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Life-Cycle Assessment of $Ti_3C_2T_x$ MXene Synthesis

Mostafa Dadashi Firouzjaei, Srinivasa Kartik Nemani, Mohtada Sadrzadeh, Evan K. Wujcik, Mark Elliott,* and Babak Anasori**

MXenes, 2D transition metal carbides, nitrides, and carbonitrides, have been investigated for diverse applications since their discovery; however, their life-cycle assessment (LCA) has not been studied. Here, a "cradle to gate" LCA is performed to assess the cumulative energy demand (CED) and environmental impacts of lab-scale synthesis of $Ti_3C_2T_x$, the most researched MXene composition. Electromagnetic interface (EMI) shielding is selected as it is one of MXenes' most promising applications and LCA of $Ti_3C_2T_x$ synthesis is compared to aluminum and copper foils, two typical EMI-shielding materials. Two laboratory-scale MXene synthesis systems—gram and kilogram batches—are examined. The CED and environmental implications of $Ti_3C_2T_x$ synthesis are investigated based on its precursor production, selective etching, delamination processes, laboratory location, energy mix, and raw material type. These results show that laboratory electricity usage for the synthesis processes accounts for >70% of the environmental impacts. Manufacturing 1.0 kg of industrial-scale aluminum and copper foil releases 23.0 kg and 8.75 kg of CO_2, respectively, while 1.0 kg of lab-scale MXene synthesis releases 428.10 kg. Chemical usage is less impactful than electricity, which suggests that recycled resources and renewable energy can make MXene synthesis more sustainable. Understanding MXene LCA helps the industrialization of this material.

1. Introduction

Resilient energy generation and storage are crucial as the first-generation power resources are being phased out[1] and sustainable development goals are being incorporated into energy planning.[2] Nanomaterials, due to their high surface areas and unique conductive, optical, and thermal properties, have been proposed as a viable option for low-cost and sustainable energy infrastructure[3] and are being adopted in clean energy generation and storage technologies such as in lithium/sodium-ion batteries,[4] solar cells,[5] and fuel cells.[6] Among various types of nanomaterials, 2D MXenes have gone from discovery to commercial products in only a decade.[7]

MXenes are a group of inorganic 2D nano carbides, nitrides, and carbonitrides that are only a few atoms thick with a thickness of about one nanometer.[8] Since their discovery in 2011,[9] MXenes have quickly found applications in materials science and nanotechnology.[7a] More than 150 precursor compositions of MXenes (the MAX phases[10]) and ≈50 MXene compositions have been synthesized to date while many more have been predicted theoretically.[8,11] To date, MXenes have found applications in many sectors, including supercapacitors,[12] energy storage devices,[13] and electromagnetic interference (EMI) shielding.[14]

Thus far, all the studies on MXenes have focused on characterizing lab-scale synthesized MXenes, corresponding to batch sizes

M. Dadashi Firouzjaei, S. K. Nemani, B. Anasori
Department of Mechanical and Energy Engineering
Purdue School of Engineering and Technology and Integrated Nanosystems Development Institute (INDI)
Indiana University-Purdue University Indianapolis
Indianapolis, Indiana 46202, USA
E-mail: mdfirouzjaei@crimson.ua.edu; banasori@iupui.edu

M. Dadashi Firouzjaei, M. Elliott
Department of Civil, Environmental, and Construction Engineering
University of Alabama
Tuscaloosa, AL35487, USA
E-mail: melliott@eng.ua.edu

M. Sadrzadeh
Department of Mechanical Engineering
10–367 Donadeo Innovation Center for Engineering
Advanced Water Research Lab (AWRL)
University of Alberta
Edmonton, AB T6G 1H9, Canada

E. K. Wujcik
Materials Engineering and Nanosensor [MEAN] Laboratory
Department of Chemical and Biomedical Engineering and the Advanced Structures & Composites Center [ASCC]
The University of Maine
Orono, ME 04469, USA

B. Anasori
School of Materials Engineering
Purdue University
West Lafayette, IN 47907, USA

The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/adma.202300422

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from <1 gram to 50 grams.[15] However, even the same MXene composition including the most studied $Ti_3C_2T_x$, can be synthesized via myriad pathways using various etching routes, leading to varying yields and functionalities.[16] To date, the environmental impacts of MXene synthesis have not been assessed systematically. The lack of this knowledge might result in missed opportunities to incorporate green-ness into the scale-up and industrialization of MXene production.

Here, we investigate the "cradle to gate" (from raw material extraction to manufacturing) in-scope life-cycle assessment (LCA) to calculate the cumulative energy demand (CED) and environmental impacts of producing $Ti_3C_2T_x$ MXene as a coating layer for communications satellites' EMI shielding. EMI shielding was selected because it is one of the MXene applications with detailed and generalizable performance metrics and due to the broad scope of its potential application.[17] Any electronic device that distributes, uses, or transmits electrical energy generates EMI, which can negatively affecting the environment and the device's performance.[14a] A significant increase in EMI can cause electronics to fail and degrade when they work at faster speeds and with smaller parts.[18] If no shielding is offered, this rise in electromagnetic pollution may also have an impact on people's health and the environment.[19]

MXene, particularly $Ti_3C_2T_x$, has high electrical conductivity, layered structure, and high surface areas, making it ideal for a variety of applications, including EMI shielding.[7b] Additionally, MXenes are hydrophilic, enabling them to bond readily to other substances and can be used for surface coatings.[20] MXenes have a high degree of solubility in specific solvents and can be integrated into different metal and ceramic matrices, which allows them to be used in the fabrication of composite materials.[21] These combinations of MXenes' properties makes them highly desirable for EMI shielding, which resulted in substantial research on this application.[17] In comparison, traditional EMI-shielding materials, such as copper and aluminum, can be heavy, bulky, and difficult to work with and to deposit on different surfaces.

As MXene is not yet employed for industrial-scale applications,[22] we evaluate two lab-scale sizes of MXene synthesis in this study. A small lab scale (19.2 g per batch) that will be referred to as a gram-size batch, labeled as g-$Ti_3C_2T_x$ MXene, and a large laboratory scale (800 g per batch) that will be referred to as a kilogram-size batch and labeled as kg-$Ti_3C_2T_x$ MXene. We curated the inventory data from our lab data and various published studies on laboratory-scale syntheses of MXene. Additionally, we look into the effects of laboratory location and energy mix on the CED and environmental impacts of MXene, and the usage of TiO_2 instead of Ti as the raw material for producing the MXene precursor. The present work is the first report on the LCA of any MXene composition. LCA requires a highly specific application and ideally, a performance comparison between the proposed and incumbent technologies. While EMI shielding has many specific applications, we selected communication satellites in this study because it is a well-known platform that requires EMI shielding and for which the detailed data required for LCA were available. To the authors' knowledge, no prior research has evaluated the CED and environmental impacts of MXene production. The information and findings from this study aim to provide directions for green synthesis and future sustainable MXene research while also filling informational gaps in the current life-cycle inventory.

2. Experimental Section

2.1. Synthesis of $Ti_3C_2T_x$ MXene and Scope of the Analysis

$Ti_3C_2T_x$ MXene can be synthesized via different routes. The LCA described in this article was based on experimental data collected during the synthesis of $Ti_3C_2T_x$ MXene in a laboratory using an aqueous acid mix that was known to give high-quality MXene flakes[23] and it is scalable across the range of masses used in laboratories.[15] The first step in the $Ti_3C_2T_x$ MXene synthesis was to make the precursor structure, known as the MAX phase, from the raw elemental powder mixture. Titanium, aluminum, and graphite powders in a stoichiometric ratio of 3:1:2 (molar ratio) were mixed in a tumble ball mill for 18 h. The mixture was then placed in a tube furnace and heated to 1400 °C with a 3.5°C min^{-1} heating rate and held for 2 h, followed by furnace cooling. MAX phase crushing to powder was not considered in LCA calculations. In LCA, this synthesis portion was referred to as MAX phase production.

One gram of Ti_3AlC_2 was then etched for 24 h at 35 °C in 3 mL of 48% HF, 18 mL of 37% HCl, and 9 mL of deionized (DI) water. Post-etching, the solution will be centrifuged repeatedly to obtain a neutral solution (50 min of centrifugation was considered for kg-$Ti_3C_2T_x$ and 25 mins for the g-$Ti_3C_2T_x$ in the etching process). After that, the multilayered MXene will be filtered and stored overnight under a vacuum. In our LCA, this step in the synthesis was referred to as the etching process, which leads to MXene multilayer particles. The next step in MXene single-to-few flake solution synthesis was the delamination of the multilayer particles. Delamination can be done using different intercalants, such as fluoride or chloride salts. In our method, 1 g of multilayered $Ti_3C_2T_x$ MXene is mixed with 1 g of LiCl and 50 mL of DI water. This mixture was then stirred at 65 °C under an argon atmosphere for 3 h before being subjected to cycles of washing and centrifuging to remove $Ti_3C_2T_x$ MXene. In this step, the total time of centrifugation for the kg-$Ti_3C_2T_x$ was 7.5 h and 3.75 h for the g-$Ti_3C_2T_x$. This part was called the delamination process in LCA. This method of etching and delamination (HCl-HF with LiCl) leads to high-quality $Ti_3C_2T_x$ MXene flakes with fewer defects and higher electrical conductivity[23,24] and it was scalable because of its solution-processability (**Figure 1**).[15]

2.2. Life-Cycle Assessment Methodology

This study aims to evaluate the energy and environmental impacts of producing $Ti_3C_2T_x$ MXene for EMI shielding of a communication satellite. First, three materials and four systems: copper foil and aluminum foil, as the two metals with high EMI-shielding effectiveness were evaluated, and two $Ti_3C_2T_x$ MXene systems (gram batch and kilogram batch). Second, the three fundamental steps in fabricating $Ti_3C_2T_x$ MXene: precursor MAX phase production, etching, and delamination processes were examined. Third, the effects of LCA flow types by three primary categories: I) waste, II) chemicals, and III) electricity were examined. Fourth, the flows in the chemical group and compare

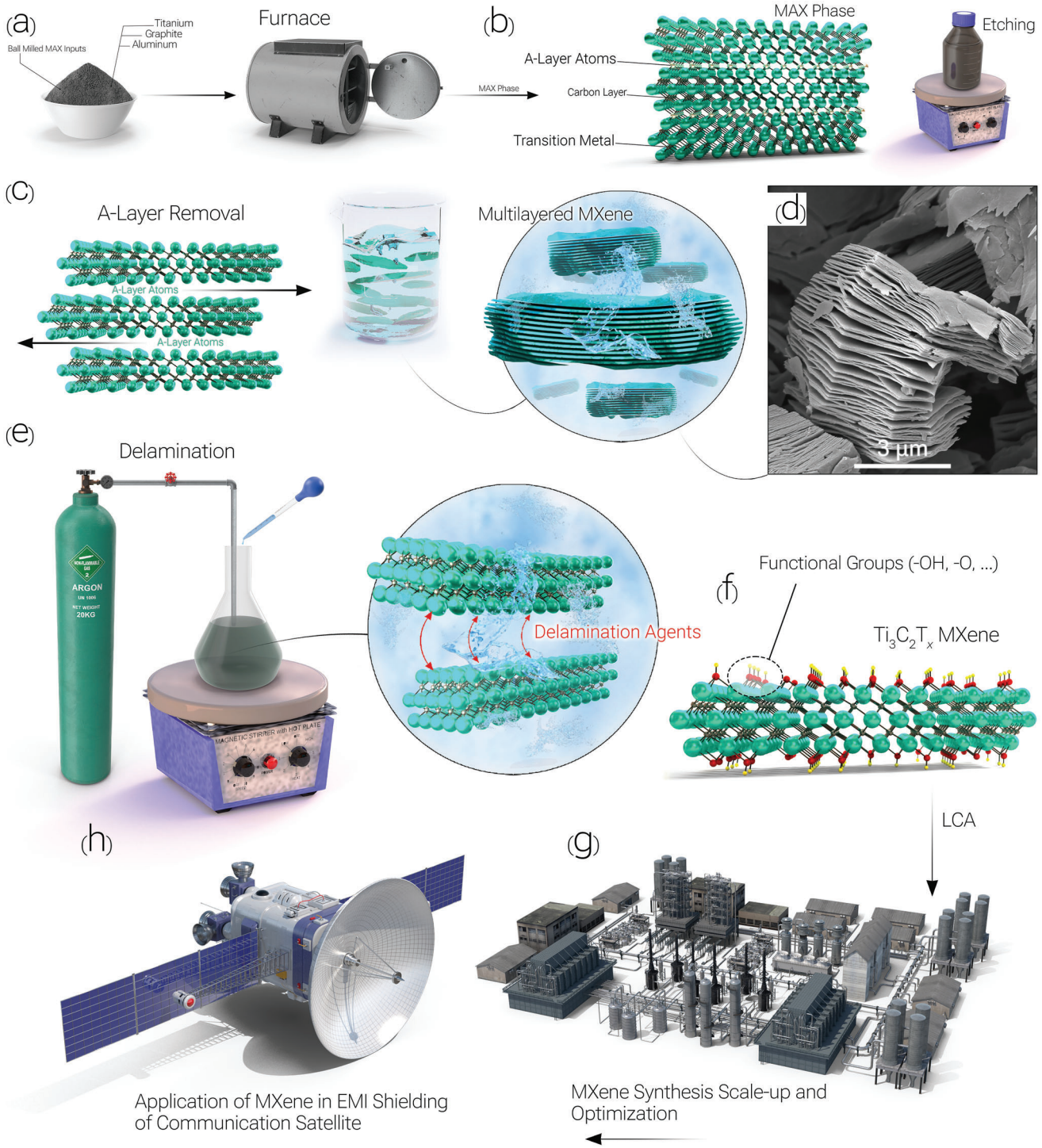

Figure 1. Schematic representation of the production of MXene on a small scale for potential industrial use. a) In this study, aluminum, titanium, and graphite powders are mixed and then heated in a tube furnace to produce the MAX phase. b) The chemical structure and etching procedure of Ti_3AlC_2 MAX phase. c) The A-layer atoms (aluminum) are first removed through selective etching in the topochemical production of MXene, leaving behind stacked MXene flakes.[25] To separate the layers and create MXene, additional processes are required. d) Scanning electron microscopy (SEM) image of multilayered MXene. e) The delamination procedure. Delamination agents are used in this stage to intercalate between the stacks of MXene flakes and separate the single flake MXene from multilayered MXenes. f) The $Ti_3C_2T_x$ MXene structure. The MXene surface can be functionalized with a variety of functional groups that are appropriate for the intended use, depending on the agents used in the etching and delamination phases.[26] g) A schematic for the LCA-based optimization of MXene synthesis and its potential for large-scale synthesis. h) The MXene surface coating for EMI shielding of communication satellites is the intended use of this work.

Table 1. The definition of case studies. The column shows the materials used for LCA and compares their properties..

	Thickness t [cm]	SSE/t [dB cm^2 g^{-1}]	Shielding effectiveness constant [dB]	Production amount [kg]	Ref.
$Ti_3C_2T_x$ MXene	0.0011	25 863.0	60	2.3	[14a]
Aluminum Foil	0.0008	30 555.0	60	2.0	[14a]
Copper Foil	0.001	7812.0	60	7.7	[14a]

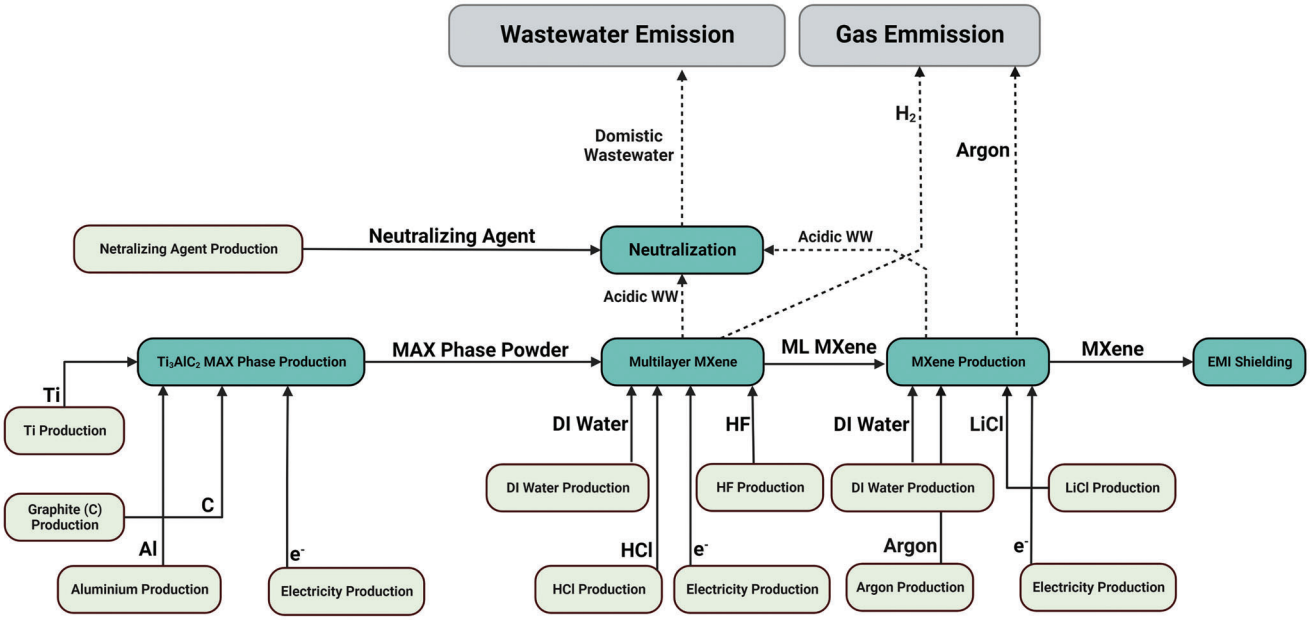

Figure 2. The conceptual synthesis schematic of $Ti_3C_2T_x$ MXene illustrating the processes involved in the production of MXene. Four key steps are involved in manufacturing MXene: waste treatment, MAX phase synthesis, multilayered MXene production, and single flake MXene production. Ball milling and heat treatment in a furnace is used in the first stage of MAX phase manufacturing to create a precursor for the synthesis of MXene. Creating MXene is a topochemical process that begins with removing the A-layer (mainly aluminum). Multilayered MXene is provided at this stage and must be delaminated. The delamination process allows MXene flakes to be extracted using inorganic salts and centrifugal/ultrasonic mechanical force. These procedures produce waste that must be treated prior to disposal.

the impact of each chemical used in $Ti_3C_2T_x$ MXene production was expanded. We also assess the impact of replacing titanium powder as the raw material in the precursor (MAX phase) synthesis with titanium dioxide. Finally, it was investigated how the lab's location affects the environmental impacts of manufacturing $Ti_3C_2T_x$ MXene. The calculations were performed using the ecoinvent database and the OpenLCA software.

2.2.1. Functional Unit, System Boundary, and Life-Cycle Impact Assessment

In this system, EMI shielding of a communication satellite with a known surface area as the application for the synthesized MXene was selected. Based on the assumption for the outer surface area of communication satellites, a surface size of 100 m^2 that requires a constant 60 dB shielding was estimated. $Ti_3C_2T_x$ and Ti_3CNT_x MXene films were known to have the highest EMI-shielding effectiveness among all nanomaterials, along with copper and aluminum foil.[14a,27] Specific EMI-shielding effectiveness (SSE) was used as a metric to compare various materials with different densities. However, thickness plays a critical role in EMI shielding as greater thickness of films leads to higher SSE while also increasing the launching cost associated with increased weight.[28] To include the thickness in shielding effectiveness, SSE/t was defined as SSE divided by material thickness (t). In our LCA calculations, we used SSE/t to determine the mass of materials required and selected constant shielding effectiveness of 60 dB, which corresponds to 99.9999% shielding efficiency (**Table 1**). The cradle-to-gate system boundaries for using the LCA methodology to synthesize $Ti_3C_2T_x$ MXene were shown in **Figure 2**. Aluminum and copper foil LCA calculations were performed using the ecoinvent database.[29] For both aluminum and copper foil production, two sets of sheet rolling were considered along with one section bar extrusion. In each rolling step, sheets with ultimate thicknesses of 0.2 to 6.0 mm were produced by hot and cold rolling of aluminum/copper ingots of 500- to 700-mm thickness. The copper cathode used in this study includes steps such as ore grounding, gravity concentration, ore preparation before hydrometallurgy, dump leaching for copper recovery, solution cleaning, and separation; all were included in the

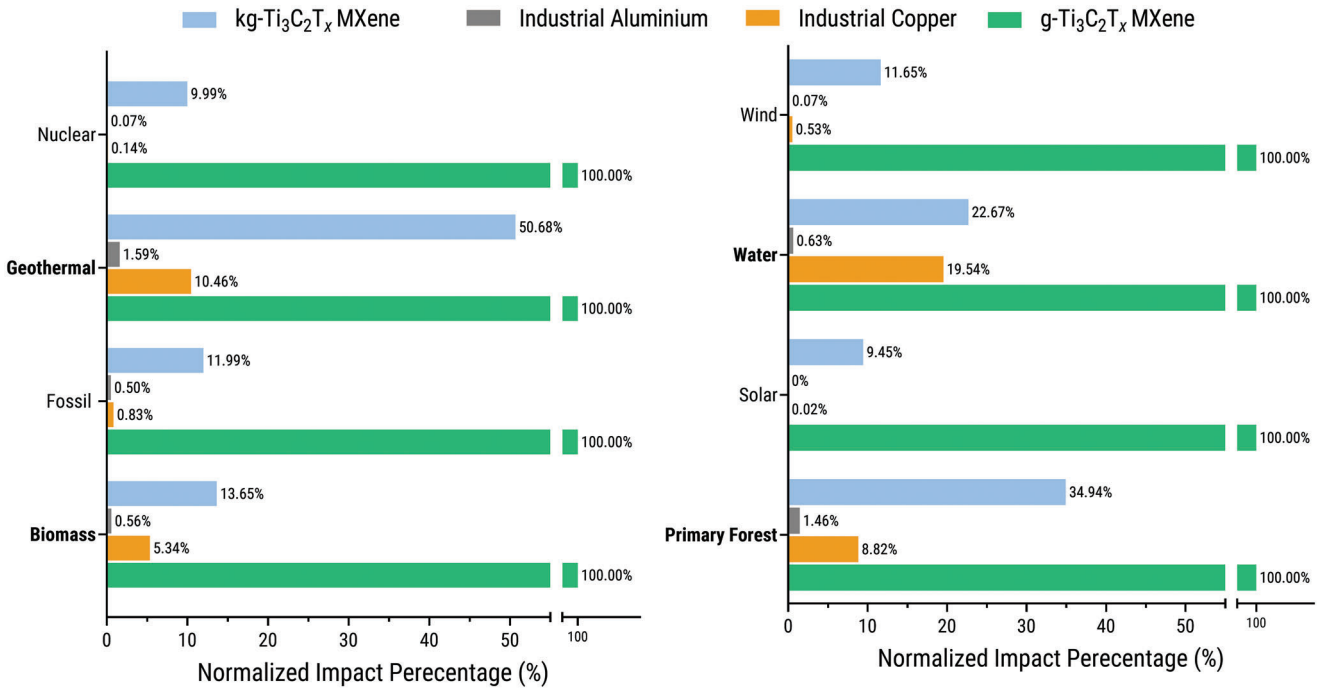

Figure 3. The normalized energy demands of producing kg-$Ti_3C_2T_x$, g-$Ti_3C_2T_x$, copper, and aluminum foil. g-$Ti_3C_2T_x$ MXene serves as a reference for the rest of the systems.

dataset. Production infrastructure used directly for mining was also included, as is the disposal of overburden and tailings.

Moreover, the dataset for aluminum ingot manufacture considers molten aluminum from the electrolytic process that was placed into a holding furnace and heated to 750 °C using natural gas. Magnesium, silicon, and manganese were added to aluminum for strength, corrosion resistance, and other qualities. Clean, sorted scrap may be introduced at this stage; however, scrap remelting was excluded from this dataset. During furnace charge and preparation, aluminum dross develops on molten aluminum. Aluminum oxides were remelted to recover lost metal. Metallurgical analysis ensures the metal fulfills client requirements before molten, alloyed (or pure, unalloyed) aluminum was cast into products of dimensions, weighed, packed, and strapped for shipping.

Two distinct systems, a small laboratory scale (19.2 g per batch, g-$Ti_3C_2T_x$) and a large laboratory scale (800 g per batch, kg-$Ti_3C_2T_x$), were studied to synthesize $Ti_3C_2T_x$ MXene. The Supporting Information contains the materials inventory lists. Except for the location-based calculations, which employed the electricity mix of each location, Indianapolis, USA, has been designated as the location for the LCA calculations (laboratory location). Life-cycle impact assessment methods were applied to get the products' Cumulative Energy Demand (CED), and Tool for the Reduction and Assessment of Chemical and other Environmental Impacts (TRACI 2.1)[30] was applied to get the related environmental impacts of the functional units. It was realized that choosing amongst these impact categories was a normative choice based on what each user values. The United States Environmental Protection Agency (US EPA) started a taxonomy analysis of potential consequences (and impact categories) that could be included to be entirely thorough in the initial selection of impact categories. More information on the LCA methods and the detailed definition of each impact category and a complete inventory list of all calculations have been provided in the Supporting Information.

3. Results

3.1. Cumulative Energy Demand of $Ti_3C_2T_x$ MXene Production

The cumulative energy demand (CED) values for producing two $Ti_3C_2T_x$ MXene systems (kg-batch scale and gram-batch scale), industrial aluminum and copper foils, are displayed in **Figure 3** and Table S1, Supporting Information. Table S1, Supporting Information, presents the CED absolute scores, while Figure 3 displays the normalized results. The ecoinvent inventory database calculates CED for aluminum and copper foil industrial manufacturing by fabricating a primary ingot for both materials. This is followed by one set of section bar extrusion and two sets of sheets rolling from the ecoinvent inventory. Compared to kg-$Ti_3C_2T_x$ MXene, the worst-case scenario for a laboratory with low-capacity appliances has been considered for g-$Ti_3C_2T_x$ MXene. The energy consumption for manufacturing kg-$Ti_3C_2T_x$ MXene is about one-ninth that of g-$Ti_3C_2T_x$ MXene, which serves as the benchmark for normalization. However, compared to MXenes, the energy needed for industrial aluminum and copper foil manufacture is substantially lower. The CED to produce aluminum and copper is 0.517 GJ-eq and 1.131 GJ-eq, respectively, while this number for g-$Ti_3C_2T_x$ and kg-$Ti_3C_2T_x$ MXene is 153.291 and 17.364 GJ-eq, respectively. Although for most of the CED power sources, both aluminum and copper have more than 20% lower energy demand compared with kg-$Ti_3C_2T_x$ MXene, in other

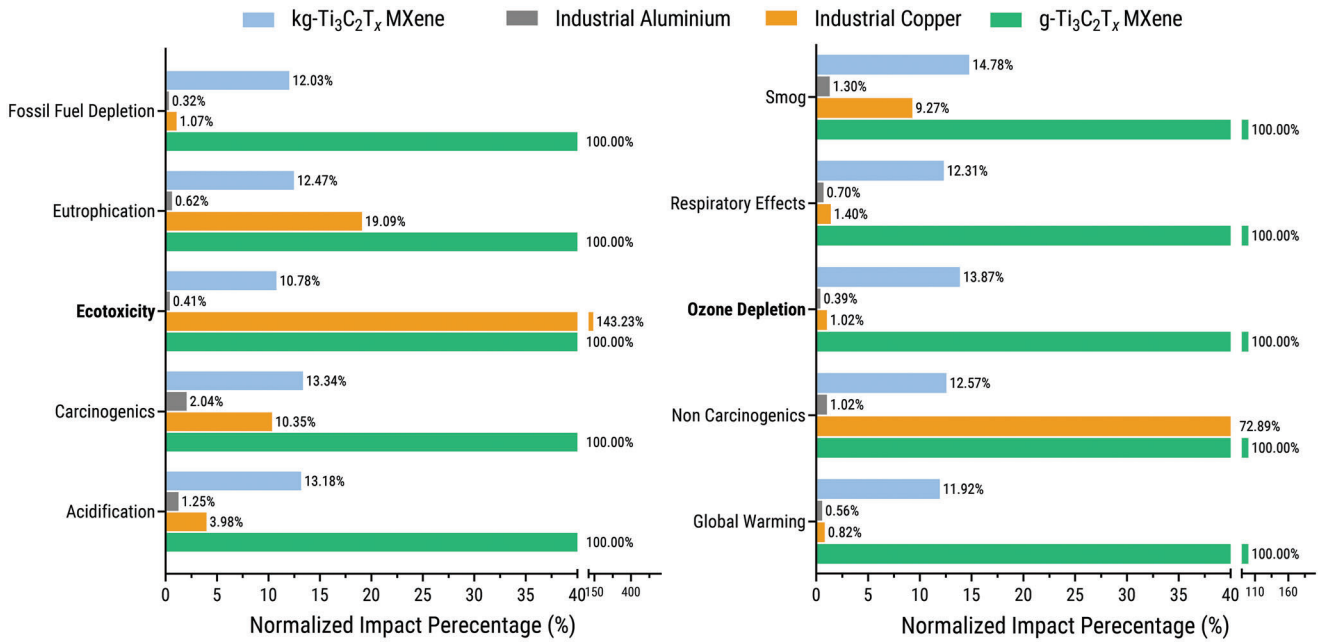

Figure 4. The normalized environmental impacts of producing kg-$Ti_3C_2T_x$, g-$Ti_3C_2T_x$, copper, and aluminum foil. g-$Ti_3C_2T_x$ MXene serves as a reference for the rest of the systems.

variables, such as water, this difference is less than 10%. The demand for non-renewable fossil energy resources for all materials contributed more than 60% of the total CED, more than any other category. Primary forest energy resources had a negligible effect, contributing less than 0.0001% of the total CED. Figures S1 and S2, Supporting Information, show the effect of the tube furnace time for MAX phase synthesis on the CED of kg-$Ti_3C_2T_x$ and g-$Ti_3C_2T_x$. The trend was the same for both systems and CED was reduced by ≈10% when furnace time was cut in half from two to one hour and raised by ≈20% when furnace duration was doubled from 2–4 h.

3.2. Environmental Impacts of $Ti_3C_2T_x$ MXene Production

Figure 4 and Table S2, Supporting Information, display the environmental impact results per functional unit. $Ti_3C_2T_x$ MXenes have more substantial environmental impacts than copper and aluminum in most categories, which is consistent with CED results. Industrial copper, however, has the largest adverse effects in the categories of non-carcinogenics and ecotoxicity. In eight categories, the gram size batches of MXene, g-$Ti_3C_2T_x$, have the greatest adverse impact, but by scaling up to kg-$Ti_3C_2T_x$, the impacts drop by about ten-fold. Figures S3 and S4, Supporting Information, show the environmental impacts of kg-$Ti_3C_2T_x$ and g-$Ti_3C_2T_x$ as a function of the time spent in the tube furnace during MAX phase synthesis. Both systems followed the same general trend, with around a 10% decrease in impacts when furnace time was cut in half from 2 to 1 h and around a 20% increase when furnace time was extended from 2–4 h.

Figure 5 shows the ratio of chemicals, waste, and electricity in the scores (normalized to 100%) for the manufacturing of $Ti_3C_2T_x$ MXene (based on the information in Table S2, Supporting Information). Figure 5 demonstrates that more than 90% of the share for g-$Ti_3C_2T_x$ MXene is electrical, with the remaining 10% being chemical. However, in the case of kg-$Ti_3C_2T_x$ MXene, electricity accounts for ≈70% of the share, and chemicals make up the remaining. For both systems, the waste flow contribution was negligible. The intensive use of electrical machinery in MXene synthesis, particularly in MAX phase production, is the cause of this high share of electricity. Sintering at a temperature of ≈1400 °C is required for at least 1–2 h (or more) during MAX phase synthesis. The etching and delamination process also involves many cycles of centrifugation and temperature-controlled operations in addition to MAX phase formation. Table S3, Supporting Information, displays the contribution of each piece of equipment to the MXene synthesis electricity flow. For the two MXene systems, the values are quite similar. Findings show that the tube furnace accounts for ≈57% of MAX synthesis' total electrical consumption, followed by the stirrer/hot plate (28%), the centrifuge (12%), the ball mill (2%), and the vacuum pump (1%).

Figure 6 displays the processes' normalized share of the scores for manufacturing $Ti_3C_2T_x$ MXene. Here, the flows connected to each process are divided into categories, and the impact of these flows, along with waste flows, is calculated. The findings indicate that for both MXene systems, MAX phase preparation has the greatest impact, accounting for 60% of the total, followed by etching (≈20%) and delamination (≈15%). The waste management process has a marginal effect with less than 1% share in both g-$Ti_3C_2T_x$ MXene and kg-$Ti_3C_2T_x$ MXene production. The MAX phase production uses a tube furnace with a high electric power requirement. As a result, MAX phase production has the most significant impact proportion compared with other processes.

When comparing the materials utilized in MAX phase synthesis to those that could influence the process, titanium has the highest share. Figure 5 illustrates that the overall influence

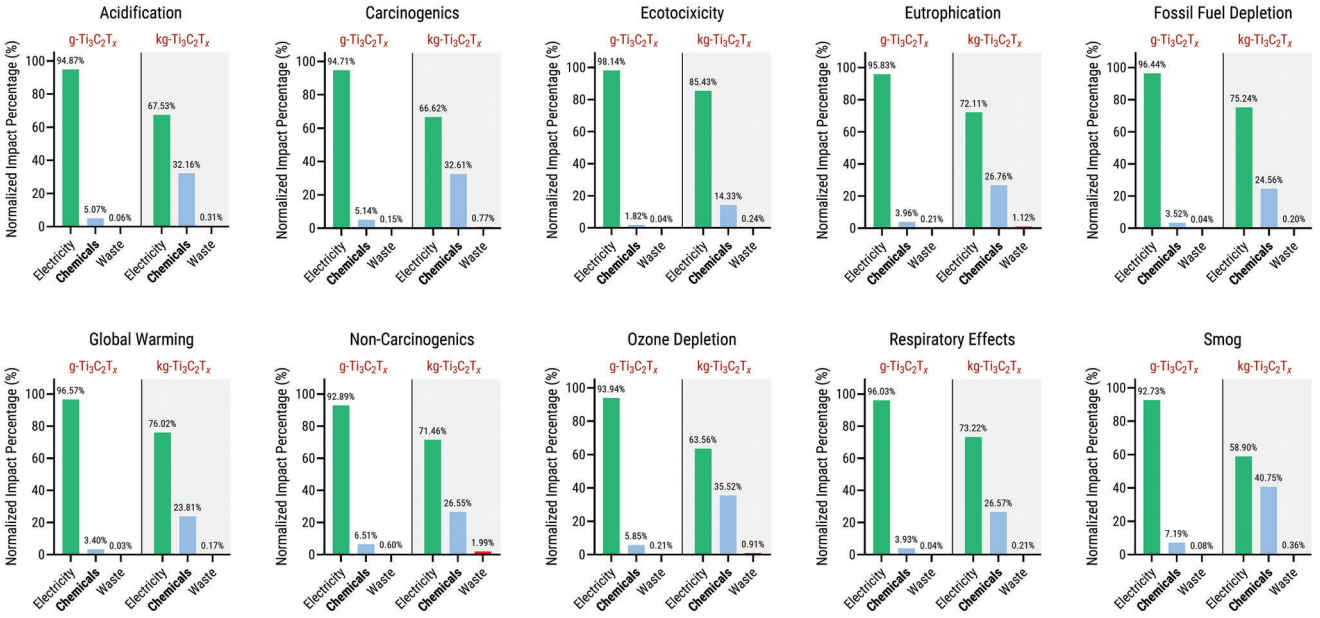

Figure 5. The normalized impact of three groups—electricity, chemicals, and waste flows—on the environmental effects of producing kg-$Ti_3C_2T_x$, and g-$Ti_3C_2T_x$. The flows associated with each of these categories are totaled and weighed in relation to the other groups for these calculations. The contribution of electricity will increase with the duration of operation of the electrical equipment. It is emphasized, though, that the production mass of the two systems is equal.

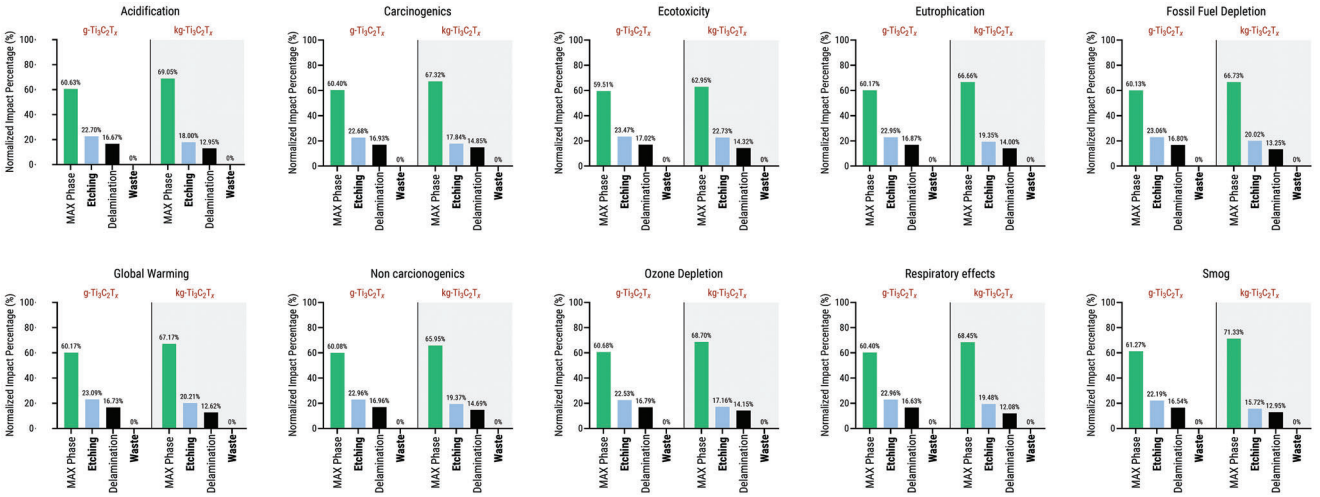

Figure 6. The normalized contribution of each synthesis process to the environmental impacts of the production of kg-$Ti_3C_2T_x$ and g-$Ti_3C_2T_x$ MXenes.

of the chemical flows is ≈60% less than the electrical flows. It is required to raise the temperature to ≈1400 °C in a controlled atmosphere to form the MAX phase. Therefore, there is no economically feasible replacement for the furnace power supply except for using other renewable energy sources like solar panels.

Figure 7 displays the normalized share of the various substances and materials in the scores for the synthesis of $Ti_3C_2T_x$ MXene (the chemical share in Figure 5). Since the chemical stoichiometry for both processes is the same, the share of the chemicals is roughly the same for g-$Ti_3C_2T_x$ MXene and kg-$Ti_3C_2T_x$ MXene. In comparison to the others, titanium has a much greater impact, accounting for ≈75% of the total. Aluminum comes in second place among chemicals (≈15%), while LiCl comes in third with a roughly 10% overall impact. Argon, hydrochloric acid (HCl), hydrofluoric acid (HF), graphite, and DI water are the remaining chemicals, and their combined impact is less than 2%.

3.2.1. Impact of Transition Metal Source on LCA of $Ti_3C_2T_x$ MXene

Because ≈¾ of the MXene chemical adverse impacts are attributable to the transition metal (Ti for Ti_3AlC_2), we examined the impact of Ti sources on the LCA of kg-$Ti_3C_2T_x$ MXene in this section (**Figure 8**). The source of titanium used in the Ti_3AlC_2 MAX phase precursor synthesis step is the only distinction

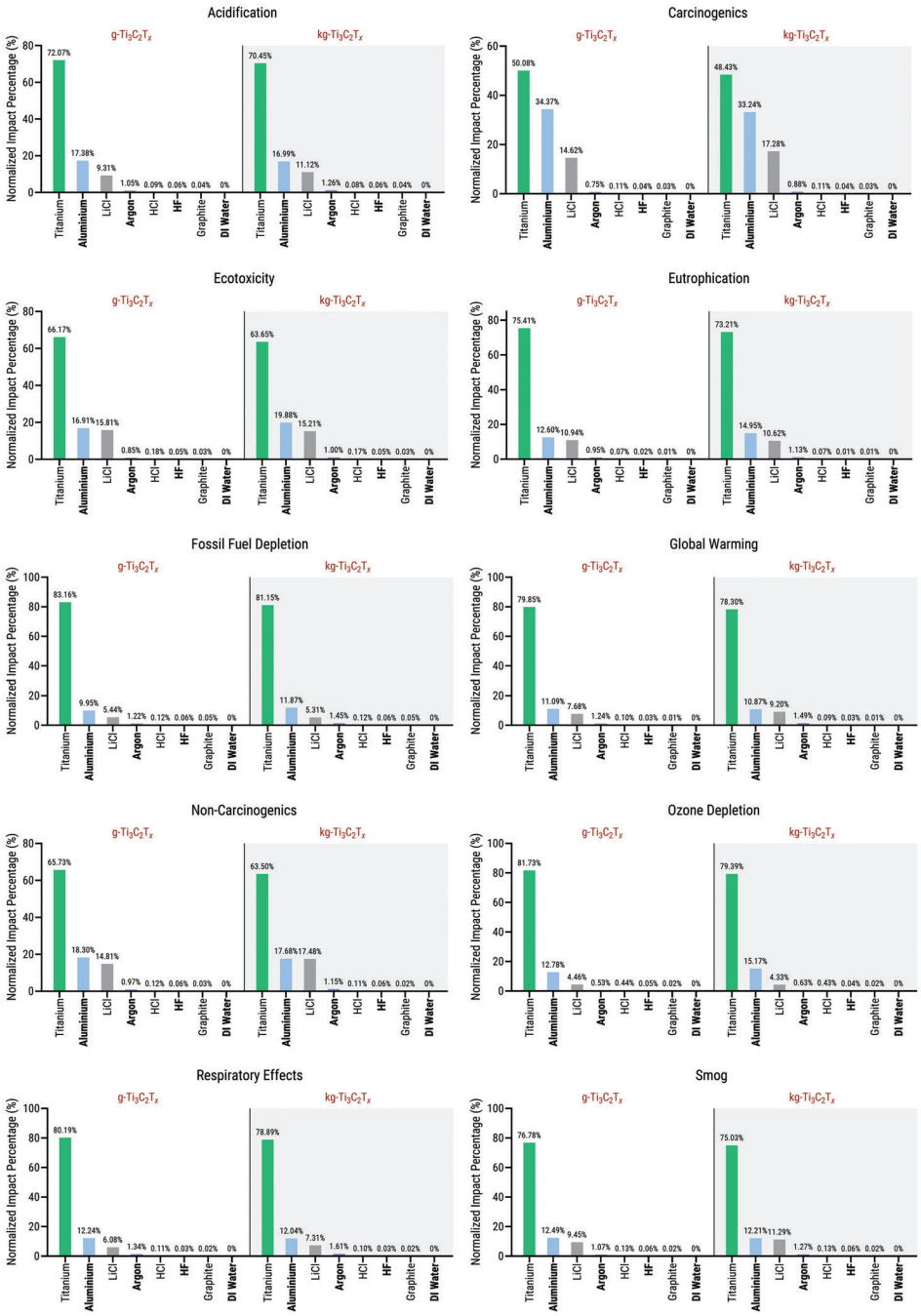

Figure 7. The normalized contribution of each chemical to the environmental impacts of the synthesis of kg-$Ti_3C_2T_x$ and g-$Ti_3C_2T_x$ MXenes. With almost 75% of the total, titanium provides the most significant contribution, followed by aluminum and LiCl.

between the systems shown in Figure 8. One employs titanium dioxide (TiO_2) as the source, whereas the other uses the same pure titanium as the rest of the LCA in earlier sections. The Ti_3AlC_2 MAX system that uses TiO_2 as the source of titanium had substantially greater adverse impacts in four categories (ecotoxicity, carcinogenics, acidification, non-carcinogenics) and substantially less adverse impacts for only ozone depletion; for the remaining categories, the Ti and TiO_2 systems were close (within 0.4% to 5.4%).

3.2.2. Impact of Location on the LCA of $Ti_3C_2T_x$ MXene

To evaluate the effects of the location of laboratory sites on environmental impacts, California, Texas, Indiana, China (Shanghai), Sweden, and Japan were selected (**Figure 9**). MXene fabrication in Texas has the greatest adverse effects in six categories, followed by China with the most adverse significant influence in three. Sweden, however, has the most negligible impact across all categories. The disparities in energy generation, administration, and

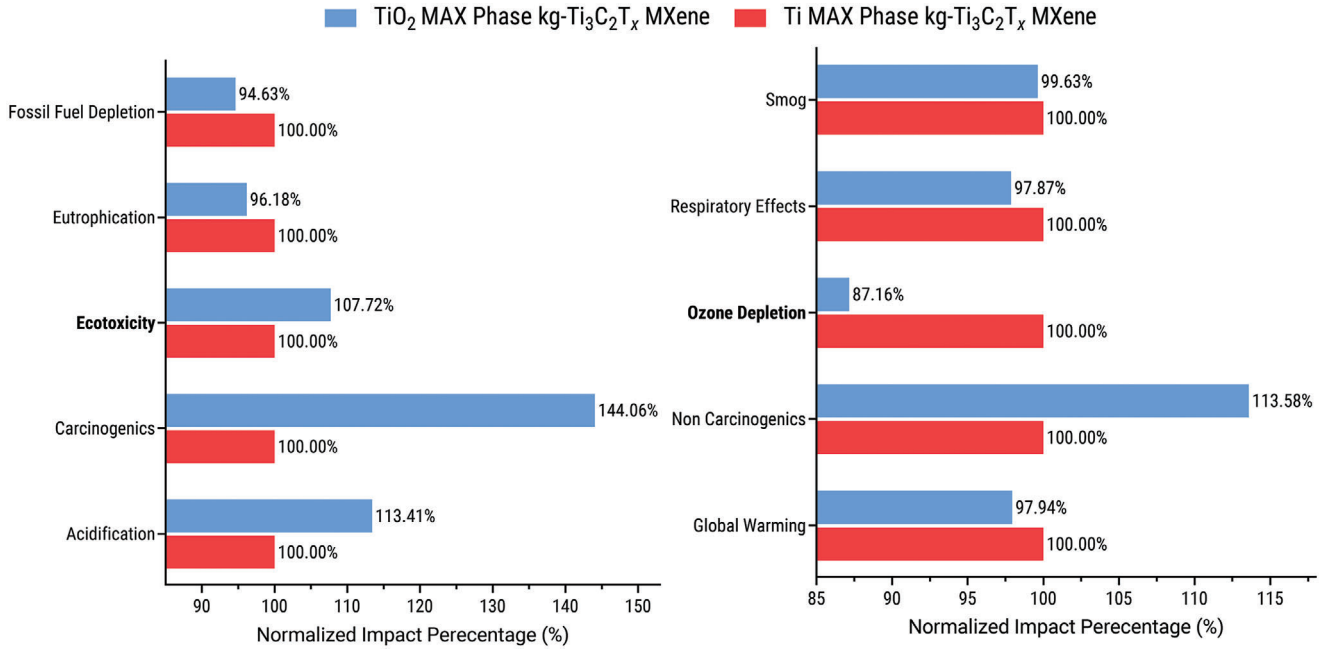

Figure 8. The normalized impact of producing kg-$Ti_3C_2T_x$ using titanium or TiO_2 as input for MAX phase production. Figures S5–S7, Supporting Information, provide more detailed information on the groupings for TiO_2-based LCA of MXene, the same as Figures 5–7.

treatment are primarily responsible for these differences. Sweden is a global leader in the utilization of renewable energy. The CED for kg-$Ti_3C_2T_x$ MXene synthesis in various areas is shown in Figure 9c and Table S4, Supporting Information. According to the CED findings, Sweden gets 26.6% of its energy from renewable sources, assisted by its geographic location; in contrast, Texas gets only 8.7% of its energy from renewable sources. This outcome is not surprising as Sweden has 15 times more hydropower than Texas, given its abundance of flowing water and 63% forest cover, which directly impacts the LCA implications.

4. Discussion

This study investigated the CED and environmental impacts of $Ti_3C_2T_x$ MXene synthesis on two laboratory scales. Industrial aluminum and copper foil were used as references. As a target application for this study, we selected coverage of the communication satellite's surface with these materials to achieve 60 dB of EMI shielding. Based on the SSE of each material and 100 m^2 area, 2.3 kilograms of $Ti_3C_2T_x$ MXene, 2.0 kg of aluminum foil, and 7.7 kg of copper foil are required to perform this function. When two MXene systems, kg-$Ti_3C_2T_x$ MXene and g-$Ti_3C_2T_x$ MXene, are compared, kg-$Ti_3C_2T_x$ MXene is significantly more efficient than g-$Ti_3C_2T_x$ MXene in terms of energy demand and environmental implications. Compared to g-$Ti_3C_2T_x$ MXene, the total CED for kg-$Ti_3C_2T_x$ MXene is around nine times lower. The power mix for both systems is the same if they are fabricated in the same location (e.g., Indianapolis in the USA). As a result, the two systems' environmental effects roughly follow the same pattern. However, the use of equipment and electricity in the two systems differs. Better-equipped and larger laboratories will tend to use larger batches, represented by the kg-$Ti_3C_2T_x$ MXene system, whereas g-$Ti_3C_2T_x$ MXene would be typical of smaller and more poorly equipped laboratories. Comparing these two laboratory-scale systems suggests that the $Ti_3C_2T_x$ MXene's significant environmental impact is due to its energy sources, mainly electrical devices.

Electricity consumption plays the most important role in the environmental impacts of $Ti_3C_2T_x$ MXene synthesis in the laboratory. For kg-$Ti_3C_2T_x$ MXene, electricity consumption accounts for over 70% of adverse environmental effects, and for g-$Ti_3C_2T_x$ MXene, it accounts for 90%. As a result, the nature of the energy resources determines most of the environmental impact. Therefore, synthesis in Sweden had the least adverse effects on the environment compared to the other five locations examined. According to the CED data, Sweden uses 73.39% of its power from non-renewable energy sources, whereas Indiana uses 96.56% for kg-$Ti_3C_2T_x$ MXene. The geography and limitations of the laboratory also have a significant impact on energy resources. Therefore, the location might be significant in defining the LCA. However, changes to the chemical sources of the process, at least in the case of employing titanium dioxide instead of titanium in MAX phase synthesis, did not significantly influence the environmental consequences, as shown in Figure 8.

Among chemical flows, titanium contributed more than 70% of the adverse environmental effects. Aluminum contributed 15%, and LiCl contributed 10%. The total impacts from the chemical group accounted for less than 10% of the adverse impacts in most impact categories, although it contributes more than 30% in certain kg-$Ti_3C_2T_x$ MXene cases. This suggests that some adverse impacts could be addressed using recycled titanium metal as the primary metal source for $Ti_3C_2T_x$ MXene. The amount of recycled titanium from scrap in the US from 2005 to 2019 is depicted in **Figure 10**a. Given that the MXene family uses a range of metal sources, this trend illustrates the potential for employing recycled metal sources as the precursor for MXene synthesis. Figure 10b displays the general formula for MXenes, various

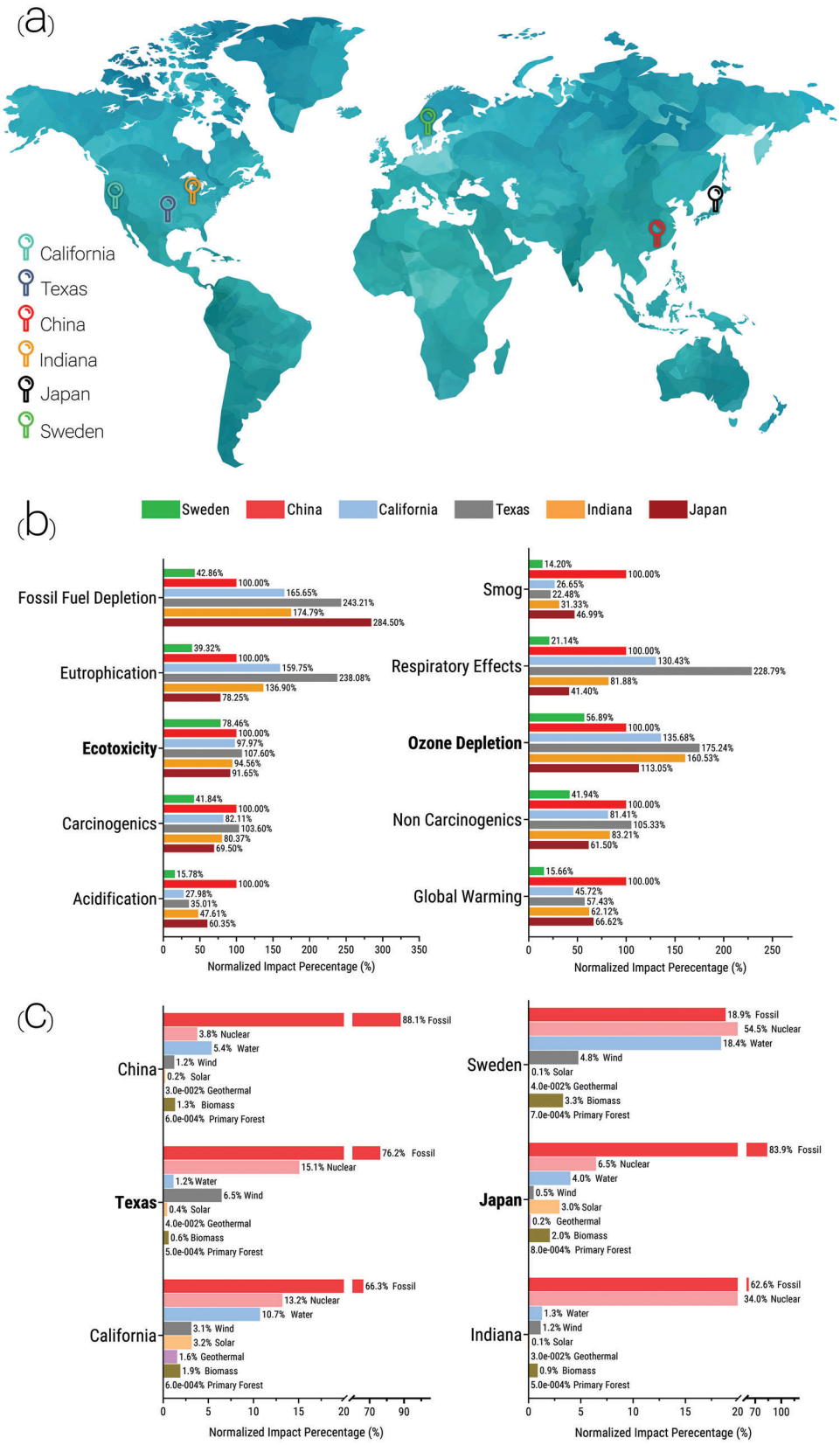

Figure 9. a) The location-based investigation of CED and b,c) environmental impact of the normalized environmental impacts (b) and energy demand (c) of producing kg-$Ti_3C_2T_x$ MXene in five locations. The environmental impacts are normalized using China as the reference, while energy demand categories are normalized within their categories.

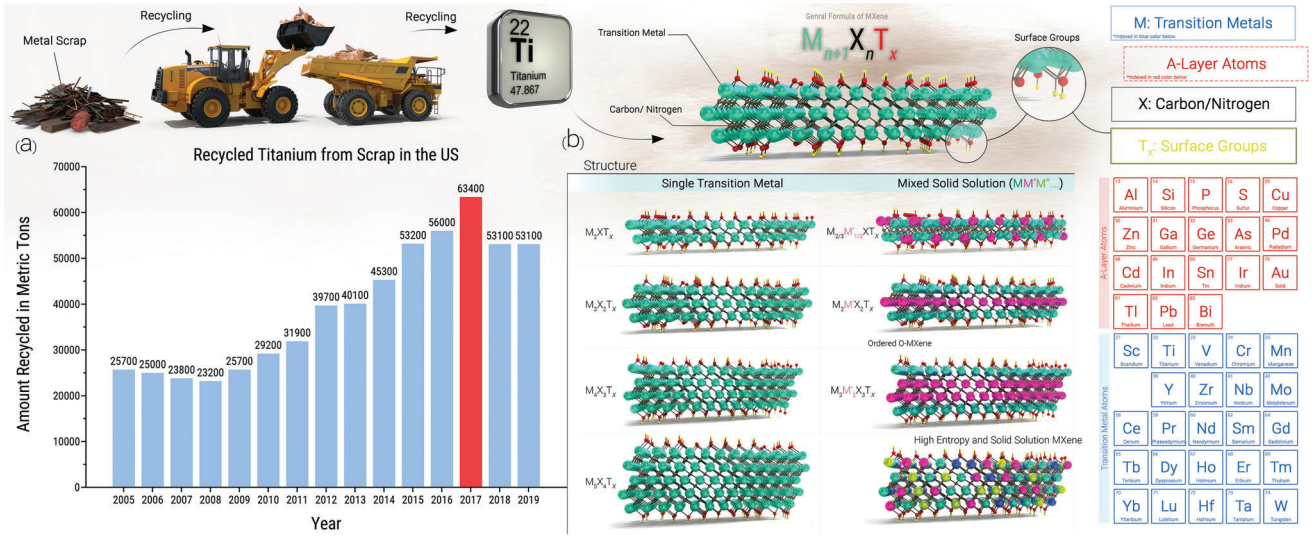

Figure 10. a) The amount of recycled titanium from scrap in the US from 2005 to 2019. b) Schematic representations of general MXene formula and several MXene structures. $Ti_3C_2T_x$, an $M_3X_2T_x$ MXene sample, was the first MXene identified in 2011, while M_2XT_x and $M_4X_3T_x$ were discovered in 2012. Among the most recent additions to the MXenes family are the $M_5X_4T_x$ solid solution MXene, and the high-entropy M_2XT_x and $M_4X_3T_x$ MXenes. Early transition metals in MXenes are represented by the colored spheres in green, yellow, pink, and blue. Randomly dispersed and attached to the outermost atomic layer of the MXene structure, primarily comprising O, F, or OH groups, are surface terminations of MXenes.

synthesized MXene structures to date, and the elements employed in the MAX structures. If the cost and application permit, this tunability in structure enables flexibility between elements and metals that are more ecologically benign, particularly for transition metals to reduce the total impact.

The results demonstrate that both g-$Ti_3C_2T_x$ MXene and kg-$Ti_3C_2T_x$ MXene are less environmentally friendly than the two external EMI references on a per functional unit basis. However, we only considered lab-scale manufacturing of $Ti_3C_2T_x$ with almost no optimization for industrial scale. Proportional to copper and aluminum foil, the production of kg-$Ti_3C_2T_x$ MXene requires ≈15 and 33 times more energy. However, in the case of g-$Ti_3C_2T_x$ versus kg-$Ti_3C_2T_x$, enlarging the synthesis amount by choosing different equipment decreased 90% of the CED, even on a laboratory scale. This demonstrates that MXene has substantial industrialization potential, especially considering the ongoing optimization of process, product, and yield. It would be desirable if more renewable energy sources were employed for the synthesis rather than non-renewables, such as fossil fuels.

The findings for other applications will differ because this study is predicated on how well these materials shield EMI. In other words, risks also depend on the relative performance improvements that MXene-enabled technologies offer, such as the increased clean energy that can be produced (due to efficiency gains enabled by nanotechnology) compared to energy-intensive manufacturing processes necessary to synthesize MXenes. Because no single MXene or its supply chain is representative of all MXenes, each has unique properties, performances, costs, and environmental effects that change from initial production to functionalization, incorporation into a product, and ultimately use in a final application. However, the most important factor that influences the CED and LCA of its synthesis is the quality and performance of MXene. MXene performance must therefore be considered for applications where they outperform other materials. It should be emphasized that the calculations for MXenes in this article are based on experimental laboratory data, where equipment use is not optimized, providing a high upper limit forCED, and leaving room for more efficient equipment use in future studies. In contrast, aluminum and copper foils are optimized and used at the industrial level. Both MXene systems were created in the software and simulated independently, albeit only on a small scale (compared to the other two systems).

Based on this research, several suggestions can be made to reduce the energy consumption and environmental impacts of the synthesis of $Ti_3C_2T_x$ MXene. As the primary suggestion, reducing the energy consumption of electrical equipment and lowering the synthesis time should be considered. MXenes' adverse environmental impacts are primarily caused by electrical appliances. It is worth noting that tube furnaces account for more than half of the total amount of power used in MXene synthesis. However, the hot plate/stirrer and centrifuge account for 28% and 12% of the power consumption, respectively. An example of one of the possible pathways to decrease the adverse environmental impacts of MXene synthesis is provided below.

The high-temperature reactive sintering step required to produce the MAX phase precursor contributes more than 60% to the overall energy consumption of the MXene synthesis process. Therefore, energy consumption reduction during the MAX phase production, such as improved furnace insulation and heat recovery, as well as the use of renewable energy resources are crucial to developing more sustainable and cost-effective synthesis methods. These strategies, along with other innovations in energy-efficient manufacturing, can be achieved in the coming years to support more sustainable and greener MXene synthesis. For example, a 10% reduction in heat loss due to improved furnace insulation could save ≈8.7 kWh of electricity per kg of MAX. Additionally, a 20% waste heat recovery, by using a heat exchanger to capture waste heat and preheat incoming raw

materials, could save ≈17.3 kWh of electricity. Ultimately, the use of renewable energy sources, such as solar or wind power electricity, reduces and potentially eliminates the dependence on fossil fuels and lowers the overall carbon footprint. Accordingly, the electricity consumption for MAX phase fabrication using a tube furnace can be reduced from 86.6 kWh (for kg-$Ti_3C_2T_x$ MXene) to 60.6 kWh (Green-$Ti_3C_2T_x$ MXene), representing a significant reduction in energy consumption and environmental impact. Here, we defined the Green-$Ti_3C_2T_x$ MXene as the synthesis route with lower energy consumption that uses 100% renewable energy resources compared to kg-$Ti_3C_2T_x$ MXene that uses fossil-based energy resources.

To better understand the effect of MAX synthesis, we recalculated the environmental impacts and CED for the kg-$Ti_3C_2T_x$ assuming 100% renewable energy, labeled as **Green**-$Ti_3C_2T_x$ MXene synthesis and compared it with the kg-$Ti_3C_2T_x$ MXene synthesis method (Figure S8 and Table S5, Supporting Information). In general, the Green-$Ti_3C_2T_x$ MXene synthesis method shows less environmental impacts (50% or more) across all impact categories compared to the kg-$Ti_3C_2T_x$ synthesis method, as discussed in detail in the Supporting Information. Specifically, the Green-$Ti_3C_2T_x$ MXene synthesis method shows ≈70% reduction in global warming potential, meaning it generates less greenhouse gas emissions compared to kg-$Ti_3C_2T_x$ MXene synthesis. For CED, the results also show that the method has a 52% reduction in cumulative energy demand compared to the kg-$Ti_3C_2T_x$ method. The largest contributors to the cumulative energy demand for both methods are fossil and nuclear energy resources, which account for 42% and 33% of the energy demand for the kg-$Ti_3C_2T_x$ MXene synthesis method, and 42% and 47% of the energy demand for the Green-$Ti_3C_2T_x$ MXene synthesis method, respectively.

Overall, these results suggest that the Green-$Ti_3C_2T_x$ MXene synthesis method has the potential to yield substantial energy savings and environmental benefits compared to the kg-$Ti_3C_2T_x$ method and that LCA can be a useful tool for evaluating and comparing the environmental impacts of different MXene synthesis methods. However, it is essential to note that the results are based on specific assumptions and conditions and may vary depending on the specific implementation and context of each method. Further research and evaluation are needed to confirm and refine these results and to identify additional opportunities to improve the environmental sustainability of MXene synthesis processes.

The second suggestion for reducing the energy consumption, cost, and environmental impacts of the synthesis of $Ti_3C_2T_x$ MXene is utilizing less expensive and recycled A-layer and carbon sources (for the X-layer). A-layer elements can be found at reasonable prices from metal scraps; for instance, there are 33 million tons of aluminum scraps worldwide. In comparison to bauxite ore, recycled aluminum is less expensive and emits fewer greenhouse gases. Additionally, using recycled carbon from tires in place of graphitic carbon through a straightforward sulfonation–pyrolysis procedure could cut the cost of producing carbon by up to 50%.[31] Jolly et al.[31] produced $Ti_3C_2T_x$ MXene from the Ti_3AlC_2 MAX phase made from secondary aluminum, titanium dioxide, and tire-recycled carbon using recycled resources as input. While the electrical conductivity for this MXene, 5857 ± 680 S cm^{-1},[31] is about half of that for MXene made from pure Ti, Al, and C sources, this $Ti_3C_2T_x$ MXene as a supercapacitor electrode performed in an identical manner comparable to that of $Ti_3C_2T_x$ MXenes made conventionally from elemental powders. This technique created a new way to reduce the manufacture of MXene's adverse environmental impact, CED, and costs.

As MXenes application performance improves, less material and energy are required to achieve the desired level of performance, resulting in lower environmental impacts. This can be seen in our study, where environmental impacts of MXene were compared with conventional EMI-shielding materials. It was discovered that the environmental impacts of MXene were comparable to those of copper and aluminum, as currently used in industry for EMI shielding, which could potentially be reduced with improved EMI-shielding performance. As a result, improving the performance of MXenes is critical because it can lead to a significant reduction in the environmental impacts associated with their production, making them more sustainable and environmentally friendly materials.

Our results show that the environmental impacts of MXene are comparable to those of copper and aluminum as currently used in industry for EMI shielding, which suggests improvement in MXenes' performance can lead to a significant reduction in the environmental impacts associated with EMI-shielding production. This can be accomplished by improving the purity and morphology of MXene flakes, optimizing the synthesis process, and exploring new MXene-based composites. These methods can further unlock the full potential of MXene and improve its environmental sustainability by addressing the performance-related challenges associated with its production and use.

More than 10000 articles have been published on MXenes or MXene-based materials in more than 400 journals since the discovery of MXenes. This explosive growth of MXene research involved more than 1450 institutions from 62 various countries. In 2020, there were almost 3000 published papers on MXene. MXene was the subject of more than 1493 and 903 publications published in 2020 and 2019, respectively, compared to 469 and 226 in 2018 and 2017. The quality of MXenes will continue to improve as research activity continues, enabling optimization for use in industrial applications.[8,11]

While this first screening-level LCA showed that current, laboratory-scale techniques for synthesizing $Ti_3C_2T_x$ MXene had substantially more adverse environmental impacts than comparable EMI reference materials, upscaling from a laboratory-scale synthesis usually entails the establishment of a mini-plant, a pilot plant, and a production-scale plant. A screening-level LCA may not accurately predict the environmental burdens by a direct scale-up because scaling up can introduce additional uncertainties. Therefore, higher reaction yields, the recycling of reagents, and more efficient equipment are expected to reduce the associated environmental impact and energy required for the unit mass of $Ti_3C_2T_x$ MXenes produced at the industrial scale compared to those at a laboratory scale.

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.

Data Availability Statement

The data supporting the findings of this study are available in the supplementary material of this article. Additional raw data, not included in the supplementary file, can be obtained from the corresponding authors upon reasonable request.

Keywords

energy, environment, industrialization, life-cycle assessment, MXenes, nanomaterials, nanotechnology, sustainability

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