MXene Based Nanocomposites for Recent Solar Energy Technologies

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The MXene family of materials among 2D nanomaterials has shown considerable promise in enhancing solar cell performance because of their remarkable surface-enhanced characteristics. Firstly, there are a variety of approaches to making MXene-reinforced composites, from solution mixing to powder metallurgy. In addition, their outstanding features, including high electrical conductivity, Young's modulus, and distinctive shape, make them very advantageous for composite synthesis. In contrast, its excellent chemical stability, electronic conductivity, tunable band gaps, and ion intercalation make it a promising contender for various applications. Photovoltaic devices, which turn sunlight into electricity, are an exciting new area of research for sustainable power.

1. Perovskite-Based Solar Cells

Since PVSK solar cells have such good light-harvesting qualities, they have developed rapidly in recent years, and numerous milestones have been attained in this sector, such as a high PCE of up to 23.2%, stability for more than a thousand hours, and so on. However, in order to meet its potential PCE limits (30–33%), a number of complex difficulties, such as the higher crystal size and fewer grain boundaries, must be handled. Two-dimensional MXene ($Ti_3C_2T_x$) was initially suggested as an additive in PVSK solar cells by Guo et al. in their paper [1][2][3][4][5]. Inserting a Ti_3C_2-MXene has an energy level that is higher than the carbon electrode, which lowers PVSK's conduction and valence band, thereby decreasing the pace at which the photocurrent is transferred and accelerating the transfer of the hole [6]. By inserting a thin layer of Ti_3C_2-MXene, it is possible to passivate the PVSK flake surface and create a direct conducting channel between Ti_3C_2-MXene and $CsPbBr_3$, which speeds up carrier transport to the carbon electrode. Recently, 2D Ruddlesden–Popper PVSK solar cells have been suggested as a way to improve the long-term stability of operation. Jin et al. [7] demonstrated perovskite solar cells with $Ti_3C_2T_X$ MXene-doped PVSK flakes, which increased the device's current density. In addition, a MXene-$MAPbBr_3$ heterojunction is formed using the in situ solution growth method.

2. Fabrication of MXene Composite

2.1. Solution Mixing

Solution mixing techniques have produced most MXene-reinforced polymer nanocomposites due to the hydrophilic character of MXene nanosheets supplied by the functional groups [8][9]. MXene nanoparticles are often distributed in polar solvents such as water [10], N,N-dimethylformamide (DMF) [11], and dimethylsulfoxide (DMSO) [12]. Due to their mutual solubility, polymer components might potentially be dissolved in the same dispersant or a different one [11]. These solutions, which consist of the polymer and MXene, are combined and blended to produce a homogeneous slurry of MXene composites. It should be emphasized that the solubility of MXene in nonpolar polymers or those with weakly polar groups is still problematic; thus, a proper surface pretreatment is required to improve dispersibility [13][14]. Solution mixing is a straightforward procedure that takes advantage of the hydrophilicity of MXene nanoparticles, but serious limitations, such as the formation of an abnormal quantity of environmental waste, poor mechanical qualities associated with the resulting composites, and laborious evaporation of solvents, generally prohibit its application [15].

2.2. Hydrothermal Process

The hydrothermal technique, also known as solvent thermal or solvothermal, is an often-documented procedure for producing a variety of new substances, new materials, and new compounds [16][17][18][19][20], especially MXene ceramic nanocomposites because of its simplicity, low cost, and widespread use. The amount of restacking required by this approach is low, and the resulting distributional uniformity is adequate [21][22][23][24]. For instance, $BiFeO_3$ (BFO)/Ti_3C_2

nanohybrid was produced by using a straightforward and cheap double solvent solvothermal process for the break-down of organic dye and colourless contaminants [22]. In another study, tetrabutyl titanate $Ti(OBu)_4$ was used in a straightforward hydrothermal process at a low temperature to create a Ti_3C_2/TiO_2 composite [25]. High oxidation or interdiffusion is unavoidable due to the method's use of excessive temperatures, and achieving a uniform dispersion of particles is difficult in comparison to other techniques [26][27].

The significant rise in PCE value is primarily attributable to the synergistic effects of the hydrothermal method and the one-of-a-kind layered morphology of conductive MXene nanosheets and their cocatalysts with CoS nanoparticles. These two factors contribute to the catalytic activity of the material. According to the findings of Chen et al., MXene-based composite CE materials show a great deal of promise for high electro-catalytic activity in QDSCs. These materials generate an abundant number of catalytic active sites, have good permeability, and exhibit outstanding charge transfer and ion-diffusion performance [28].

2.3. Powder Metallurgy

Powder metallurgy reduces waste, makes smooth surfaces, and the process produces less than 3% scrap. Tooling expenses, on the other hand, may be justified in large-scale manufacturing [13][29] An aluminum (Al) matrix containing 10% $Ti_3C_2T_x$ in a polypropylene container was tested for chemical stability using powder metallurgy [30]. After cold pressing, the pellet was sintered without applying pressure at a temperature between 500 and 7001 degrees Celsius [30]. Pressureless sintering followed by a hot extrusion technique was used by [31] to generate $Ti_3C_2T_x/Al$ with a MXene concentration of 0–3 wt%, while [13] used spark plasma sintering to produce $Cu/Ti_3C_2T_x$ with improved tribological characteristics. Self-lubricating Ti_3C_2 nanosheet/copper (Ti_3C_2/Cu) composite coatings were studied by [32], who used an electrodeposition approach at room temperature to create the coatings using Ti_3C_2 nanosheets. Similarly, Refs. [32][33] developed a novel MXene-Ag nanowire composite using a simple electrodeposition approach [27].

3. Role of Surface Termination Groups

MXenes cleared the way for the possible construction of innovative optoelectronic devices based on developing surface termination groups. Surface termination groups may adjust the band gap without altering the Ti_2CT_x MXene's original structure, and this is a valuable technique for regulating the material's electrical characteristics [34][35]. On the other hand, theoretical investigations have shown that surface termination groups affect the electronic structure of Ti_2CO_2 [36]. The pristine MXenes (Ti_3C_2) have a metallic structure. In contrast, $Ti_3C_2(OH)_2$ terminated with –OH displays semiconducting properties [37]. As a result, surface functional groups (–OH and –F) show semiconducting behavior with a valence band–conduction band energy differential of 0.05–0.1 eV [38]. Enyashin et al. theorized that the band gap of –OH terminated Ti_3C_2 within the range of 0–0.042 eV [39]. While the work function of –O and –OH terminated Ti_3C_2 MXenes was shown by Schultz et al. [40]. According to the researchers, the kind of OH termination has little effect on the variations of strain energies in titanium carbide TiC_x nanotubes, but it does affect the relative stability of the planar parent phases [39].

Controlling the amount of TiO_2 and Ti_3C_2 in the resulting TiO_2/Ti_3C_2 composite affects the separation of charge carriers based on: (i) the surface alkalization processes of pure Ti_3C_2; (ii) hydrothermal oxidation temperature; (iii) calcination temperature; (iv) surface termination groups (–F, –OH, or –O); and (v) hydrothermal reaction time [41]. The chemically reactive M-A bonding in the $M_{n+1}AX_n$ phase makes selective etching of the interleaved A element a viable option for separating $M_{n+1}AX_n$ layers. In 2011, Naguib et al. used a Ti_3AlC_2 MAX phase powder to investigate Ti_3C_2 MXenes (graphene-like morphology) [42].

4. MXene-Reinforced Nanocomposites

Combining MXenes with polymers, ceramics, metals, and nanoparticles yields composites with improved performance. Their exceptional optical, electrical, structural, mechanical, and thermal qualities result from their one-of-a-kind chemical and physical properties. Many other nanomaterials, including graphene derivatives, metal oxides, metals, and polymer monomers, have been successfully merged with MXene to create MXene-based hybrid nanocomposites, which improve upon the characteristics and practicality of pure MXene.

4.1. MXene-Metals/Ceramics Composite

MXenes are often employed to reinforce polymeric materials, but they can also be utilized to reinforce metallic or ceramic materials [43][44][45]. Reinforcement agents like graphene and CNTs have previously been tried in metals. On the other hand, metal matrix composites have faced significant difficulties due to agglomeration and poor wettability [46]. Pure

MXene has been successfully combined with a wide range of nanomaterials, including graphene derivatives, metal oxides, and metals, to create Mxene-based hybrid nanocomposites [15].

4.2. MXene-Polymer Composite

Using MXenes, polymer-based composites get a significant advantage in mechanical performance [15][47][48]. MXenes offer a wide range of applications as composite components because of their unique chemistry [49][50][51]. MXenes could greatly affect how spherulites grow and how polymeric materials crystallize [52][53]. Since the MXene sheets have a high aspect ratio and the -OH termination groups provide hydrogen-bonding interactions, the $Ti_3C_2T_x$ was found to significantly alter the glass transition temperature (Tg), and the mechanical strength increased by 23 percent, from 104.6 MPa for pure Nafion to 128.4 MPa for the composite sample [54]. Polymeric molecules respond better to MXene's functional groups than to Graphene's. These functional groups include the $–O_2$, –OH, and –F. Graphene devoid of surface terminations is often insufficient for composite production [55]. Due to its hydrophilic nature, MXene sheets have excellent wettability with a broad range of materials. It makes it easy to disperse and spread the sheets in various liquids [56]. Currently, MXenes have been employed in several types of polymeric matrices, including polyurethane (PU) [47][57], polyacrylic acid (PAA) [58], polylactic acid (PLA) [49], poly-vinyl alcohol (PVA) [59], nylon-6 [60], chitosan [61], and polyvinylidene fluoride (PVDF) [11], etc.

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