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2D MBenes: A Novel Member in the Flatland

Varun G. Nair, Magdalena Birowska, Dominika Bury, Michał Jakubczak, Andreas Rosenkranz,* and Agnieszka M. Jastrzębska**

2D MBenes, early transition metal borides, are a very recent derivative of ternary or quaternary transition metal boride (MAB) phases and represent a new member in the flatland. Although holding great potential toward various applications, mainly theoretical knowledge about their potential properties is available. Theoretical calculations and preliminary experimental attempts demonstrate their rich chemistry, excellent reactivity, mechanical strength/stability, electrical conductivity, transition properties, and energy harvesting possibility. Compared to MXenes, MBenes' structure appears to be more complex due to multiple crystallographic arrangements, polymorphism, and structural transformations. This makes their synthesis and subsequent delamination into single flakes challenging. Overcoming this bottleneck will enable a rational control over MBenes' material–structure–property relationship. Innovations in MBenes' postprocessing approaches will allow for the design of new functional systems and devices with multipurpose functionalities thus opening a promising paradigm for the conscious design of high-performance 2D materials.

1. Introduction to MBenes' Unique Structure

Boron, a light element with three valence electrons, can form multicentered bonds being useful to overcome its electron deficiency, thus resulting in a high reactivity with metal ions.[1] Therefore, the presence of boron in a material gives an excellent opportunity to create an enormous variety of complex multidimensional boride structures including various transition metal–borane organic complexes such as $Na[H_3BMn(CO)_3PPh_3]$ or $Na[H_3BCo(CO)_4]$[1] or inorganic boride compounds, which are formed between boron and other less electronegative elements.[2] Among the extraordinary variability of inorganic boron compounds, 2D structures such as early transition metal borides or transition metal boride (TMB) phases with a layered structure can be found.

TMB phases have been well known since the early 1940s, after their first discovery by Halla and Thury in 1942.[3] During the 1960s, research on TMBs bloomed, with contributions made by Stadelmaier[4] and Jeitschko[5] regarding the structure and magnetic properties of Fe_2AlB_2 and MoAlB, respectively. In 1973, Chaban and Kuz'ma discovered Cr_2AlB_2,[6] thus adding another member to the M_2AB_2 family. In 2015, the work of Ade and Hillebrecht[7] on Cr_4AlB_6, Cr_2AlB_2, and Cr_3AlB_4 boosted research on TMBs, which was further inspired by the success of MXenes.[8] They compared the $(CrB_2)_nCrAl$ (n = 1–3) structure of these TMB phases with the structure of ternary carbides and nitrides with the chemical formula of $M_{n+1}AX_n$ (MAX) phases and coined the terminology "MAB phases" due to similarities discovered.

MAB phases are usually composed of an early transition metal (M), metals from groups 13 and 14 of the periodic table (A), and boron (B), having variable structures and stoichiometries (**Figure 1**a). Taking aluminum as an example of the alternating A element, MAB phases can be categorized into MAlB with *Cmcm* crystal space group, M_2AlB_2 with *Cmmm*, M_3AlB_4 with *Pmmm*, and M_4AlB_6.[9] MAB phases contain stacked M–B blocks, comprising face-sharing BM_6 trigonal prisms, interleaved by A atom layers or intermetallic complexes of A layers as visible in $M_3Al_2B_2$.[9c]

The renaissance of TMB phases as MAB phases motivated scientists around the globe to delaminate them by breaking the M—A bonds, thus creating a new class of 2D materials named MBenes.[10] Based upon MAB phases, their corresponding 2D counterparts (MBenes) are composed of M and B (Figure 1b), but different lattice symmetries clearly differentiate them from MXenes with $M_{n+1}X_n$ stoichiometry, and only hexagonal lattices are observed for MXenes. For instance, MBenes with a stoichiometry of M_nB_{n+1} can exhibit both hexagonal and orthorhombic lattices. As displayed in Figure 1c, different stoichiometries including MB, M_2B_3, and M_3B_4 are possible (please refer to structurally stable MBenes summarized in Table S1 in the Supporting Information). Additionally, novel 2D Mo_2B_2 structures with tetragonal and trigonal lattices (Figure 1d) have recently

V. G. Nair, D. Bury, M. Jakubczak, A. M. Jastrzębska
Faculty of Materials Science and Engineering
Warsaw University of Technology
Woloska 141, Warsaw 02-507, Poland
E-mail: varun.gopalakrishnan_nair.dokt@pw.edu.pl;
agnieszka.jastrzebska@pw.edu.pl

V. G. Nair, M. Birowska
Faculty of Physics
University of Warsaw
Pasteura 5, Warsaw 02-093, Poland

A. Rosenkranz
Department of Chemical Engineering, Biotechnology and Materials
University of Chile
Avenida Beauchef 851, Santiago 8370459, Chile
E-mail: arosenkranz@ing.uchile.cl

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been discussed.[11] Moreover, hexagonal Mo_2B with different lattices and possible transitions induced by tensile strains has been theoretically predicted.[12]

Recent studies demonstrate that the elemental space of MAB phases can be expanded by creating $M'_{4/3}M''_{2/3}AB_2$ alloys.[13] Novel, chemically ordered and disordered alloys have been predicted to be thermodynamically stable (Figure 1e), and experimentally verified by the synthesis of two ordered phases ($Mo_{4/3}Y_{2/3}AlB_2$ and $Mo_{4/3}Sc_{2/3}AlB_2$).[13a] Yao et al.[13b] further expanded the possible MAB compositions by considering other A elements such as Si, Zn, Ga, and In with a hexagonal symmetry, thus predicting additionally 25 thermodynamically stable phases. Ab initio calculations revealed that the substitutional incorporation of M″ atoms with larger atomic radii and reduced electronegativities compared to the M′ atom tends to enhance the stability of the alloyed phases. In these alloys, the formation of kagomé-like structures of A atoms has been observed, which strengthens the A—A bonds.[13] Finally, we anticipate that the range of MBenes' compositions can be greatly enhanced by similar metal-alloying approaches (Figure 1f) as explored for MAB phases.

In terms of theoretical predictions, it has been shown that $M'_{4/3}M''_{2/3}B_2$ alloys could be exfoliated from their parent $M'_{4/3}M''_{2/3}AB_2$ alloys, thus holding great promise for their successful exfoliation in experimental procedures.[13b] Furthermore, it has been suggested that it is possible to obtain ordered vacancy structures in MBenes. Zhang et al.[14] verified the stable formation of Mo vacancies in Mo_2B_2. Moreover, doping Mo_2B_2 with Ti, V, Cr, Mn, Fe, Co, Ni, or Cu resulted in negative binding energies, and a high structural stability.[15]

Here, we comprehensively summarize the state-of-the-art MBenes, regarding their atomic structure/arrangement, synthesis routes, prospective properties, and potential applications. Herein, we emphasize that since MBenes are novel structures with challenging synthesis procedures, theoretical predictions are indispensable to understand their properties. Currently, the majority of theoretical predictions considering these 2D materials are based on ab initio approaches in the framework of density functional theory (DFT),[16] which is one of the most powerful techniques to obtain reliable, accurate predictions of a variety of material properties. Therefore, the theoretical predictions presented here are entirely based on DFT, and should be understood as a motivation for further post-DFT studies and experimental studies on these exciting 2D materials. Since our work addresses the broad topic range from atomic structure over synthesis to properties and applications, we expect that our Perspective can serve as an inspiration for researchers associated with 2D materials, who search for both excellent and challenging model 2D materials.

2. The Quest for MBenes' Synthesis

Even the most accurate theoretical predictions and optimistic predictions demonstrating MBenes' outstanding physical properties cannot become true if researchers are not able to experimentally synthesize them. Consequently, all MBenes' applications need to wait for their successful synthesis. The structure of MBenes presents some similarities to early transition metal carbides and nitrides (MXenes), which are etching products of MAX phases. Similar to MXenes, MBenes have weaker M—A bonds and stronger A—B bonds, facilitating etching and delamination into single 2D flakes.[17] Additionally, M—A bonds can be significantly weakened by applying mechanical strains up to 30% along the *z*-direction,[18] which helps to mechanically exfoliate MBenes.

Significant ionic and covalent contributions (M—B bonds) greatly contribute toward MBenes' thermodynamic and mechanical stability. This is especially important for acid-based delamination processes, in which the material must withstand harsher conditions. A comparison of the resulting M—B, B—B, and M—M bond strengths proves that the B—B is the strongest bond, while M—M tends to be the weakest one. This tendency also holds true for bare and terminated MBenes with the following order of B—B > M—O > M—F ≈ M—OH > M—B > M—M.[9a] Consequently, superficial M—O bonds make B—B bonds stiffer, while weakening M—M bonds, due to the removal of electrons from the π^* state.[9a] Similar to MXenes, this allows for an easier processing while preventing the formation of defective single flakes.[9a,19] However, despite the presence of weaker M—A bonds in MAB phases compared to M—B and B—B, MBenes' synthesis is yet to be fully realized, while different approaches are pursued. Like MAX phases, the A layers of MAB phases need to be selectively removed. To do so, the starting phase in form of bulk powder or a thin film[20] is subjected to chemical wet etching. However, in contrast to MAX phases, it has been verified that MAB phases are not easily etchable.

First attempts to chemically etch MAB phases were carried out by Alameda et al.[21] MoAlB single crystals were tested in hydrofluoric acid (HF) and a combination of sodium fluoride (NaF) and hydrochloric acid (HCl), which is known as a mild-type delamination method with in-situ-formed HF used for Ti_3AlC_2 etching. However, this approach did not satisfy the expectations. The underlying reason is that the etching of the MoAlB phase occurred via cavities and branches that appear in the structure along [100] and [010] directions. A high stacking fault energy of two Al zigzag layers additionally hindered the complete etching. Subsequent studies tried to modify the etching conditions for MAB phases, thus analyzing the underlying mechanisms and looking for alternatives to MAB phases as starting materials.

A schematic illustration of the recently explored synthesis approaches for ternary MAB phases and binary borides is presented in **Figure 2**. While taking aluminum as an A interleaving element, the protocol may start with the layered, ternary M_2AlB_2 phase (Figure 2a, "first pathway"). However, the etching procedure of ordinary MAB phases using HF resulted in serve oxidation to oxiboride, structural transformations, and material dissolution.[21] For Mo_2AlB_2, the Mo_2AlB_2/MoAlB phase transformation coupled with oxidation ended up in AlO_x.[22] Since etching with HF has certain limitations, the alloying of the early transition metal (M) could provide more opportunities for the synthesis of MBenes. Zhou et al. reported obtaining $Mo_{4/3}B_{2-x}$ by selectively etching out Y—Al or Sc—Al layers from alloyed $(Mo_{2/3}Y_{1/3})_2AlB_2$ and $(Mo_{2/3}Sc_{1/3})_2AlB_2$ MAB phases, respectively.[23] The etching procedure made use of 40 wt% aqueous HF for about 3 h. Tetrabutylammonium hydroxide (TBAOH)

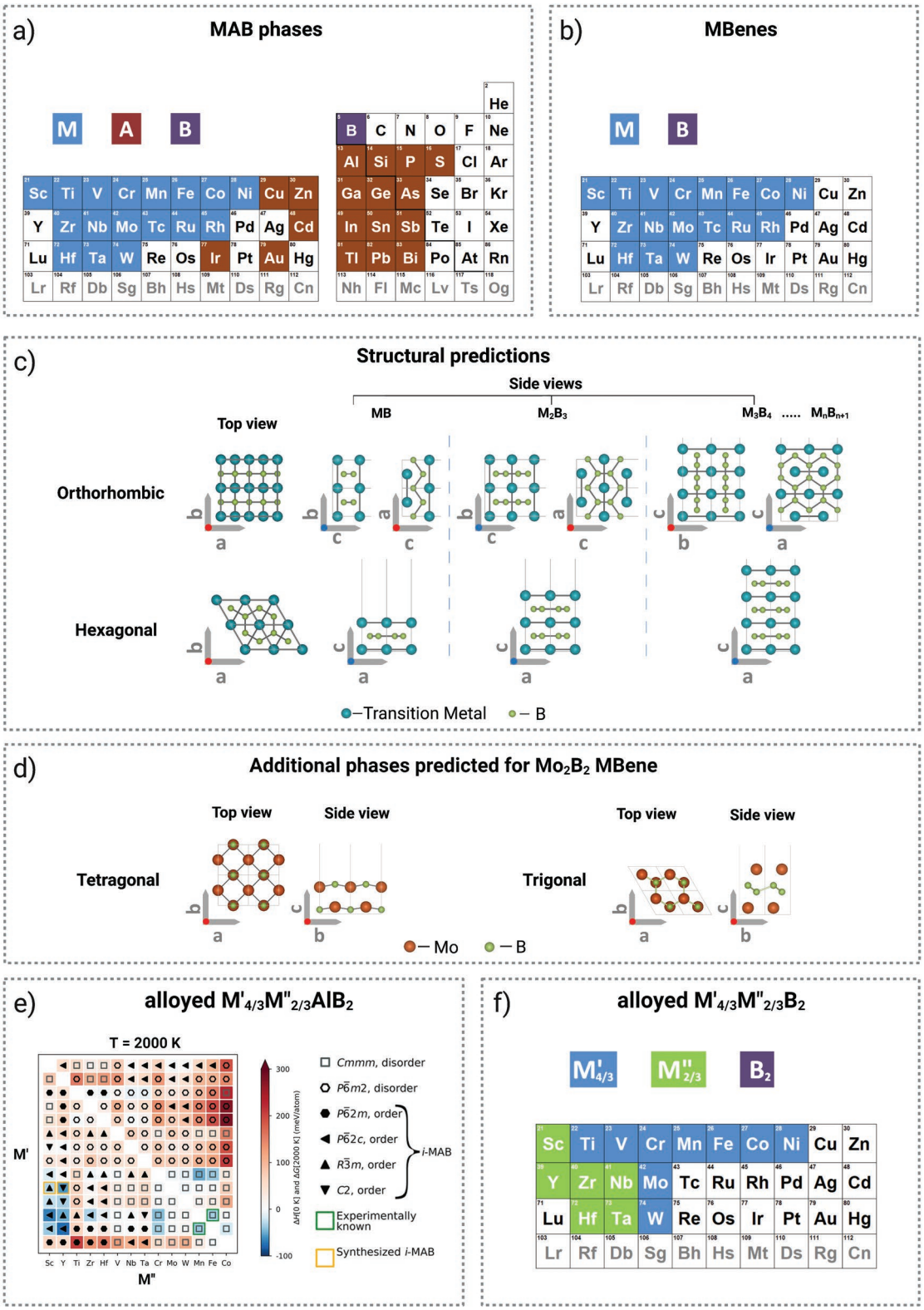

Figure 1. MBenes' possible compositions and structures. The variety of elements from the periodic table to be used to compose a) MAB phases and b) MBenes. c) Schematic atomic arrangements (orthorhombic and hexagonal lattices) predicted for ordinary MBenes. d) Additional phases with tetragonal and trigonal lattice structures predicted for Mo_2B_2 MBenes. e) Prediction of alloyed $M'_{4/3}M''_{2/3}AlB_2$ phases. Colored boxes in heat map represent the most stable elemental and structural arrangements. f) Corresponding alloyed $M'_{4/3}M''_{2/3}B_2$ MBenes that could be obtained from their parental alloyed MAB phases via experimental approaches. a–d,f) Created with Biorender.com. e) Adapted under the terms of the ACS AuthorChoice with CC-BY license (https://pubs.acs.org/page/policy/authorchoice_ccby_termsofuse.html).[13a] Copyright 2020, American Chemical Society.

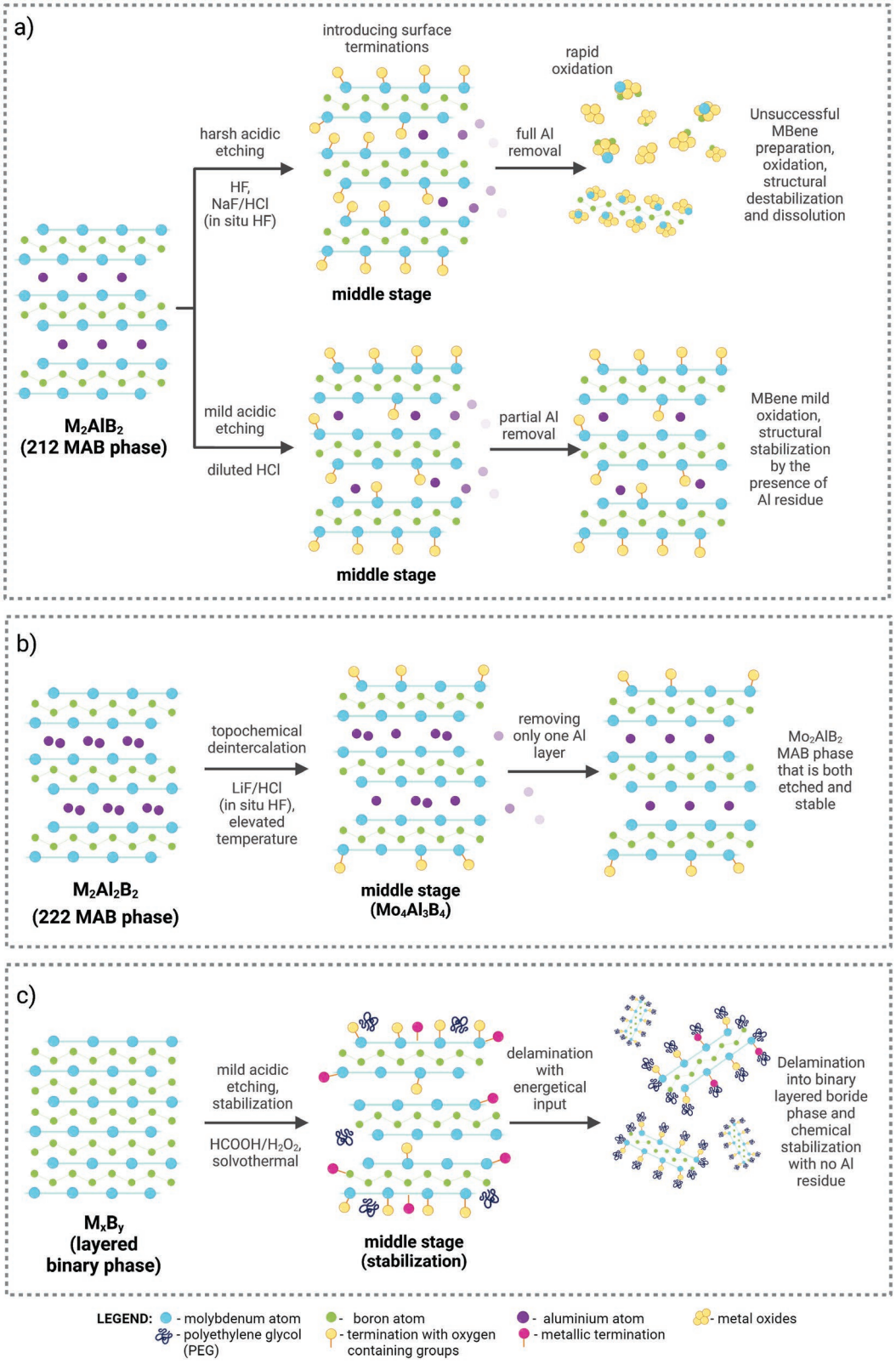

Figure 2. Schematic illustration of various synthesis routes tested for MBenes' synthesis yielding various results. While taking aluminum as the A interleaving element, the procedure may start with: a) layered, ternary M_2AlB_2 MAB phases, b) $M_2Al_2B_2$ phases, and c) bulk layered binary boride phases having an M_xB_y composition. The corresponding wet chemical routes include harsh acidic etching (HF) and mild acidic etching (using HCl or HCOOH). Delamination can be further assisted by various stabilization/capping approaches, temperature, and pressure. a–c) Created with Biorender.com.

was used for further delamination. Notably, $Mo_{4/3}B_{2-x}$ formed 2D boridene sheets with ordered metal vacancies.

Similar to MAX phases, the successful etching of MAB phases was realized using milder acidic conditions (Figure 2a, "second pathway"). Zhang et al. prepared 2D CrB nanosheets by completely removing the Al layers from Cr_2AlB_2 using diluted 0.5 mol L^{-1} HCl solutions (etching time about 7 days at room temperature).[24] Wang et al. demonstrated the possibility of etching Ti_2InB_2 (space group $P6m_2$) with diluted HCl thus obtaining 2D TiB_2 (6.3 wt% of the final product was Ti_2InB_2).[25]

Kim et al. further etched $Mo_2Al_2B_2$ having an orthorhombic crystal structure with 3 M lithium fluoride (LiF)/10 M HCl (aqueous solution) at an elevated temperature of 40 °C for 24 h.[26] During etching, only single Al layers were topochemically etched from the MAB phase (Figure 2b). The $Mo_2Al_2B_2$ etching into Mo_2AlB_2 was confirmed by changing the MoB interlayer distance from 7.1 to 6.1 Å. Interestingly, the etching process involved a phase transformation with $Mo_4Al_3B_4$ being the intermediate phase.

The last synthesis approach is based on the delamination ability of nanolaminated binary M_2B_2 borides (Figure 2c). The use of properly selected etching mixtures and energetic input allows for the generation of 2D flakes, which have the same composition and structure as the original bulk phase. This method was employed by Fan et al. for the bulk MgB_2 phase, which was delaminated into 2D MgB_2 flakes via sonication in a mixture of acetic acid (CH_3COOH) and hydrogen peroxide (H_2O_2).[27] The addition of poly(vinylpyrrolidone) (PVP) resulted in capping of 2D sheets thus facilitating their stabilization. Microwave-assisted MnB defragmentation was developed by Jin et al. for bulk MnB,[28] which was dispersed in ethylene glycol (EG) and etched with CH_3COOH and H_2O_2. During defragmentation, the surface of 2D nanosheets was modified by bismuth ions and additionally capped with PVP. Similar routes were explored for ZrB_2[29] and GdB_6 binary phases.[30]

Due to the possibility of synthesizing MBenes via wet etching approaches, we hypothesize that the existence of surface terminations on the outer MBenes' surface and between the layers is inevitable. Considering the available knowledge about MXenes' surface terminations, we anticipate that similar surface terminations including −O, −OH, −F, and −Cl groups will be present for MBenes.[9c,31] The existence of surface terminations on MBenes has also been experimentally confirmed for CrB MBenes derived from Cr_2AlB_2 via HCl etching (**Figure 3**a). The obtained X-ray diffractograms of the synthesized MBenes could not be fully assigned with the numerically predicted diffractogram of bare CrB without surface terminations (Figure 3b). However, when considering CrB with various arrangements of −OH surface terminations (Figure 3c), the experimental data were accurately fitted with the greatest overlap found for $(CrB)_2(OH)_{ac}$.[32]

In summary, we note that nonalloyed Mo-based phases undergo only partial etching. In contrast, the change from Mo

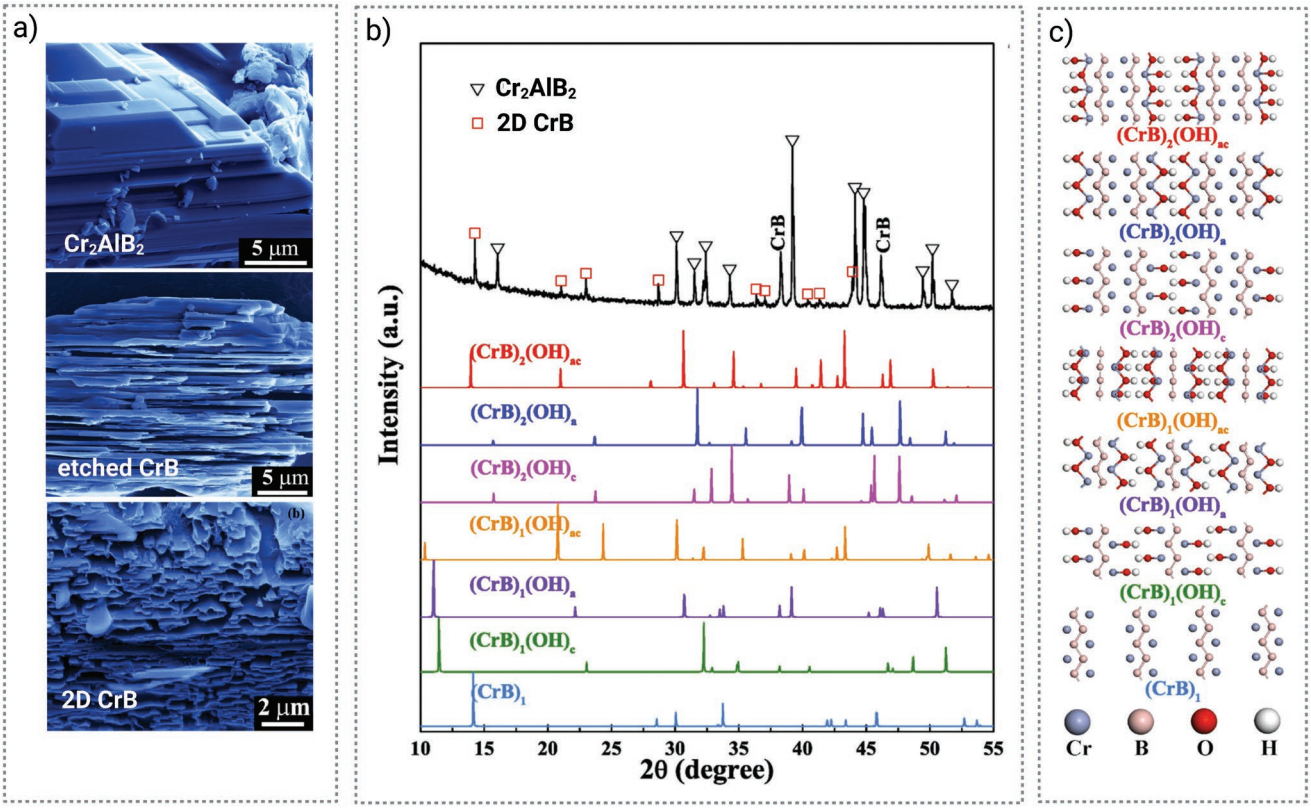

Figure 3. a) Microstructure of Cr_2AlB_2 MAB prior to and after treatment with diluted HCl solutions to obtain 2D CrB MBenes. b) Experimentally measured X-ray diffractograms of Cr_2AlB_2 MAB and derived 2D CrB MBenes were compared with numerically predicted diffractograms of CrB MBenes having different surface terminations. c) Schematic illustration of numerically predicted surface terminations with various spatial arrangements. a–c) Adapted with permission.[32] Copyright 2018, Elsevier.

to Cr allowed for etching under milder conditions. Further oxidation and dissolution of the resulting MBenes as well as potential recrystallization or structural transformations indicate that the removal of Al layers from MAB is a complex process and not completely similar to MAX phases. Ultimately, there are many existing challenges to overcome for MBenes' synthesis and more research needs to be dedicated toward improved synthesis routes.

3. Mechanical Properties of MBenes

The mechanical properties of MBenes are important for a wide range of applications. High-throughput screening based upon DFT calculations allowed for the prediction of MBenes' mechanical properties over a wide range of compositions and stoichiometries.[9a,c,33] Similar to layered ternary carbides and nitrides (MAX phases), MAB phases possess metallic M—A bonds, being weaker than the rest of the bonds thus enabling their reactive liquid-phase delamination.[17] Based upon the Allen scale, the electronegativity of boron (2.05 eV) is lower compared to carbon (2.54 eV) and nitrogen (3.07 eV),[19] which implies a reduced charge transfer for MBenes compared to MXenes ($M_{n+1}X_n$ with X being either carbon or nitrogen). Consequently, we deduce that the M—B bond is expected to be weaker than M—C and M—N bonds in carbide and nitride systems, which points to a reduced thermodynamic stability of MBenes.[19]

Besides metallic bonds, ionic and covalent contributions need to be considered for MBenes. Regarding the ionic contribution, a detailed analysis reveals that there is always a charge transfer from the early transition metal to boron irrespective of the early transition metal considered.[9a] Due to differences in electronegativity when considering the bond between various early transition metals and boron, it has been demonstrated that Hf donates the most electrons to B thus resulting in an increased ionic strength of Hf—B bonds due to a greater charge separation. Less electrons are transferred from Zr and Ti to the boron atoms thus resulting in the lowest ionic strength for Ti—B bonds.[9a]

Moreover, it is well accepted that M—B bonds have covalent contributions. In this regard, M—B bonds are shown to be much stronger than M—A bonds, implying a significant covalent bond contribution in MBenes. Considering different early transition metals, the covalent strength of Hf—B is enhanced compared to Ti—B and Zr—B bonds. We anticipate that this has significant consequences for MBenes' synthesis including liquid-phase delamination as even small changes in the bond strength decide on the ability to generate stable 2D sheets or their potential oxidation.

Based upon the bonding characteristics, the mechanical properties of 2D MBenes, such as in-plane stiffness, can be derived. As demonstrated in **Figure 4**a, the in-plane stiffness of bare MBenes with surface terminations has been predicted to lie between 85 N m^{-1} (Au_2B) and 396 N m^{-1} (V_3B_4).[33] The latter is comparable or even higher than other 2D materials including borophene (398 N m^{-1}),[31] graphene (350 N m^{-1}),[34] $Ti_3C_2T_x$ (326 N m^{-1}),[35] h-BN (273 N m^{-1}), and MoS_2 (125 N m^{-1}).[36] MBenes with an atomic ratio of 1:1 (CrB, MnB, FeB, among others) show predicted in-plane stiffnesses of about 200 N m^{-1}. The origin of the in-plane stiffness could be related to the interplay between B—B and V—B covalent bonding oriented parallelly to the load plane.[37]

Based upon these stiffness values, the gravity-induced monolayer deformation and in-plane strains are estimated to be on the order to 10^{-4} and 10^{-8}, respectively. These values let us hypothesize that MBenes have a sufficient bending rigidity to create freestanding membranes without an underlying substrate.[33] The resulting elastic modulus of pristine MBenes has been shown to be anisotropic (please refer to Table S2 in the Supporting Information). Moreover, the elastic moduli tend to increase with increasing layer thickness in both in-plane directions.[14] Similar to the in-plane stiffness, the elastic moduli of MBenes reach higher or comparable values than other state-of-the-art 2D materials.[14] As displayed in Figure 4b,c, the existence of surface terminations in $Zr_2B_2T_2$ and $Zr_3B_4T_2$ enhances their resulting mechanical properties (e.g., elastic constants, elastic modulus, shear modulus, and Poisson's ratio).

Moreover, MBenes have been predicted to be mechanically stable based upon the Born elastic stability criteria.[38] These criteria are fulfilled for Cr-based MBenes with different stoichiometries including $Cr_{n+1}B_{2n}$ (n = 1, 2, or 3),[14] TiB,[39] MnB,[18a] Mo_2B_2, and Fe_2B_2.[10]

Moreover, Mo-based MBenes, particularly Mo_2B, have been theoretically predicted to form two thermodynamically stable structural configurations (H- and T-types).[12] The H-type configuration of MoB (space group *187*) is structurally similar to MoS_2 and consists of a layer of boron atoms sandwiched by Mo atoms. In contrast, the T-type arrangement shows structural similarities with MoC_2 and belongs to the space group *164*. Both configurations present an energetical difference of only 0.06 eV, while the H-type structure has been predicted to be slightly more stable. Due to small energy difference between both configurations, Zha et al. speculated about the possibility of inducing structural phase transformation between both configurations by applying tensile strains.[12] Considering the energy difference predicted and the existing knowledge about similar transformations happening in other member of the 2D family,[40] we hypothesize that the overall discussion about potential phase transformations in MoB_2 is highly relevant. Therefore, we emphasize that more theoretical and experimental work should be dedicated toward the validation of these initial concepts. This aspect may be particularly important when using MBenes in applications in which mechanical stresses are experienced, such as undergoing tensile stresses or strains (e.g., mechanical sensors, solid lubricant coatings, or lubricant additives).[41]

Taking all these aspects together, MBenes hold great potential to exhibit beneficial mechanical properties, which are comparable to and even superior with respect to other 2D nanomaterials. Phonon calculations[18,42] and molecular dynamics (MD) simulations[17,18,42b] showed the dynamic stability for MBenes with different stoichiometries including MB (M = Sc, Ti, V, Y, Zr, Nb, Mn, Mo, Fe, Hf, Ta, and W), MB_2 (FeB_2, RuB_2, and OsB_2), M_2B_2 (V_2B_2, Fe_2B_2, Cr_2B_2, and Mn_2B_2), and M_3B_4 (Nb_3B_4, Ta_3B_4, and Cr_3B_4).[18,42] Moreover, MD calculations proved the room-temperature stability of Mn_2B_2 and Mn_3B_4 monolayers.[17]

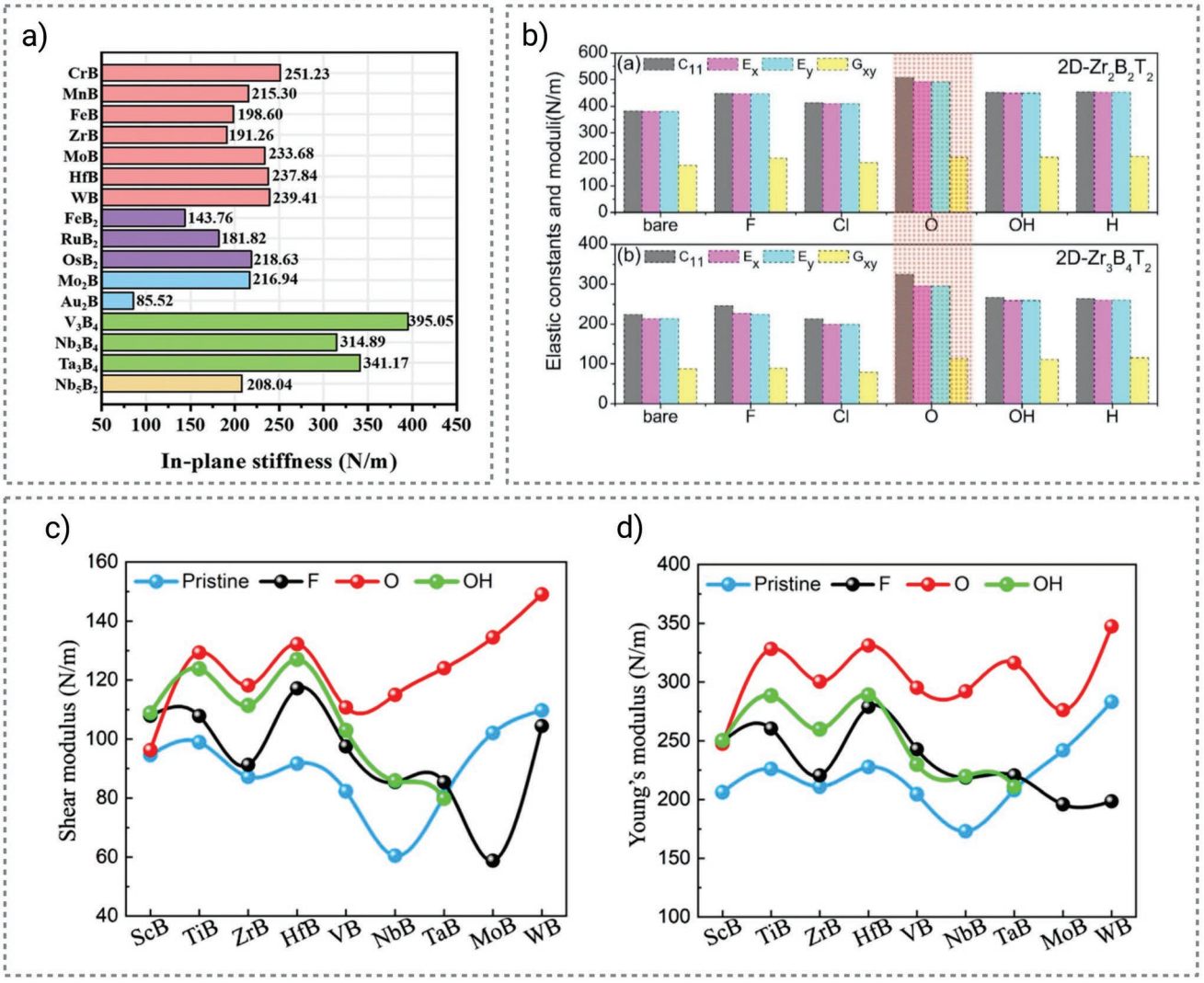

Figure 4. a) In-plane stiffness of 16 different pristine MBenes with variable stoichiometry and early transition metals. Adapted with permission.[33] Copyright 2021, Wiley-VCH. b) Numerically predicted elastic constants, elastic modulus, and shear modulus for $Zr_2B_2T_2$ and $Zr_3B_4T_2$ with different surface terminations. Adapted with permission.[19] Copyright 2020, American Chemical Society. c) Predicted shear and d) Young's modulus for MBenes with different early transition metals and surface terminations. c,d) Adapted with permission.[9a] Copyright 2021, IOP Publishing.

4. Prospective Physical Properties of MBenes

Defects, dopants, terminating groups, and vacancies play a crucial role in tailoring physical properties of atomically thin materials. MBenes' modifications and structural diversity can lead to drastic changes of various properties including their electronic properties reflected in band structure calculations, which might be further confirmed by experimental studies. In general, pristine MBenes such as Fe_2B_2, Cr_2B_2, W_2B_2, ScB, Mo_2B_2, or Mn_2B_2 are metallic in nature.[9a,10,17] Their electrical conductivity originates from the d states of transition metals, which lie in close proximity of the Fermi level (E_F).[9a,11,17] Depending on the synthesis route and the chemical reactivity of transition metals, various surface terminations are present. Surface terminations including C, F, O, and OH for Sc-, Mo-, V-, W-, Ti-, Zr-, Hf-, Nb-, and Ta-based MBenes preserve the metallic or semimetallic character of the mother compounds. In contrast, ScBO has been predicted to be an indirect-bandgap semiconductor.[9a] The electronic properties of various surface-terminated MBenes are summarized in Table S4 (Supporting Information).

However, it is important to point out that predictions of the electronic structure significantly depend on the calculation method used. It is well known that standard exchange-correlation functionals notably underestimate the bandgaps, thus often predicting metallic states. Moreover, 3d open shells of early transition metals are delocalized and generally wrongly aligned with respect to Fermi level in generalized gradient approximation (GGA) or local density approximation (LDA) approaches.[43] Furthermore, except DFT+U, other methods such as GW calculations,[44] hybrid,[45] or meta-GGAs' functionals[46] are highly computationally demanding. Although GW (where G stands for the one-body Green's function and W for the dynamically screened Coulomb interaction) approaches are considered to accurately describe the electronic structure of many systems,[47]

they have still restrictions regarding the number of atoms considered in the supercell and the involved computational effort. Thus, experimental results are urgently needed to back up theoretical claims, thus helping to refine numerical modeling.

Most ceramic systems are semiconductors, and the observed bandgap-related exception for MBenes may open doors for new types of structures for functional devices. Since MBenes do not exhibit a bandgap, the lack of optical properties should also be expected, and quantum-confinement effects have not been fully explored. Nevertheless, as metallic systems, MBenes may exhibit surface plasmon resonance (SPR)[9a,48] of the conduction band electrons undergoing collective oscillations (surface plasmons) thus enabling the fabrication of highly advanced real-time biosensors.

Additionally, high electrical and thermal conductivities have been reported for specific structural configurations of Mo_2B.[12] Similar to $Sc_2C(OH)$ and Mo_2CF_2 MXenes, which exhibit exceptional thermoelectric properties,[49] semiconducting MBenes with good electrical conductivity are expected to possess large Seebeck coefficients. This makes them promising thermoelectric materials, potentially suitable for energy-conversion applications. Moreover, the TiBF monolayer exhibits interesting topological features and can be considered as a new 2D topological metal.[50]

Regarding MBenes' properties, their magnetic properties are worth consideration, since these properties are important for their application in data storage, water purification, energy generation, and biomedicine. While these applications are generally based on using conventional 3D magnets, the application of atomically thin and light materials, reducing the size of the corresponding devices, is highly desirable. The first experimental observation of the intrinsic magnetic order was reported in 2017,[51] generating enormous attention to the field of 2D magnetic crystals and the search of novel atomically thin magnetic materials. Although 2D magnets are extremely difficult for practical applications, they could be potentially realized using MBenes. MBenes' magnetic properties arise from the partially filled d orbitals of the early transition metals.[18a,42a] Ferromagnetic ground states have been predicted for bare Cr_2B_2, Ti_2B, and Mn_2B_2 monolayers.[18b,42a] In particular, Mn_2B_2 is a metallic material exhibiting robust ferromagnetism with a Curie temperature (T_C) of about 345 K, which was determined by Monte Carlo simulations. The T_C value can be greatly enhanced by surface functionalization with −OH (600 K) and −F (405 K) groups. Interestingly, the T_C of pristine MnB is greater than the values of other 2D magnetic materials such as FeC_2 (245 K), MnO_2 (140 K), or MnPc (150 K).[18a] This exemplifies that MBenes can be a source for 2D magnets operating at room temperature. Another study has already demonstrated that Fe_2B_2, Ni_2B_2, Fe_2B_2, Cr_2B_2, and Mn_3B_4 tetra-Cr_2B_2 structures exhibit antiferromagnetism.[17]

Additionally, M-alloying in the case of tetra-$CrMnB_2$ and tetra-$CrVB_2$ unlocks ferromagnetic states[11] with tunable magnetic anisotropy for tetra-$CrMnB_2$ and tetra-$CrVB_2$.[52] This implies that antiferromagnetic to ferromagnetic transitions can be induced by modifying the dopant concentration. Like other layered materials, we hypothesize that magnetic phase transitions in MBenes could also be realized by applying strains, changing the doping concentration, applying voltage, or modifying the magnetic properties via adjacent layers coming from van der Waals heterostructures.

5. Applications Envisioned for MBenes

The structural and morphological features play an essential role in achieving unique properties for MBenes at the micro- and nanoscale, thus enabling various applications, which are schematically depicted in **Figure 5** and span from energy harvesting to specific biological responses. In terms of energy harvesting, Ma et al. calculated the theoretical gravimetric capacity of Na-intercalated MBenes thus verifying that they have an excellent Na-intercalated chemical stoichiometry with a great potential to be used as anode materials.[53] Gunda et al. confirmed MBenes' excellent ionic conductivity together with an enhanced intercalation efficiency for Na ions between MB monolayers compared to transition metal dichalcogenides.[54] Additionally, small diffusion energy barriers and increased storage capacities for Li atoms were found for MBenes.[33] Taking all these aspects together, we assume that MBenes are prospective electrode materials for Na- and Li-ion batteries.[11]

MBenes are expected to have excellent catalytic properties. Their catalytic activity is determined by their chemical composition, metallic properties, and negligible hydrogen adsorption. Liu et al. theoretically demonstrated that the value of the Gibbs free energy (ΔG) decreases with an increasing H adsorption on the surface of Mn_2B_2 and Fe_2B_2.[17] Moreover, the calculated energy levels of the d-band center for these MBenes satisfied the target criterion for catalysts (from −6.4 to −5.5 eV).[17] Zhang et al. showed an increasing catalytic activity of Cr-based MBenes with the formula $Cr_{n+1}B_{2n}$ with increasing n from 1 to 3. Cr_4B_6 MBenes used as hydrogen evolution reaction (HER) electrocatalysts showed an overpotential of 0.003 V when fully covered with a H layer on the surface.[14] This value was significantly lower than Pt's overpotential (0.009 V) thus demonstrating the excellent electrocatalytic properties of Cr_4B_6 MBenes.[14] Moreover, Zhang et al. showed the possibility of using TM@Mo_2B_2 and Ni@Mo_2B_2 as HER catalysts for water splitting with low ΔG (−0.09 eV) when covered with a 1/4 of H atoms on the surface.[15]

MBenes can be also used for the nitrogen reduction reaction (NRR),[55] or as a bifunctional electrocatalyst in the oxygen evolution reaction (OER) and oxygen reduction reaction (ORR).[15] For instance, Cu@Mo_2B_2 showed a lower OER/ORR overpotential (0.31 V) compared to IrO_2 (0.56 V) and Pt (0.45 V).[15] Based on these findings, we emphasize that MBenes are an interesting alternative to current electrocatalysts based on Pt.

The prospective biological properties of MBenes were thoroughly reviewed in our previous work.[52] The key factor toward MBenes' bioactivity, as found for MXenes and other 2D nanomaterials, may be their structural and chemical properties, closely related to their synthesis route and conditions.[9c,52] The resulting structural inhomogeneity and chemical variability of MBenes[9c] points toward the existence of synthesis-induced surface terminations. We speculate that the rich surface chemistry of MBenes will determine their environmental stability. For instance, the high water stability of MgB_2 asks for future research to understand the mechanisms of interaction with biological matter.[27] Additionally, MBenes are characterized by self-activating processes thus reducing O*/OH* into H_2O*. The potential antioxidative nature of MBenes may be beneficial for the development

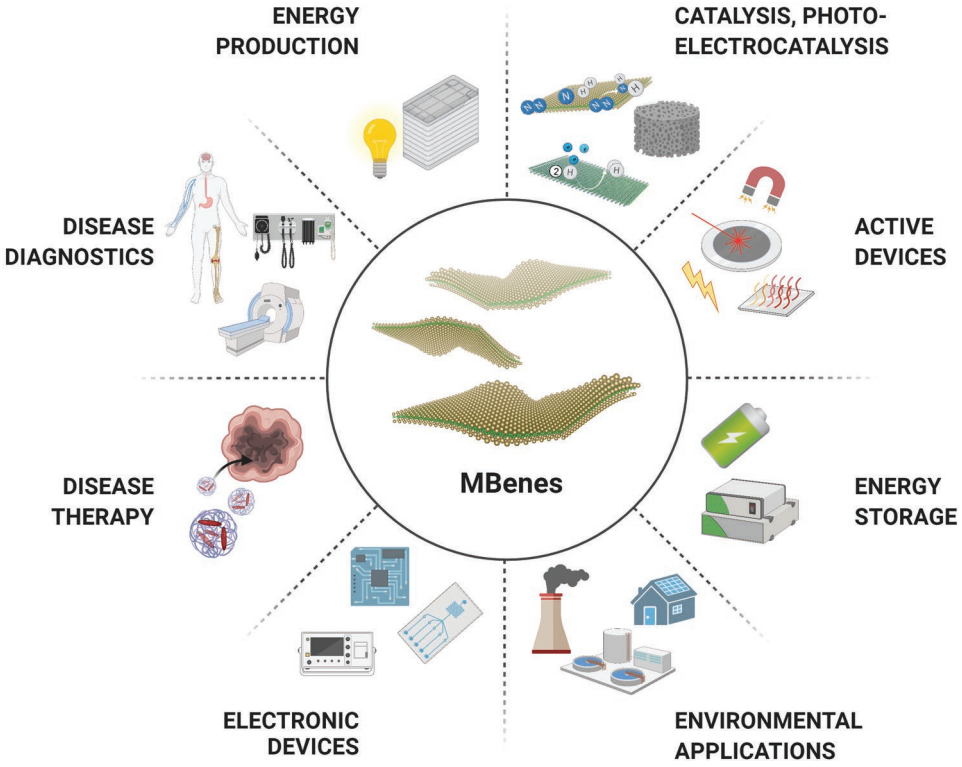

Figure 5. Schematic illustration of MBenes' wide range of potential applications. Created with Biorender.com

of drug delivery systems. Moreover, surface oxidation will additionally affect MBenes' bioactivity.[56] Surface Pourbaix diagrams combined with the selectivity analysis revealed that several MBenes (CrB, MoB, or Mo_2B) can resist surface oxidation, regardless of pH.[33]

Further active tuning of MBenes' properties is crucial for their application in many fields. As demonstrated for MXenes, it can be suspected that their properties can be tuned by chemical modification with various functional moieties due to the presence of surface terminations.[42c,52] It has already been demonstrated that Bi atoms can be anchored onto MnB_2 nanosheets. Further modifications with hyaluronic acid (HA) via borate esterification resulted in a good dispersion of monolayer Bi-anchored MnB_2 and active tumor targeting.[28] The same results were observed for zirconium boride modified with HA, for which the presence of large amounts of borohydroxyl groups facilitated their surface modification.[29] In a different approach, MgB_2 nanosheets were combined with PVP for an effective hydrogen chemotherapy. These composites were not only biocompatible, but also stable in normal tissues/blood environments.[27]

6. Summary and Outlook

This perspective summarizes the existing theoretical and experimental understanding of the material–property relationship for MBenes, thus inspiring future research on these highly prospective materials. MBenes are a new family of 2D materials with the potential to become a recognized advancement over other 2D materials. While compared to other 2D materials obtained via top-down approaches, MBenes constitute a more complex structure due to a wider range of initial crystallographic arrangements, involved polymorphisms, and potential structural transformations of MAB phases. Consequently, finding promising candidate for MBenes' synthesis is still challenging.

However, despite promising theoretical results about the strength of M—B bonds against the weakness of M—A bonds, some MAB phases (e.g., $Mo_2Al_2B_2$) turned out to undergo only partial etching due to reactions with acids. In contrast, other MAB phases (e.g., Cr_2AlB_2) experienced intense etching under mild acidic conditions. Some studies verified severe oxidation of MAB phases as well as potential recrystallization and structural transformations. However, it is still a matter of ongoing research whether these methods will be able to yield the desired efficiency.

Since MBenes have only been partially synthesized so far, thus asking for more research progress regarding the successful synthesis, experimental studies on MBenes' structure–property relationship remain scarce. Due to the very early stage of development, little is known about their physical and chemical properties, which have mainly been predicted theoretically. The conducted theoretical calculations regarding the bond strengths of M—A, M—B, and B—B bonds as well as the impact of surface terminations significantly contribute to the search of MAB phases that could be used for experimental studies. Excellent mechanical, electronic, metallic/semiconducting, capacitive, and thermoelectric properties have been predicted for MBenes. Recent developments

of ab initio methods and powerful supercomputers enable high-throughput energetical calculations for chemical reactions to be performed. Combining these approaches with machine-learning approaches will enable the screening of thousands of new MBene systems and delamination reactions, thus greatly expanding the number of their 2D derivatives, and hence, 2D material databases.

We foresee that overcoming the synthesis bottlenecks will enable a rational control over MBenes' properties. Further development of postprocessing approaches will open a door for designing new functional structures with extraordinary stability, strength, conductivity, transition properties, and energy-harvesting properties. These may be used for designing promising next-generation devices for application in spintronics, HER, NRR, OER, ORR, energy production and storage, or even in various biomedical fields.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contribution

V.G.N. and M.B. contributed equally to this work. V.G.N. and M.B. analyzed the theoretical data and provided the insight into MAB and MBenes' structures; D.B. analyzed MBenes' catalytical properties and related applications; M.J. analyzed the biological properties and relevant applications; A.R. analyzed and gave the insight into the mechanical properties of MBenes; A.M.J. developed the concept of the review study, designed the structure of the manuscript, collected and analyzed the obtained data, provided the insight into MBenes' synthesis and physicochemical features, supervised the research as a project leader, and coordinated the preparation of the manuscript. All authors helped to prepare, correct, and proofread the manuscript.

Keywords

2D structures, MAB phases, MBenes, nanolaminated, transition metal borides

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Varun G. Nair is a doctoral student at the Warsaw University of Technology, Warsaw, Poland, Faculty of Materials Science and Engineering under the guidance of Prof. Agnieszka M. Jastrzębska (Warsaw University of Technology) and Dr. Magdalena Birowska (University of Warsaw). His research interests comprises 2D materials, thin films transparent conducting oxides, using density functional theory and machine-learning methods.

Magdalena Birowska is an assistant professor at the Institute of Theoretical Physics at the University of Warsaw (UW). Her research works are concentrated in the fields of nanotechnology, condensed matter physics, and spintronics. Her research activities focus on the understanding of the physical properties of nanomaterials by means of theory and simulations, using a range of computational methods: amongst others, density functional theory, tight binding, and Monte Carlo simulations. Her current research works are devoted to the prediction of various physico-chemical properties of the novel 2D materials and van der Waals heterostructures by means of first-principles calculations.

Dominika Bury is a doctoral student at the Warsaw University of Technology (WUT), Faculty of Materials Science and Engineering, Department of Ceramic and Polymer Materials. As part of her engineer and master's thesis, she researched the efficiency of the heterogeneous Fenton process with iron catalysts in the degradation of cosmetic wastewater. Her further studies cover the analysis of the heterogeneous Fenton process in the degradation of industrial wastewater using phases of MXenes as catalysts. In addition, she analyzes the photocatalytic properties of nanomaterials and their application of the process in the degradation of pollutants.

Michał Jakubczak is a doctoral student at the Warsaw University of Technology, Faculty of Materials Science and Engineering. He graduated from Faculty of Building Services, Hydro and Environmental Engineering of the Warsaw University of Technology, where he took a special interest in microbiology and ecotoxicology. As part of his engineer and master's thesis, he redirected his research toward nanotechnology as he investigated antibacterial properties of nanooxides and MXenes. His current research interests concern 2D nanomaterials, and the efficient combination of interdisciplinary knowledge, which allows for taking a fascinating pathway toward their mechanisms of interactions and bioactivity.

Andreas Rosenkranz is a Professor forf Materials-Oriented Tribology and New 2D Materials in the Department of Chemical Engineering, Biotechnology and Materials (University of Chile). His research focuses on the characterization, chemical functionalization, and application of new 2D materials. His main field of research relates to tribology, but in recent years, he has expanded his fields of interest toward water purification, catalysis, and biological properties. He has published more than 100 peer-reviewed journal publications, is a fellow of the Alexander von Humboldt Foundation, and acts as a scientific editor for different well-reputed scientific journals including Applied Nanoscience and Frontiers of Chemistry.

Agnieszka M. Jastrzębska is a Professor at the Warsaw University of Technology (WUT). She leads an interdisciplinary research team at the Faculty of Materials Science and Engineering, Department of Ceramic and Polymer Materials. Her research works are concentrated in the area of nanotechnology for bioactive materials with multifunctional hybrid nanocomposite structures. The current fields of interest comprise biomedical, environmental, and catalytic applications of novel 2D materials with emphasis given to their cyto- and ecotoxicological effects observed at relevant exposures.