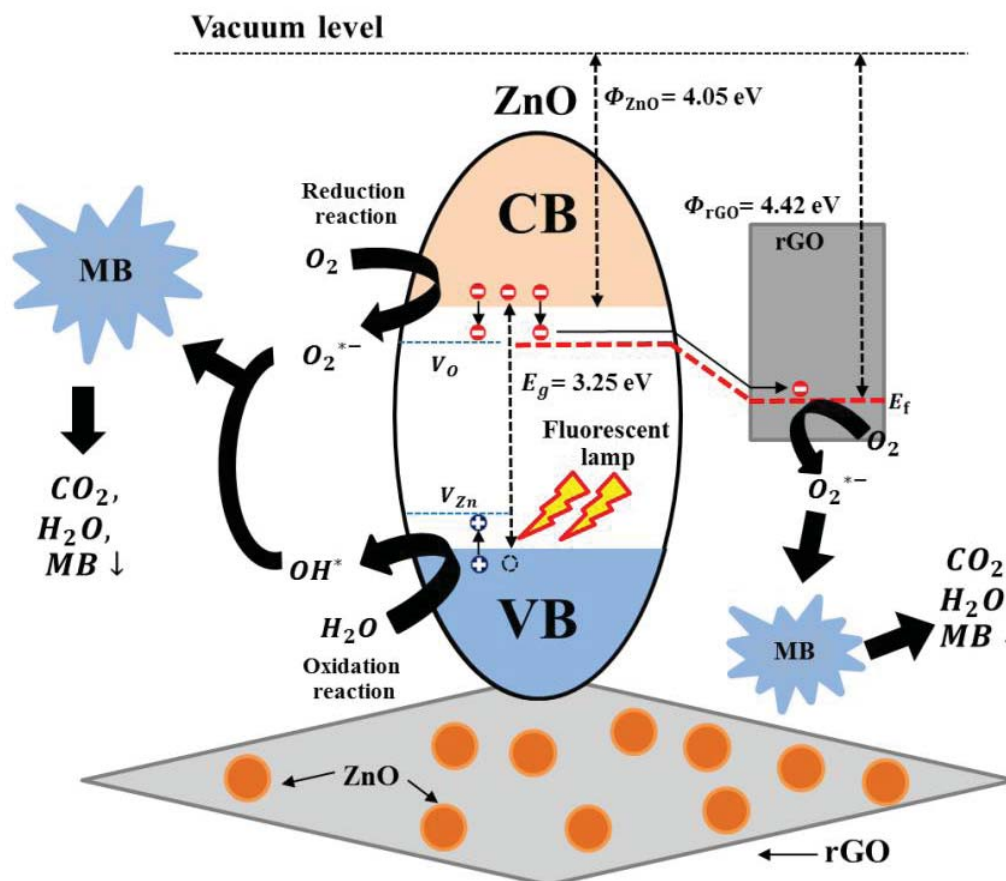


Figure 2 The photocatalytic activity of GO incorporated ZnO-based photocatalyst material. The image was taken with permission [41]. Creative Commons Attribution 2019.

Ti₃C₂T_x by controlled oxidation using ammonium persulfate, which changes F terminals into O terminals results in high capacitance performance. Jiang, et al. [53] synthesized MXene-RuO₂ composite for the supercapacitor application. The material works as an asymmetric electrode by the following pseudocapacitance, significantly increasing the device's performance.

Recently flexible micro-supercapacitors are designed to fulfill the next-generation foldable electronic devices. In this aspect, MXene based 2D materials are considered promising due to their high mechanical stability and ability to store or transport charges within the interlayer space. These flexible devices exhibit high volumetric capacitance, such as Yan et al. synthesized MXene/GO based electrode using electrostatic self-assembly method. In this, rGO was modified with poly(diallyl dimethylammonium chloride) and then inserted between the MXene layer space to design a free-standing electrode with large ion diffusion, which subsequently increases the volumetric capacitance [54]. Another study by Yang et al. reported free-standing MXene as a current collector free electrode for supercapacitor application [55]. The GO-MoS₂-WS₂ based ternary materials for efficiently used in supercapacitor applications

[56] (Figure 3). Synthesis of 2D materials for supercapacitors application. All these studies suggest the applicability of 2D materials in advanced electronic devices.

2D materials for Coronavirus

Material science and engineering are imperative for antiviral research, such as the morphology of the viral structure and biology, diagnosis, and treatment. Usually, the development of practical approaches to protecting, diagnosing, and treating viral diseases requires a detailed study of structure, transmission, and viral sequence.

Importance of structure and viral sequence: With the help of confocal microscopy, individual viruses can be tracked in cells, thereby quickly understanding the mode of action. Nanotechnology or nanopore sequencing has contributed in next-generation sequencing platforms. With the help of nanopore sequencing/gene sequencing, researchers can synthesize the viral protein, and their 3D-structure can be rebuilt by using electron microscopy, X-ray crystallography, and NMR spectroscopy. However, a higher concentration of protein and stability are required for X-ray crystallography and NMR spectroscopy analysis. In this context, single-particle cryo-electron microscopy

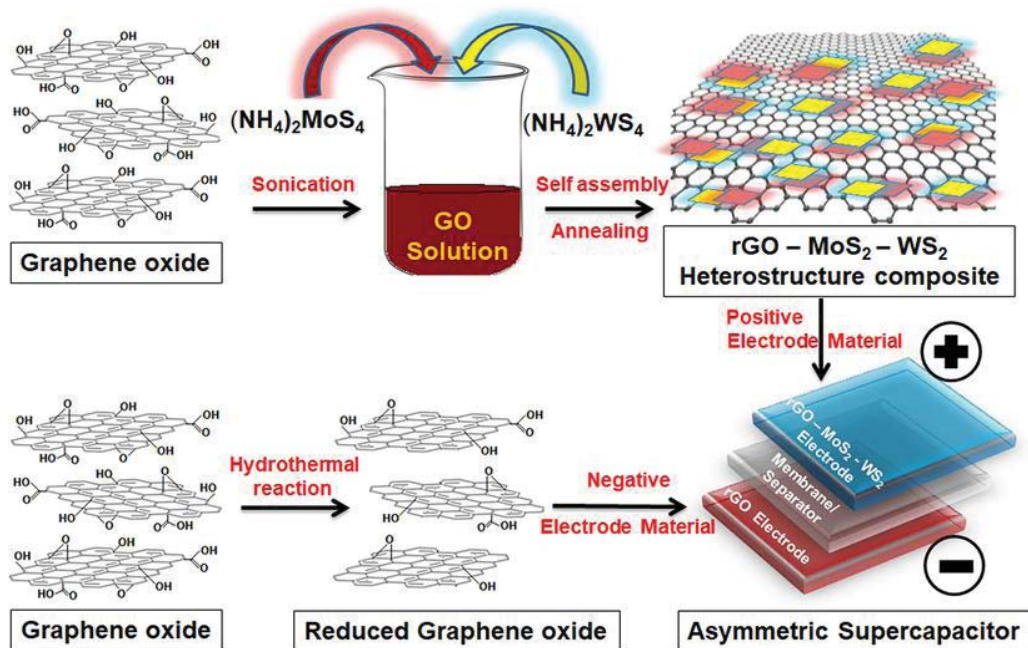


Figure 3 Synthesis of 2D materials for supercapacitors application. The image was taken with permission [56].

has the potential ability to ascertaining the morphology of the viruses. Single-particle cryo-electron microscopy quickly determined the structure of viruses, including SARS-CoV-2. Interestingly, the understanding of material science and viruses has played an essential role in enhancing the sensitivity and selectivity of the particular biomolecules, including SARS-CoV-2 [57,58].

Protection against infection: Usually, viruses replicate within the living cells and are transmitted through air, blood, bloodsucking insects, mucus, anal, vaginal fluid, semen, saliva, and direct contact. Initially, SARS-CoV-2 binds with the host cell using the binding of S protein to the angiotensin-converting enzymes-2 (ACE-2) receptor that allows it to enter the cell and release viral RNA. In other words, the virus captures the host cell to synthesize RNA and produce structural protein that gathers into the new virus, which is released from the host cell. This process is repetitive; thereby SARS-CoV-2 infects human as well as animal. Usually, gloves, masks, face shields, and protective suits are the direct process for the protection against SARS-CoV-2. The surgical masks made of different layers protect against the entry of viruses. Numerous materials such as polymeric film with nanopores, carbon-based materials, and 2D materials were used to synthesize protective coating. However, due to safety and cost concerns, these nanomaterials have not been used to protect viruses, especially SARS-CoV-2. Researchers continue to focus on the toxicity aspects of nanomaterials, including 2D-materials, which suggest that most nanomaterials, mainly carbon-based nanomaterials have insignificant toxicity, which is safer to be used as protective agents.

Detection of SARS-CoV-2: Usually, rapid identification or detection of SARS-CoV-2 infected patients helps to control the viral infection. The immunoassay and Polymerase Chain Reaction (PCR) are extensively used to detect SARS-CoV-2 infection through protein and nucleic acid. The sensitivity and selectivity of the immunoassay mainly depend on the materials and instruments. Numerous 2D materials, such as graphene, have been used to detect SARS-CoV-2 or its variant COVID-19 [59-61]. For example, Fathi-Hafshejani, et al. [62] fabricated the WSe2 based Fet-based COVID biosensor. The data suggested that the SARS-CoV-2 antibody was immobilized onto the WSe2 through 11-mercaptopundecanoic acid-activated N-hydroxysuccinimide and carbodiimide hydrochloride, thereby efficiently detect SARS-CoV-2 infection. Seo, et al. [63] fabricated graphene (as a sensing material) based FET sensor to detect SARS-CoV-2 infection. The data suggested that the graphene conjugated with the spike protein via 1- pyrene butyric acid N-hydroxysuccinimide ester. The prepared biosensor is highly sensitive and detects SARS-CoV-2 in the clinical sample. Muratore, et al. [64] fabricated the MoS2 based biosensor for the detection of SARS-CoV-2 and influenza virus. The data suggested that the sulfur vacancy of MoS2 aided advantages to bind ACE-2 enzymes with the SARS-CoV-2 samples. The angiotensin converts ACE-2 enzyme for the spike protein of SARS-CoV-2 that modified protein acted as recognizing element for the detection of SARS-CoV-2.

In general, functionalized 2D-material-based biosensors offer simple, cost-effective, sensitive, and highly responsive for detecting SARS-CoV-2. The pandemic of COVID-19 required newer technologies that efficiently combat the

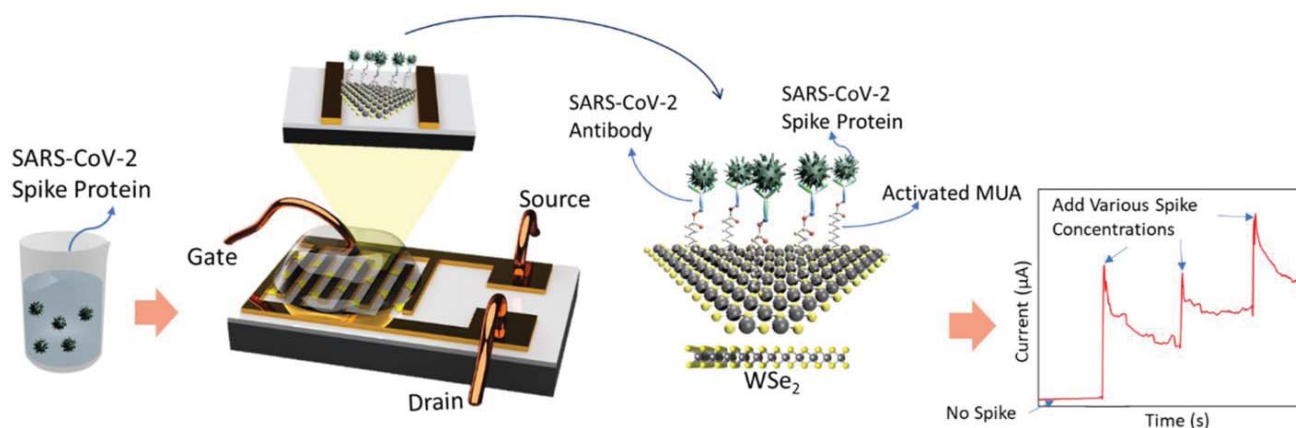


Figure 4 A schematic illustration of the WSe₂ based FET sensor for the detection of SARS-CoV-2. The image was taken with permission [62].

life threatens viruses. The exceptional characteristics such as high electrical, mechanical and functional ability of the 2D-materials like graphene and its derivative make a suitable candidate for making a novel and innovative sensing device [65-69]. Figure 4 shows the schematic illustration of the WSe₂ based FET sensor for the detection of SARS-CoV-2. The 2D-materials-based novel sensing device might be efficiently tackled COVID-19. Moreover, 2D materials provide a technological platform for the protection, detection, and treatment of life-threatening viral diseases.

CONCLUSION

In summary, 2D materials are a promising candidate for advanced environments, energy devices, and biomedical applications. The technological advancement eventually depends on structural modifications of 2D materials. Several strategies such as band gap tuning, deformation control, and surface chemistry modifications are essential to enhance performance. Environmental application of 2D materials needs specific bonding toward analyte to remove the analyte from solution. However, energy application requires high surface area, active sites, mechanical stability, and flexibility. 2D materials need more understanding as they may have both positive and negative responses towards biomedical application in terms of toxicity and impact over the cell. Hence, future demand of 2D materials concluded that specific modification promotes the applicability of 2D material in several end applications, including energy, environment, and biomedical.

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