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Semiconducting polymer-MXene blends with improved charge carrier mobilities and their application in field-effect transistors

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ABSTRACT

$Ti_3C_2T_x$ is the first successfully obtained member of the MXene family. Due to its many excellent properties such as high metallic conductivity, solubility and capacitance, it has attracted a wide interest in potential applications such as supercapacitors and energy storage devices. In the presented work, we have successfully produced various semiconducting thin-films consisting of Poly(3-hexylthiophene-2,5-diyl) (P3HT) organic semiconductor (OS) blended with MXene flakes with different MXenes concentrations. Time-of-flight photoconductivity (TOFP) measurements revealed a 370 % enhancement in charge carrier mobility compared to neat P3HT. Organic field-effect transistors (OFETs) were also fabricated using these blends, showing a 20 % improvement in field-effect mobility. This discrepancy arises due to contact resistance and interface effects in OFETs, which are absent in TOFP measurements. These results highlight the promise of P3HT:MXene blends for advanced electronic applications, where high mobility and straightforward processing are essential.

Introduction

The two-dimensional (2D) $Ti_3C_2T_x$ titanium carbide, where T_x is the surface termination, was first synthesized in 2011, marking the discovery of MXenes – a growing family of 2D transition metal carbides and nitrides [1]. Given their properties like exceptional electrical conductivity, high charge carrier mobility and solution-processability [2], MXenes have the potential to address a key limitation in organic semiconductors (OSs) – their inherently low charge carrier mobility, which restricts performance in organic field-effect transistors (OFETs).

In this study, we investigate the enhancement of charge carrier mobility in organic thin films by incorporating $Ti_3C_2T_x$ MXene flakes into poly(3-hexylthiophene-2,5-diyl) (P3HT), a commonly used organic semiconductor known for its commercial availability, solution processability and relatively good hole transport properties [3]. By blending MXenes with P3HT, we demonstrate the formation of a semiconducting ink with enhanced charge transport properties, achieving a mobility increase from 1.05×10^{-3} cm^2/Vs (pristine P3HT) to as high as 4.75×10^{-3} cm^2/Vs, as measured by the time-of-flight photoconductivity (TOFP). This technique directly probes the charge carrier mobility of semiconducting films, unaffected by interface effects or contact resistance, making it especially valuable for evaluating the true transport potential of blended materials.

Furthermore, OFET devices fabricated from these hybrid blends exhibit a mobility enhancement from 1.67×10^{-3} cm^2/Vs to 2.01×10^{-3} cm^2/Vs, while even improving the high on/off current ratio characteristic of P3HT. By comparing charge transport in bulk and interface-limited regimes, we elucidate MXenes role in improving organic semiconductor performance, addressing a gap in systematic studies of blended systems and highlighting their potential for high-performance, solution-processable electronics.

Experimental part

Full experimental details, including materials, device fabrication and characterization protocols, are provided in the Supplementary Information. Below is a concise overview.

Materials and preparation

Commercial P3HT (shown in Fig. 1**a**) powder was dispersed in dichlorobenzene (DCB), producing a 5 mg/ml solution, while the

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$Ti_3C_2T_x$ MXenes (Fig. 1**b**) were prepared using the HF etching method, resulting in the surface termination T_x of –F, –OH and =O, followed by their dispersion in dimethylformamide (DMF).

P3HT:MXene blends were prepared by mixing a constant volume of MXene (in DMF) with varying concentrations with the same volume of P3HT (in DCB), resulting in MXene weight fractions of 0 %, 0.5 %, 1 %, 2.5 %, and 5 %. The 0 % reference sample was prepared by adding only DMF (without MXene) to account for any solvent effects. All blends were then spin-coated to form thin films for charge transport measurements. Higher MXene concentrations were not evaluated, as they caused aggregation in DMF, resulting in poor mixing with P3HT, inhomogeneous films and degraded TOFP performance.

Characterization techniques

Charge transport in the blended layers was characterized using two methods. The first, time-of-flight photoconductivity (TOFP), involved illuminating samples (100 μm electrode spacing) with 3 ns laser pulses near one electrode. A variable bias was applied, and the resulting time-dependent current $I(t)$ was measured as a voltage drop across a resistor at the opposite electrode.

For OFETs, charge transport was analyzed by fitting transfer curves to the standard field-effect transistor model, yielding the field-effect mobility (μ_{FET}) and on/off current ratio, which reflects device switching performance. Additionally, the contact resistance (R_C) at the electrode/OS interface was determined from I-V characteristics using the transfer-length method (TLM) [4], enabling quantification of injection-related effects in the OFETs.

Results and discussion

The morphology of P3HT:MXene blends was examined using scanning electron microscopy (SEM) and is presented in Fig. 2, revealing that higher MXene concentrations correspond to an increased flake density within the films (Fig. 2**a**). This trend is further supported by quantitative analysis of the flake density (Fig. 2**b**), confirming a systematic increase in MXene flake density with concentration. These morphological changes are expected to influence charge transport properties, as discussed below. Flake counting and density analysis were performed using ImageJ (Fiji) [5].

Fig. 3**a** shows TOFP I(t) curves for P3HT:MXene blends at bias voltage (V_b) of 100 V and an excitation wavelength of 530 nm, corresponding to P3HT's maximum absorption [6]. The bias polarity was set for hole drift toward the collecting electrode. The photocurrent drops sharply when the fastest carriers arrive, marked by a slope change in $I(t)$. The time of this change is taken as the hole transit time (t_{tr}), indicated by the arrow in the figure.

The measurements performed at varying V_b (presented in Fig. S3) show consistent results – the cusp shifts to shorter times as the bias increases. We extract t_{tr} position by using a Scher–Montroll-based model that approximates the line shape before and after the slope change [7]. From the value of t_{tr} we can calculate the TOFP charge carrier mobility (μ_{TOF}) by using equation:

$$\mu_{TOF} = \frac{\pi}{8}\frac{L^2}{t_{tr}V_b}. \quad (1)$$

Extracted mobilities values for different concentrations of MXenes at each V_b are summarized in Fig. 3**b**, presented in boxplots. The mean μ_{TOF} value of the neat P3HT layer is 1×10^{-3} cm^2/Vs. As more MXene flakes are added to the P3HT matrix, the mobility increases, reaching 4.75×10^{-3} cm^2/Vs at 5 %. This corresponds to a more than 370 % increase, demonstrating a favorable role of MXene flakes on the charge transport in these blends.

In OFET measurements, transconductance curves were acquired for 4 transistor devices for each MXene concentration. Fig. 4**a** shows the square root of the drain-source current I_{DS} versus the gate voltage V_{GS}, representative for each sample, while Fig. 4**b** presents boxplots of the extracted field-effect mobilities μ_{FET}. A trend of mobility increase is observed with the addition of MXenes, with it going from 1.5×10^{-3} cm^2/Vs for neat P3HT up to 2.0×10^{-3} cm^2/Vs for a 2.5 % MXene blend. However, at 5 % MXene content, a decrease in mobility is observed.

The observed 20 % enhancement in OFET mobility at 2.5 % MXene loading is accompanied by a notable reduction in contact resistance R_C (from 19 to 8 kΩmm), as shown in Fig. 4**c**. This reduction directly supports improved charge injection at the electrode/semiconductor interface – a critical bottleneck in organic transistor performance. However, at higher concentrations (5 % MXene), contact resistance increases sharply to 27 kΩmm – likely due to interface effects or non-uniform flake distribution near contacts, rather than bulk transport limitations. This is supported by the continued increase in TOFP mobility at 5 wt%.

Moreover, the improved on/off current ratio (Fig. 4**d**) and retained switching characteristics indicate that the incorporation of MXene flakes does not degrade the semiconducting behaviour of the P3HT matrix. This is particularly important given that MXenes are highly conductive materials and their presence could potentially introduce shorting pathways or increase leakage.

TOFP measures bulk charge transport at low carrier densities, where mobility reflects intrinsic semiconductor properties, free from injection barriers or contact resistance [7]. In contrast, OFETs operate at high carrier densities, where transport is influenced by the semiconductor/dielectric interface and contact resistance [8]. Similar to P3HT:graphene blends [9], MXenes in P3HT enhance mobility in TOFP by creating low-resistance pathways. However, in OFETs, charge injection barriers, contact resistance and charge trapping at the polymer-dielectric interface hinder the intrinsic mobility. Blends with doped metal oxide nanoparticles, such as Mg- and Ca-doped ZnO, have also been used to improve P3HT performance via energy level alignment, gate-induced surface potential modulation and trap density reduction in the active layer [10,11]. In contrast, the conductive MXene flakes primarily

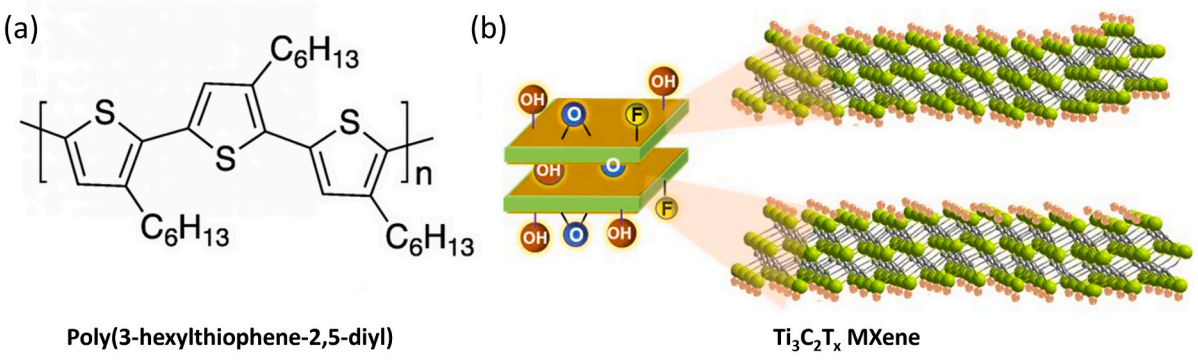

Fig. 1. a) Chemical structure of poly(3-hexylthiophene-2,5-diyl), commonly known as P3HT. b) Schematic view and atomic structure of two $Ti_3C_2T_x$ MXene layers.

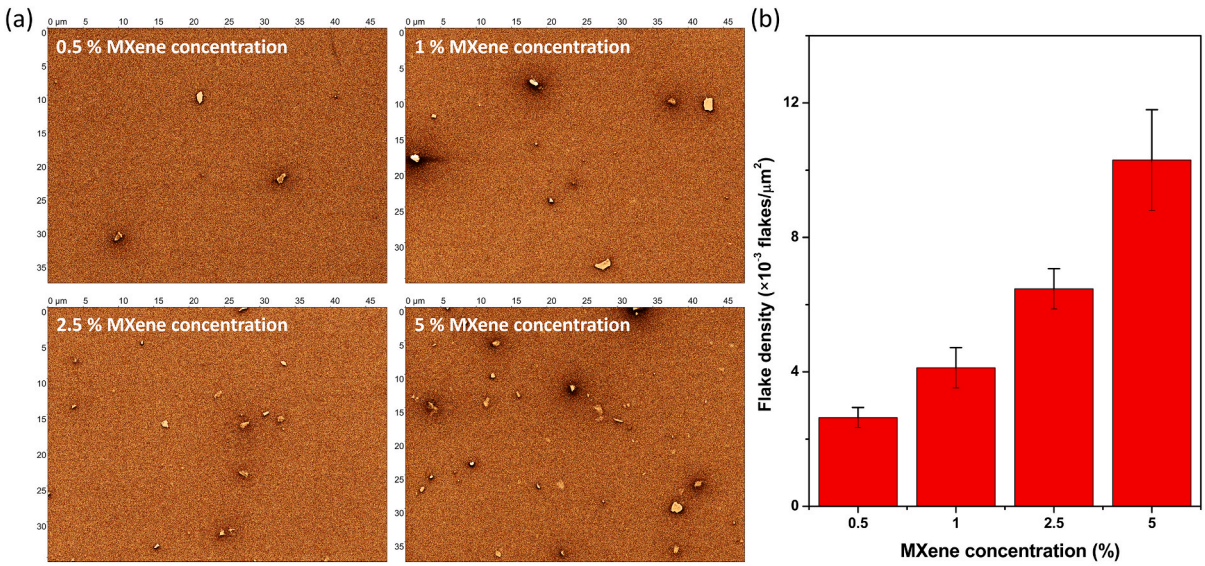

Fig. 2. a) SEM images of OFET active layers based on P3HT:MXene blends with varying MXene concentrations. The micrographs illustrate the dispersion and morphology of MXene flakes within the polymer matrix. b) The MXene density distribution is estimated from the SEM images.

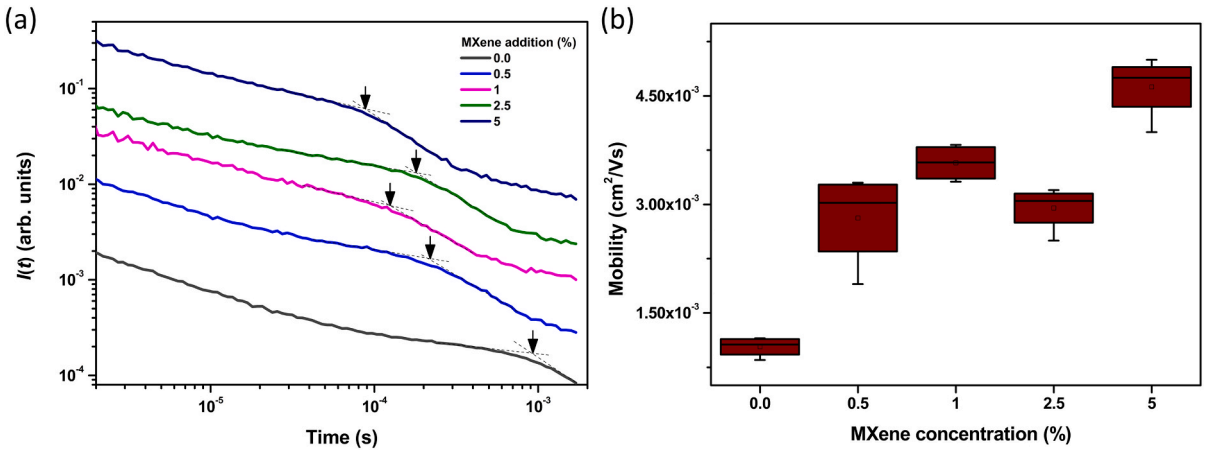

Fig. 3. a) TOFP of P3HT film with added MXene amount of 0–5 % at fixed V_b = 100 V in double-logarithmic plot. Arrows represent the transit time t_{tr}. b) The summarized mobilities for different P3HT:MXene blends, presented in a boxplot.

enhance transport by facilitating percolation and reducing contact resistance, indicating a different, more transport-driven mechanism.

Conclusion

In summary, we have demonstrated that incorporating MXenes into P3HT enhances charge transport, with the extent of improvement dependent on the measurement regime. TOFP measurements, which assess bulk charge transport under low-carrier density conditions, revealed a consistent increase in mobility with MXene addition. In contrast, OFET measurements, which probe interface-limited transport at higher carrier densities, showed a mobility increase at lower MXene concentrations (2.5 %) but a decline at higher concentrations (5 %). This reduction in field-effect mobility is attributed to increased contact resistance and interfacial charge trapping, likely caused by MXene aggregation at the semiconductor-electrode and semiconductor-dielectric interfaces.

By systematically evaluating charge transport in both bulk and interface-dominated regimes, we demonstrate that optimized P3HT:MXene composites can be tailored for different device architectures, balancing bulk transport benefits with interfacial stability. This highlights the potential of MXene-doped organic semiconductors for high-speed organic transistors and flexible sensor applications, where both bulk transport and interface effects play crucial roles. Our findings emphasize the need for controlled MXene dispersion to mitigate interfacial issues, ensuring robust device performance across different operational conditions.

CRediT authorship contribution statement

Jurij Urbančič: Writing – original draft, Visualization, Validation, Investigation, Conceptualization. **Huanhuan Shi:** Resources, Investigation. **Ali Shaygan Nia:** Resources, Investigation. **Egon Pavlica:** Writing – review & editing, Validation, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

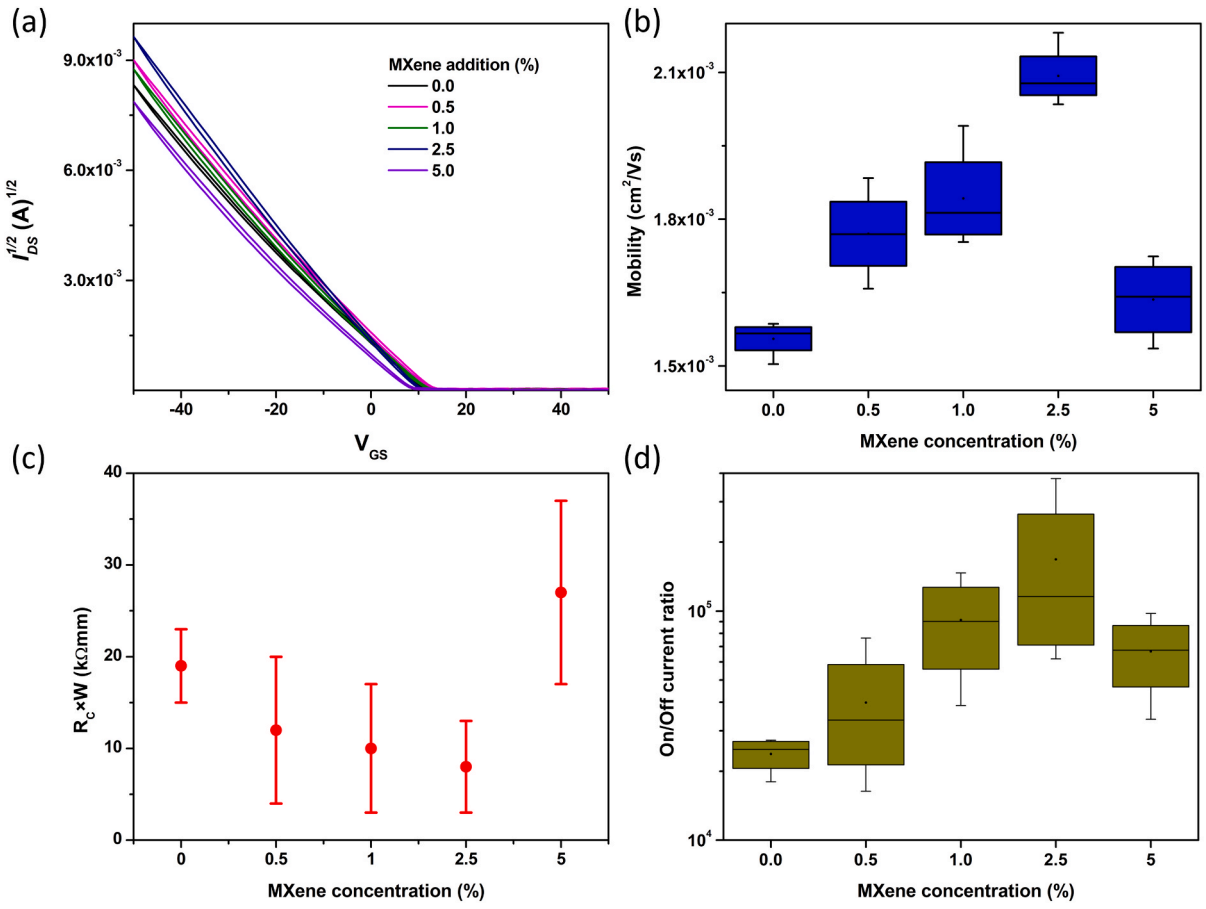

Fig. 4. a) Square root of the drain-source current vs gate voltage characteristics representative for each P3HT:MXene blend. The extracted b) mobilities, c) contact resistance and d) on/off current ratio of OFET devices.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.mlblux.2025.100244.

Data availability

Data will be made available on request.

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