

MXene-Based Photothermal Fabrics Via Dip-Coating for Solar-Driven Evaporation Of Seawater

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Abstract

Solar-driven interface evaporation (SDIE) is a promising and sustainable seawater desalination approach that can perform long-term application. Unlike conventional desalination method, which does not support in off grid area, SDIE offers a viable solution because of its reliance on solar energy and its simple setup. In this work, a MXene/Polypyrrole (PPy) cotton-based fabric was prepared via a dip-coating method to serve as the SDIE system's solar absorber. The MXene and PPy modification endows the fabric with excellent photothermal ability. The optimal MXene/PPy fabric was determined based on two factors (volume of MXene and PPy) and two responses (surface temperature and coating stability). The optimized MXene/PPy fabric, containing 3 ml of MXene and 100 μ l of pyrrole, demonstrated minimal coating leaching of 0.026 grams with the ability to provide surface temperature of 64°C. Outdoor performance testing under sunny day showed an average evaporation rate of 0.041 L/m²·h with low conductivity of 0.347 μ S/cm, indicating its effectiveness in desalination applications.

1. Introduction

Freshwater scarcity has become a global issue, endangering human health and perhaps their lives [1]. As widely known that the ocean covers around 71% of the earth's surface and thus seawater represents a reliable source of freshwater. As a result, extracting freshwater from the sea has garnered significant attention by both academia and industry. The desalination process typically involves forcing seawater through a semipermeable membrane such as reverse osmosis or thermal methods, which involve heating seawater into vapor, which is then condensed as freshwater. These processes effectively remove salt and impurities, resulting in drinkable water. Solar desalination, a sustainable approach within the thermal method category, uses solar energy to provide heat for water evaporation, with freshwater obtained upon condensation of the water vapor, leaving impurities and salt behind. This technology requires photothermal material to harvest solar energy and turn it into heat to evaporate water. It is therefore desirable for the photothermal materials to have enough light absorption across the entire solar spectrum (280–2500 nm) [2]. Photothermal materials should also be harmless and biocompatible for the potential use in treating seawater water, in gaining drinkable water.

Solar desalination offers several key benefits, making it an attractive solution for addressing water scarcity issues. This method significantly reduces carbon emissions by utilizing abundant and renewable solar energy, making it environmentally friendly and sustainable [3]. Moreover, solar desalination can be cost-effective in regions with ample sunlight, lowering energy expenses compared to conventional desalination processes. It operates with reduced energy consumption, supports off-grid and remote areas with limited access to freshwater, and can be scalable to meet various water demand levels. Additionally, it produces less brine, thereby mitigating environmental concerns, and yields high-quality freshwater with fewer impurities. Conventional thermal desalination methods like Multistage Flash (MSF) and Multi-Effect Distillation (MED) have long been employed to convert seawater into freshwater through evaporation. These methods typically rely on fossil fuels or electricity to generate the necessary heat, resulting in relatively high energy consumption and environmental impact.

Scientists have recently shown growing interest in MXene, a novel two-dimensional material, as a photothermal material in solar desalination due to its remarkable properties, having excellent electronic, optical, elastic, thermoelectric, photothermal, and magnetic properties, which promise excellent light harvesting and charge separation as well as photothermal effect [4]. Despite notable advancements, several challenges continue to limit the widespread application of MXene-based materials in solar desalination. Firstly, the photothermal conversion efficiency of MXene decreases because it is readily oxidized in air and has a high chemical activity. Secondly, MXene is frequently immobilized on a flexible polymer matrix, although this polymer may partially break down in some extreme environments (such as an acidic environment). Thirdly, following the evaporation of water, salt crystallizes and eventually precipitates on the material surface.

Incorporating MXene within a polypyrrole (PPy) polymer matrix can significantly enhance the photothermal performance of materials for solar desalination by leveraging the complementary properties of both components. MXene, renowned for its high solar absorption, is susceptible to oxidation, which diminishes its photothermal efficiency; however, encapsulation within a PPy matrix can protect MXene from oxidative degradation, thereby sustaining its performance over time. Polypyrrole itself possesses high adhesive properties, cost-effectiveness, stable performance, non-toxicity, and exceptional sunlight absorption ability [5], and when combined with MXene, the composite exhibits improved photothermal conversion efficiency due to the additive effects of both materials. Additionally, PPy's inherent heat retention properties promote a higher localized surface temperature, enhancing water evaporation rates. The flexible and porous structure of PPy also aids in preventing salt crystallization on the material's surface, as it allows for improved salt diffusion and maintains structural integrity under various environmental conditions, including acidic and saline settings. This composite structure not only resists salt buildup but also imparts greater mechanical durability to the material, supporting longer-term performance in desalination applications. Together, these synergistic effects make MXene-PPy composites promising candidates for efficient and resilient solar desalination systems.

Thereby, this study develops a photothermal fabric by integrating MXene with polypyrrole (PPy) to harness their synergistic advantages. Two key factors are considered: the volume of the PPy and MXene solutions, which are optimized to control the composite's adhesion to the fabric surface. The resulting photothermal performance, including surface temperature and coating stability, is systematically evaluated to assess the effectiveness of the MXene-PPy fabric composite in enhancing solar desalination efficiency.

2. Methodology

This part consists of procedures for the synthesis of MXene powders, followed by the preparation of MXene/PPy fabric. The concentration of MXene/PPy was controlled by adjusting the volume of MXene and pyrrole. Optimization of the MXene/PPy fabric was determined by conducting surface temperature test and stability test as responses. Chemical properties of the MXene-PPy-fabric were characterized via Fourier-transform infrared spectroscopy (FTIR). The evaporation rate was evaluated and the water that condenses from evaporation was evaluated through conductivity test.

2.1 Synthesis of MXene Powder

The exfoliation approach of selectively etching the Al element from the raw Ti_3AlC_2 MAX phase was used to develop MXene nanosheets [6]. 3 g of Ti_3AlC_2 powders was gradually added to 60 mL of 2 wt% LiF, and then the mixture was constantly stirred for 24 hours at 350°C. The resulting solution was then mixed with 60 mL of ethanol, sonicated for 10 minutes, and then centrifuged for 5 minutes at 3500 rpm. The sonication and centrifugation procedures were repeated multiple times until the pH of the supernatant reached 6. Then, the final MXene particles were obtained after vacuum drying at 600 °C overnight.

2.1.1 Characterization of MXene

Following the synthesis of MXene, characterization was conducted using FTIR to confirm the successful transformation of the MAX phase into MXene nanosheets. These techniques were verifying the structural properties, ensuring the successful synthesis of MXene from its precursor.

2.2 Alkaline Treatment of Cotton Fabric

The cotton fabric, as substrate, was submerged in a sodium hydroxide solution (NaOH) with a fixed concentration of 6%. The cotton fabric was then rinsed with distilled water eight time to eliminate the excessive NaOH on the cotton fabric. The cotton fabric was dried in oven at 80°C for another 24 hours.

2.3 Preparation of MXene/PPY-fabric

Various volume of pyrrole and MXene dispersion was added in 17 mL of deionized water. The solution was then sonicated in an ice-water bath for 10 min and agitated for 30 min. The modified fabrics were then dipped into the MXene/PPY solution. Then, 1 g ammonia persulfate was dissolved in 5 mL of deionized water and added dropwise to the mixed solution. The reaction continued for 6 h. The fabric was then taken out of the solution and repeatedly rinsed with deionized water to remove excess black particles from the surface. Then, put it to air dry.

2.4 Optimization of MXene/PPY -fabric

Design Expert software was used to create the experimental design, which suggested conducting 13 sample runs. The Box-Behnken design method was applied, incorporating two factors and two responses in the experimental setup. The factors were the volume of MXene and the volume of pyrrole, while the responses were surface temperature and stability. The MXene volume range was set between 1 mL and 3 mL, and the pyrrole volume was set between 100 μ L and 500 μ L. This combination of factors, responses, and limits resulted in a total of 13 sample runs. The fabric samples underwent surface temperature testing to evaluate their heat dissipation capabilities. This process involved subjecting the fabric to thermal conditions and using infrared thermography to precisely measure and analyze surface temperatures. Additionally, stability tests were conducted to assess the fabric's durability and resistance to environmental factors.

2.4.1 Surface Temperature Test

The MXene/PPY cotton fabric samples were put under the sun radiation for one hour. Each reading was recorded within 10 minutes. The infrared thermometer was pointed directly at the samples. Position the digital screen so that the samples were visible. The samples were captured and analyzed using Testo IRSoft software to collect precise surface temperature data.

2.4.2 Stability Test

The MXene/PPY cotton fabric were weight and recorded for initial reading. Then it was put into a beaker filled with 30 ml of dionized water and sonicated for 30 minutes. After the MXene/PPY were sonicated, it was put into drying oven at 40°C for 1 hour to let it completely dry. The dry MXene/PPY fabric were weight again for final reading. The weight loss was calculate using formula in Equation 1 below.

$$\text{Weight loss} = \text{final weight} - \text{initial weight} \quad (1)$$

2.5 Characterization of Chemical Structure of MXene/PPY-fabric

The characterization of the MXene/PPy-coated cotton fabric was conducted using Fourier Transform Infrared Spectroscopy (FTIR) (Agilent Technologies Cary 600 Series) to analyze chemical functionalities. FTIR was specifically used to identify functional groups present on the surface of the MXene/PPy fabric, providing insights into its chemical structure.

2.6 Solar evaporation experiment

The evaporator used in the evaporation experiment consisted of a light absorption layer, a heat insulation layer, and a water transport channel. Specifically, the heat insulation layer comprised a 2 cm-thick foam, the water transport channel was made from commercial cotton thread, and the light absorption layer was a 4 cm-diameter MXene/PPy fabric. Water vapor generated during the experiment was captured and condensed using acrylic. The simulated seawater used in the experiment consisted of deionized water and sea salt in a 96.5:3.5 ratio.

Throughout the experiment, an infrared camera monitored the evaporation interface, capturing thermal images. The 6-hour evaporation experiment was conducted outdoors, utilizing natural sunlight from 9:00 a.m. to 3:00 p.m [7].

2.7 Performance Test

The performance of the solar evaporation experiment was evaluated based on the quality of purified water and the evaporation rate.

2.7.1 Conductivity Test

The conductivity meter was calibrated before using. The condensed water were collected and put into a beaker. Then, conductivity electrode was dip into the water and the reading was taken.

2.7.2 Evaporation Test

The water produced through evaporation was collected in a container. The accumulated water volume was recorded over time during the evaporation process. The evaporation rate from the evaporation experiment was calculated using the following equation 2.

$$J = \frac{v}{A - \Delta t} \quad (2)$$

where V is the water volume collected (L) for sampling time (Δt , h), A is the effective MXene/PPy fabric area (m^2).

3. Result and Discussion

3.1 Characterization of MXene

MXenes was characterized by surface terminations that often include -OH, -F, and -O groups. In FTIR spectra, these would typically manifest as a broad band around $3200-3600\text{ cm}^{-1}$ due to O-H stretching vibrations. A sharp peak near 1630 cm^{-1} was associated with O-H bending vibrations or C=O stretching. If fluorine was present, a peak around 1200 cm^{-1} was expected for C-F stretching vibrations. Peaks below 700 cm^{-1} may be attributed to metal-oxygen vibrations, indicative of the MXene structure. All spectral features of MXene can be found in Figure 1.

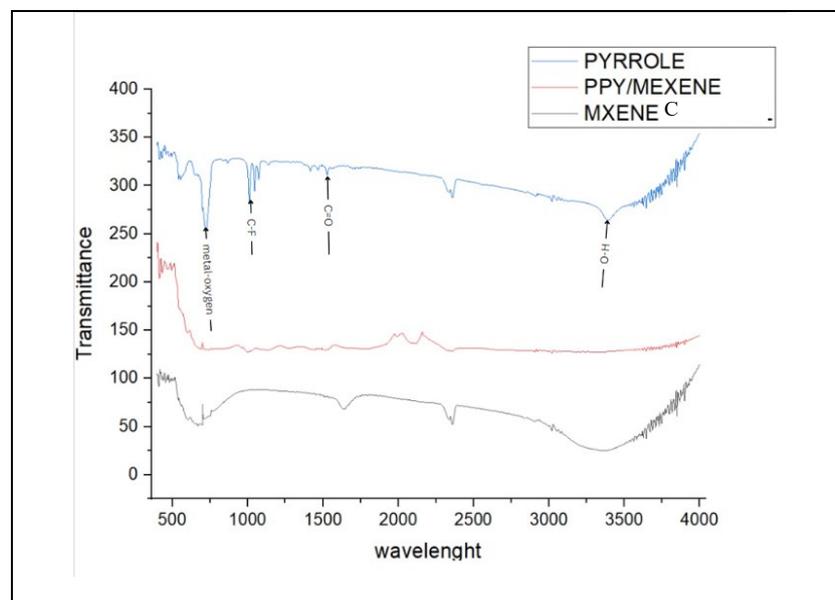


Fig. 1 FTIR spectra of pyrrole, pyrrole/MXene (PPy/MXene) and MXene colloidal (MXene C)

3.2 Preparation MXene/PPy Cotton Fabric

The preparation of MXene/PPy cotton fabric involves a careful process to ensure effective integration of the conducting polymer (PPy) and MXene nanomaterial into the cotton substrate. The first step typically involves the synthesis of PPy, which was achieved through chemical polymerization methods. MXene was synthesized and exfoliated into nanosheets, which were then dispersed into the PPy solution and were stirred for 30 minutes. The cotton fabric was then immersed in a MXene/PPy solution while stirring it for 6 hours, allowing for the penetration and adhesion of the polymer and nanomaterial onto the fabric fibers. The optimization of the MXene/PPy concentration is crucial in achieving the desired properties of the composite fabric.

3.3 Optimization of MXene/PPy Cotton Fabric

The MXene/PPy fabric's surface temperature was quantitatively assessed under thermal conditions using infrared thermography. Concurrently, the stability test was conducted to assess the fabric's durability over time. The assessment provides a comprehensive understanding of the fabric's photothermal properties and its long-term performance, offering valuable insights for practical applications. Table 1 presents the results of surface temperature and stability of fabric prepared at different run.

Table 1 Design of expert results

Run	Factor 1 MXene volume (ml)	Factor 2 Pyrrole volume (ml)	Response 1 Surface temperature (°C)	Response 2 Stability test (g)
1	0.6	300.0	59.9	0.073
2	1.0	100.0	64.6	0.035
3	2.0	17.2	66.7.0	0.034
4	2.0	300.0	67.0	0.065
5	2.0	300.0	66.4	0.063
6	1.0	500.0	67.9	0.034
7	2.0	582.8	69.0	0.048
8	3.0	500.0	63.0	0.033
9	3.0	100.0	64.0	0.026
10	2.0	300.0	64.0	0.064
11	2.0	300.0	63.2	0.055
12	2.0	300.0	63.6	0.066
13	3.4	300.0	67.0	0.043

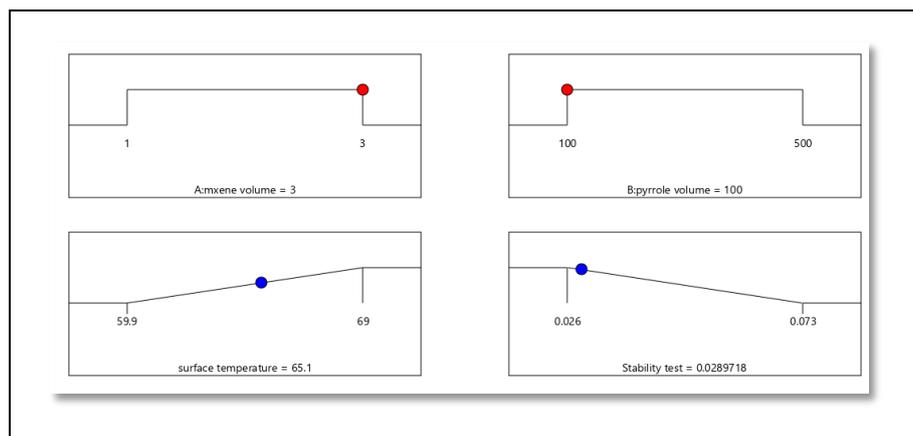


Fig. 2 Ramp graphs of MXene/PPy fabrics

As shown in figure 2, sample run 9 was selected as the optimized sample, with an MXene volume of 3 mL and a pyrrole volume of 100 μL. The optimization process was conducted using Design Expert software, which identified the sample run yielding the highest surface temperature and stability. This optimized fabric was subsequently used in performance tests to evaluate evaporation rate and water quality.

3.3.1 Surface Temperature

Surface temperature analysis is crucial to evaluate MXene/PPy fabric’s photothermal properties in converting sunlight into heat, which drives the evaporation process [8]. Figure 3 displays an infrared thermograph of MXene/PPy-coated cotton fabric under sunlight, with an ambient temperature of 43.9 °C. The temperature analysis provides some insights into the thermal behaviour of the MXene/PPY cotton fabric. Notably, the highest temperature achieved was 74.4 °C (see table 2). In contrast, the lowest temperature of 37.7 °C was observed for the pristine cotton fabric. This contrast illustrates the substantial impact of MXene and polypyrrole on elevating the fabric’s thermal performance, demonstrating a significant improvement over pristine cotton fabric. The surrounding temperature standing at 43.9 degrees, serves as a reference point, emphasizing the fabric’s ability to exceed ambient conditions. This temperature differential clearly demonstrates the active role played by MXene and polypyrrole in elevating the fabric’s temperature beyond the ambient surroundings. The enhancement of the fabric’s photothermal properties signifies the successful functionality of the MXene and polypyrrole, showcasing efficiency in harnessing solar irradiance, which underscores the fabric’s potential for diverse applications, ranging from solar-driven water evaporation to other innovative uses where photothermal properties are essential.

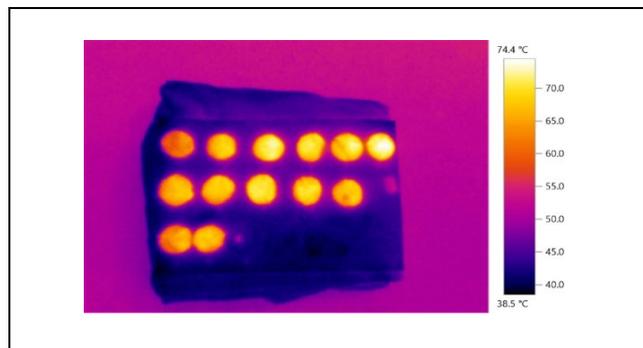


Fig. 3 Infrared thermometer image of PPY/MXene cotton fabric with ambient temperature of 43.9°C

Table 2 Average surface teperature

	Factor 1	Factor 2	Response 1
Run	MXene volume (ml)	Pyrrole volume (ml)	Average surface temperature (°C)
1	0.6	300	59.9
2	1.0	100	64.6
3	2.0	171	66.7
4	2.0	300	67.0
5	2.0	300	66.4
6	1.0	500	67.9
7	2.0	582	69.0
8	3.0	500	63.0
9	3.0	100	64.0
10	2.0	300	64.0
11	2.0	300	63.2

12	2.0	300	63.6
13	3.4	300	67.0
14	0.0	0	38.8

Following the comprehensive assessment of various concentrations of MXene/PPy fabric, the detailed findings have been systematically organized in table 2. Notably, in this dataset, it becomes evident that the MXene/PPy fabric from run number 7 exhibits the highest average temperature among all runs. A closer examination reveals that run 7 is characterized by the largest volume of pyrrole in comparison to the other runs. Contrastingly, run 14 exhibits the lowest surface temperature. This was attributed to the absence of both pyrrole and MXene in this run. Specifically, run 14 serves as an interesting case study, emphasizing that the absence of these key components leads to a significant reduction in the fabric's capacity to exhibit photothermal behaviour. It is noteworthy that the volume of pyrrole alone does not exhibit a direct proportionality to the average surface temperature across all runs. This distinction is illustrated by instances where runs with similar pyrrole volumes may have slightly different temperatures. This phenomenon suggests that other factors, possibly related to the concentration of MXene, play a role in influencing the fabric's thermal behaviour. Figure 4 below shows the graph of average temperature vs run.

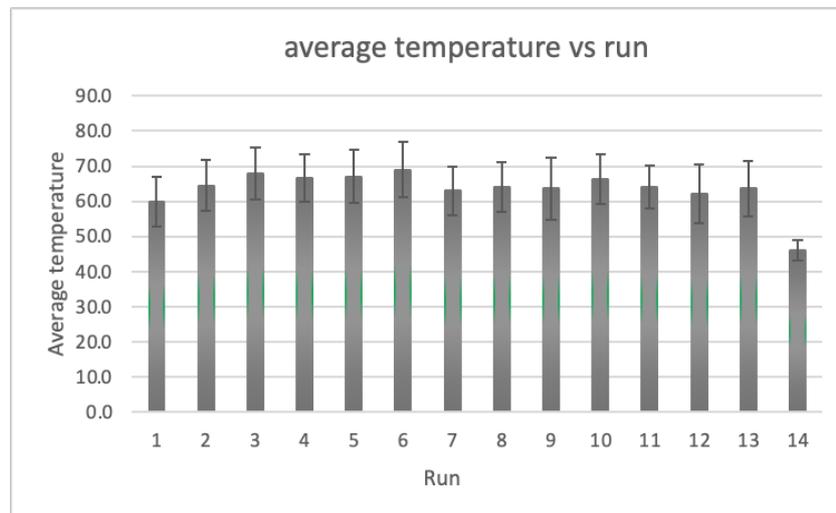


Fig. 4 Graph of average temperature vs run

3.3.2 Stability Test

The stability test, incorporating sonication and weight measurements, constitutes an important aspect of this project, designed to thoroughly assess the adhesion strength of polypyrrole and MXene on the cotton fabric. With an emphasis on real-world applications, this evaluation is critical for validating the practical viability of the developed photothermal fabrics. The application of sonication, simulating mechanical stress resembling routine washing or extended use, provides a controlled environment to scrutinize the fabric's response to environmental challenges. As can be seen in figure 5, there is a beaker with clear water and some with black water. The black water means it loss many of the polypyrrole and MXene during the sonication process. Pyrrole was not strongly adhesive to the cotton fabric. This happens due to the high-energy ultrasonic waves that generate cavitation bubbles in the liquid medium.

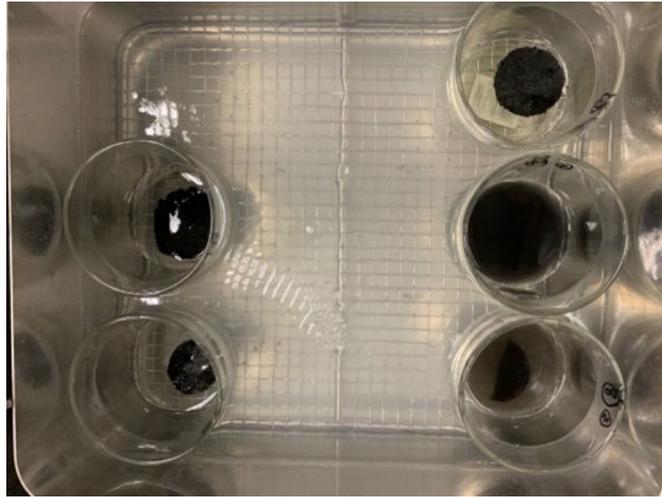


Fig. 5 Application of sonification process for the as prepared photothermal fabrics

Table 3 provides the data for the stability test. The data of stability test below were in gram unit. It indicates the weight of the MXene and polypyrrole that has fall during the sonication process. The lower the value means more stable the fabric itself. The sample of run 9 has the lowest value of material loss. This indicates that the formulation with 3ml of mxene and 100µl has the highest stability. While the trend is the stability fluctuates within up and down through each concentration. This highlights that high concentration of MXene and polypyrrole does not necessarily resulting in higher stability.

Table 3 Stability test

	Factor 1	Factor 2	Response 2
Run	MXene volume	Pyrrole volume	Stability test
	(ml)	(µl)	(g)
1	0.6	300.0	0.073
2	1.0	100.0	0.035
3	2.0	17.2	0.034
4	2.0	300.0	0.065
5	2.0	300.0	0.0063
6	1.0	500.0	0.034
7	2.0	582.8	0.048
8	3.0	500.0	0.033
9	3.0	100.0	0.026
10	2.0	300.0	0.064
11	2.0	300.0	0.055
12	2.0	300.0	0.066
13	3.4	300.0	0.043

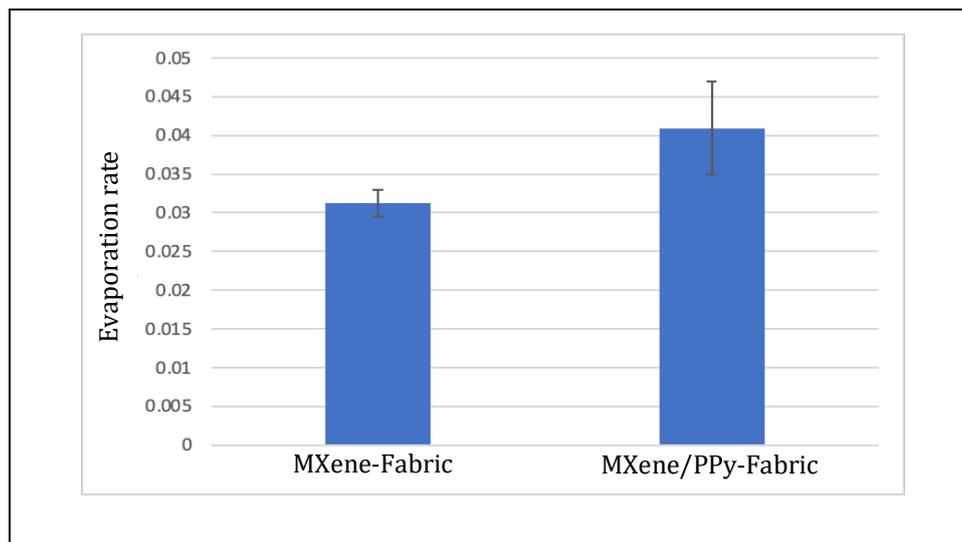
3.4 Evaporation Rate

The data provided in table 4 indicates a comparison between two types of fabrics, MXene fabric and MXene/PPY fabric, in their ability to evaporate water and allow water to pass through them. The MXene fabric and MXene/PPY fabric were respectively had the same concentration.

Table 4 Volume of water collected and water flux of MXene fabric and MXene/PPY fabric

	Sample	Volume of water collected (ml)	Evaporation rate (l/m ² .h)	Average evaporation rate (l/m ² .h)	Standard deviation
MXene fabric	1	3.50	0.0291	0.032	0.0017
	2	3.75	0.0312		
	3	4.00	0.0333		
MXene/PPY fabric	4	4.00	0.0333	0.041	0.0060
	5	5.00	0.0416		
	6	5.75	0.0479		

Each fabric type has been assessed with three samples. For the MXene fabric, the volume of water collected ranged from 3.50 ml to 4.00 ml, with an evaporation rate between 0.0291 and 0.0333 L/m².h. An improvement in the volume of water and the evaporation rate was observed for the sample with polypyrrole. The MXene/PPY fabrics exhibited collected volume of 4.00 ml to 5.75 ml, with corresponding evaporation rate between 0.0333 and 0.0479 L/m².h. It's clear that the MXene/PPy fabric achieves higher rates across all samples when compared to the MXene fabric. This is due to the addition of polypyrrole to the fabric which enhance its thermal conductivity hence supply more heat to the fabric to boost the evaporation rate. PPY's strong light absorption, especially in the visible and near infrared regions (NIR), allows for efficient solar energy conversion into heat, resulting in faster water evaporation [9]. Additionally, It is postulated that the MXene/PPy composites exhibit enhanced thermal conductivity, providing uniform heat distribution and quicker vaporization. Synergistic effects between PPY and MXene further boost performance. Moreover, the chemical and structural stability of PPy enhances the durability of the photothermal fabrics while also improving wettability, thereby enabling efficient water spreading and evaporation. These combined advantages make MXene/PPy fabrics promising for various solar-driven evaporation. The bar graph in figure 6 summarize the average evaporation rate of MXene fabric and MXene/PPy fabric.

**Fig. 6** Graph of average water flux of fabric

3.5 Conductivity

The conductivity data for both MXene fabric and MXene/PPy fabric samples, as presented in Table 5, provide an insightful comparison to the quality of the treated water. By comparison, pure distilled water is characterized by its low ionic content, generally exhibits conductivity values ranging from 0.5 to 3 microsiemens per centimeter ($\mu\text{S}/\text{cm}$).

Table 5 Conductivity of PPy/MXene fabric and MXene fabric

	Sample	Volume of water collected (ml)	Conductivity ($\mu\text{S}/\text{cm}$)	Average conductivity ($\mu\text{S}/\text{cm}$)	Standard deviation
MXene fabric	1	3.50	1.67	0.693	0.8581
	2	3.75	0.06		
	3	4.00	0.35		
MXene/PPY fabric	4	4.00	0.14	0.347	0.2050
	5	5.00	0.55		
	6	5.75	0.38		

The conductivity measurements of MXene fabric samples exhibited a conductivity ranging from 0.06 to 1.67 $\mu\text{S}/\text{cm}$, indicating relatively pure water. However, Sample 2, measured at 0.06 $\mu\text{S}/\text{cm}$, falls significantly below the normal range for distilled water, suggesting either an exceptionally pure sample or a potential measurement error. Sample 3's conductivity of 0.35 $\mu\text{S}/\text{cm}$ places it comfortably within the expected range for distilled water, suggesting minimal contamination from ions.

In contrast, the MXene/PPy fabric samples show conductivity range between 0.14 $\mu\text{S}/\text{cm}$ to 0.55 $\mu\text{S}/\text{cm}$, comparable to distilled water, indicating very few ionic impurities. It is worth to note that the result from Sample 5, having a conductivity of 0.55 $\mu\text{S}/\text{cm}$, is higher than that of distilled water and suggests significant ionic content, which could be attributable to the contamination or interactions between the water and the fabric. Sample 6 shows a conductivity of 0.38 $\mu\text{S}/\text{cm}$, aligning it with the expected range for distilled water.

4. Conclusion

In summary, a MXene/PPy fabric fabricated for photothermal conversion for solar driven interfacial evaporation was successfully prepared via dip-coating method. MAX phase was successfully synthesized into MXene, as evidence from the peak of FTIR analysis. The MXene and Pyrrole volume were varying during the fabrication of the MXene/PPy fabrics and the optimal parameters were determined using Design of Expert (DOE) based on the fabric's stability and fabric's surface temperature. The optimized parameters were obtained at 3ml of MXene and 100 μl of pyrrole with minimal coating leaching of 0.026 gram and surface temperature of 64 $^{\circ}\text{C}$. Following the optimization process, the optimized fabric was subjected to performance testing for solar interfacial evaporation to assess its efficiency in terms of evaporation rate and the quality of treated water. The average evaporation rate and water quality of the MXene/PPy fabric were 0.041 $\text{l}/\text{m}^2\cdot\text{h}$ and 0.347 $\mu\text{S}/\text{cm}$, respectively.

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Conflict of Interest

Authors declare that there is no conflict of interest regarding the publication of the paper.

Author Contribution

The authors confirm contribution to the paper as follows: **study conception and design:** Nik Ashraf Daniel, Mohd Haiqal Abd Aziz, Nur Hashimah Alias; **data collection:** Nik Ashraf Daniel; **analysis and interpretation of results:** Nik Ashraf Daniel; **draft manuscript preparation:** Nik Ashraf Daniel, Ahmad Faez Abdul Khalil. All authors reviewed the results and approved the final version of the manuscript.

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