



Defect-interface synergistic engineering of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ anodes toward fast-charging and durable sodium storage

Minghui Ma¹, Manyu Zhang², Chao Li², Mingyuan Wang¹, Jin'an Wang³, Xiang Hu⁴, Qian Sun⁵(✉), Yu Zhang²(✉)

¹ School of Vehicle and Traffic Engineering, Zhengzhou University of Science and Technology, Zhengzhou 450064, China

² College of Chemistry and Chemical Engineering, Xinyang Normal University, Xinyang 464000, China

³ National Polytechnic Institute of Mexico, Higher School of Chemical Engineering and Metallurgical Industry, Mexico City, 07738, Mexico

⁴ State Key Laboratory of Structural Chemistry, and Fujian Provincial Key Laboratory of Materials and Techniques toward Hydrogen Energy, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China

⁵ Department of Mechanical & Industrial Engineering, University of Toronto, Toronto, ON M5S 3G8, Canada

Nano Research Energy, Just Accepted Manuscript • <https://doi.org/10.26599/NRE.2026.9120289>

<https://www.sciopen.com/journal/2791-0091> on Oct. 23, 2026

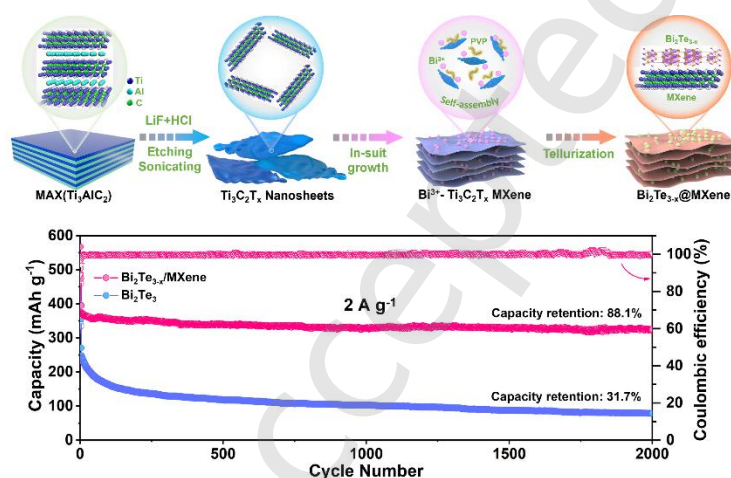
© The Authors(s)

Just Accepted

This is a "Just Accepted" manuscript, which has been examined by the peer-review process and has been accepted for publication. A "Just Accepted" manuscript is published online shortly after its acceptance, which is prior to technical editing and formatting and author proofing. Tsinghua University Press (TUP) provides "Just Accepted" as an optional and free service which allows authors to make their results available to the research community as soon as possible after acceptance. After a manuscript has been technically edited and formatted, and the page proofs have been corrected, it will be removed from the "Just Accepted" web site and published officially with volume and article number (e.g., Nano Research Energy, 2025, 4, e9120191). Please note that technical editing may introduce minor changes to the manuscript text and/or graphics which may affect the content, and all legal disclaimers that apply to the journal pertain. In no event shall TUP be held responsible for errors or consequences arising from the use of any information contained in these "Just Accepted" manuscripts. To cite this manuscript please use its Digital Object Identifier (DOI®), which is identical for all formats of publication.

Defect-Interface Synergistic Engineering of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ Anodes toward Fast-Charging and Durable Sodium Storage

Table of contents



Te-vacancy engineering and robust Ti-Te interfacial coupling synergistically regulate the electronic structure and accelerate Na^+ transport in $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$. The integrated heterostructure stabilizes conversion-alloying reactions, enabling ultralong cycling life and high energy-power output in sodium-ion batteries.



Defect-interface synergistic engineering of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ anodes toward fast-charging and durable sodium storage

Minghui Ma¹, Manyu Zhang², Chao Li², Mingyuan Wang¹, Jin'an Wang³, Xiang Hu⁴, Qian Sun⁵ (✉), and Yu Zhang² (✉)

¹ School of Vehicle and Traffic Engineering, Zhengzhou University of Science and Technology, Zhengzhou, Henan, 450064, China

² College of Chemistry and Chemical Engineering, Xinyang Normal University, Xinyang, 464000, China

³ National Polytechnic Institute of Mexico, Higher School of Chemical Engineering and Metallurgical Industry, Mexico City, 07736 Mexico

⁴ State Key Laboratory of Structural Chemistry, and Fujian Provincial Key Laboratory of Materials and Techniques toward Hydrogen Energy, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China

⁵ Department of Mechanical & Industrial Engineering, University of Toronto, Toronto, ON M5S 3G8, Canada

@ The Author(s)

Received: 23 July 2026 / Revised: 13 September 2026 / Accepted: 4 October 2026

ABSTRACT

Metal tellurides are promising anode candidates for high-energy sodium-ion batteries (SIBs) owing to their multielectron redox chemistry, but their practical deployment is limited by sluggish reaction kinetics and severe structural instability associated with repeated conversion/alloying reactions. Herein, a Te-vacancy-rich $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ heterostructure is rationally constructed via synergistic electrostatic assembly and in situ tellurization. Strong Ti-Te interfacial coupling immobilizes $\text{Bi}_2\text{Te}_{3-x}$ nanoparticles on conductive MXene nanosheets, generating a robust three-dimensional architecture with continuous electron/ion transport pathways and enhanced tolerance to volume variation. Meanwhile, Te-vacancy engineering tailors the electronic structure and creates abundant active sites, synergistically accelerating Na^+ transport kinetics. Combined electrochemical analysis and in situ/ex situ characterizations reveal a highly reversible insertion-conversion-alloying mechanism with stabilized phase evolution during cycling. Consequently, the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ anode delivers outstanding rate capability and ultralong cycling stability, retaining 324.8 mAh g⁻¹ after 2000 cycles at 2 A g⁻¹ and maintaining 317.9 mAh g⁻¹ even at 10 A g⁻¹. Moreover, the $\text{Na}_3\text{V}_2(\text{PO}_4)_3/\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ full cell achieves a high energy density of 210.6 Wh kg⁻¹ and preserves 104.7 Wh kg⁻¹ even at an ultrahigh power density of 11300 W kg⁻¹. This work highlights the effectiveness of integrating defect chemistry with heterointerface engineering to unlock fast and durable sodium storage in metal tellurides for high-energy and high-power SIBs.

KEYWORDS

sodium-ion batteries, anode, $\text{Bi}_2\text{Te}_{3-x}$, Te-vacancy engineering, ultralong cycling stability

1 Introduction

The global transition toward electrified society and renewable-dominated power grids demands electrochemical storage systems that are not only high-performing but also inherently scalable and resource-sustainable [1-3]. Sodium-ion batteries (SIBs) are therefore attracting intense interest as a compelling post-lithium technology, enabled by the natural abundance, low cost, and wide geographic distribution of sodium resources [4-8]. However, the larger ionic radius and slower diffusion kinetics of Na^+ compared with Li^+ impose stringent requirements on anode materials, especially in terms of structural robustness, reaction

reversibility, and interfacial charge-transfer efficiency under practical current densities [9, 12]. Consequently, developing high-capacity anode materials capable of simultaneously achieving fast ion/electron transport, high structural stability, and durable cycling performance remains a critical challenge for next-generation SIBs.

Among various candidate anodes, bismuth-based materials have attracted considerable attention owing to their high electronic conductivity and favorable alloying/dealloying reactions with sodium [11-15]. In particular, layered Bi_2Te_3 has emerged as a promising anode material because of its multielectron conversion/alloying chemistry, high theoretical capacity, and intrinsically fast electron transport characteristics

[16-18]. Nevertheless, its practical electrochemical performance is still limited by severe volume fluctuation during repeated sodiation/desodiation, particle pulverization, interparticle electrical disconnection, and unstable solid-electrolyte interphase (SEI) evolution. More importantly, the structural instability of Bi_2Te_3 is further aggravated under high-rate conditions, where insufficient interfacial charge-transfer efficiency and slow Na^+ transport become increasingly dominant. In essence, the fundamental bottleneck of Bi_2Te_3 -based anodes lies not only in their limited structural stability, but also in the lack of robust and dynamically stable heterointerfaces capable of simultaneously regulating electron transport, Na^+ diffusion, and stress dissipation throughout repeated electrochemical cycling.

Two-dimensional MXenes, represented by $\text{Ti}_3\text{C}_2\text{T}_x$, have recently emerged as highly attractive conductive scaffolds for advanced electrochemical energy-storage systems because of their metallic conductivity, hydrophilic surface chemistry, abundant terminal functional groups, and mechanically flexible layered structures [19-21]. Unlike graphene, which features a relatively inert sp^2 carbon surface with limited chemical functionality, MXenes provide abundant surface terminations ($-\text{O}$, $-\text{OH}$, and $-\text{F}$) and tunable interlayer galleries, enabling stronger interfacial coupling with active materials, enhanced electrolyte accessibility, and more favorable Na^+ transport kinetics. These unique structural and interfacial characteristics allow MXene nanosheets to function as conductive and flexible matrices that accommodate volume variation, suppress active-phase aggregation, and facilitate electron/ion transport during electrochemical cycling [22-24]. However, conventional hybridization approaches, such as mechanical mixing or post-growth assembly, generally suffer from weak interfacial interactions and uncontrolled active-phase distribution, leading to increased interfacial resistance, severe nanosheet restacking, and localized transport bottlenecks during cycling. As a result, achieving efficient interfacial charge transfer and structural integrity simultaneously remains highly challenging. These limitations underscore the importance of constructing strongly coupled and spatially regulated heterostructures in which the nucleation, growth, and crystallization behaviors of active materials can be precisely controlled to maximize interfacial stability and electrochemical kinetics.

Herein, we report the rational design of Te-vacancy-rich $\text{Bi}_2\text{Te}_{3-x}$ @MXene composites, in which highly conductive MXene nanosheets serve as a robust 2D matrix for Bi_2Te_3 via a combination of electrostatic adsorption and in situ tellurization strategies. In this architecture, $\text{Bi}_2\text{Te}_{3-x}$ nanoparticles are uniformly anchored on the MXene surface through strong Ti-Te covalent interactions and simultaneously interwoven into a 3D conductive framework, forming continuous pathways that enable rapid electron/ion transport while maintaining structural integrity during repeated cycling. Meanwhile, the

introduction of Te vacancies effectively tailors the electronic structure and generates abundant electrochemically active sites, thereby enhancing Na^+ adsorption capability and accelerating charge-transfer kinetics. Benefiting from these structural and interfacial merits, the $\text{Bi}_2\text{Te}_{3-x}$ @MXene electrodes exhibit markedly enhanced sodium-storage performance, delivering high reversible capacity, excellent long-term cycling stability, and superior rate capability in both half-cell and full-cell sodium-ion battery configurations.

2 Results and Discussion

The fabrication process of the Te-vacancy-rich $\text{Bi}_2\text{Te}_{3-x}$ @MXene composites is schematically illustrated in Figure 1a. Initially, few-layer $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanosheets were exfoliated from the Ti_3AlC_2 MAX precursor through a mild etching strategy [5, 25]. Assisted by ultrasonic delamination, the obtained MXene exhibits a highly exposed two-dimensional architecture with large specific surface area and excellent dispersibility (Figure S1 and S2), providing abundant active sites for the subsequent anchoring of Bi species. Subsequently, Bi^{3+} ions were uniformly immobilized on the negatively charged MXene surface via electrostatic interactions, effectively suppressing precursor aggregation. Meanwhile, PVP acted as a coordination agent to regulate the nucleation and growth of Bi-based species, where the carbonyl groups within the pyrrolidone rings coordinated with Bi^{3+} ions to retard rapid hydrolysis and agglomeration. During the subsequent in situ tellurization process, the adsorbed Bi species were gradually converted into uniformly dispersed nanoparticles on the MXene framework, ultimately forming the Te-vacancy-rich $\text{Bi}_2\text{Te}_{3-x}$ @MXene heterostructure.

The morphology and microstructure of the $\text{Bi}_2\text{Te}_{3-x}$ @MXene composites were systematically examined by field-emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM). As shown in Figure 1b and c, the $\text{Bi}_2\text{Te}_{3-x}$ nanoparticles are uniformly and intimately anchored on highly wrinkled, interconnected MXene nanosheets, constructing a well-defined three-dimensional hierarchical architecture. Notably, the intrinsic ultrathin layered configuration of MXene is well retained after the tellurization process, indicating the structural robustness of the MXene scaffold during composite formation. In sharp contrast, pure Bi_2Te_3 shows pronounced particle agglomeration and irregular bulk-like morphologies composed of densely packed nanoparticles (Figure S3), indicative of uncontrolled crystal growth and the absence of an effective dispersive substrate. These observations highlight the critical role of MXene in directing the spatially confined growth of $\text{Bi}_2\text{Te}_{3-x}$ nanocrystals and stabilizing the overall architecture. TEM analysis further confirms that ultrafine $\text{Bi}_2\text{Te}_{3-x}$ nanoparticles with an average diameter of ~ 20 nm are homogeneously dispersed and firmly anchored on the MXene nanosheets without observable aggregation (Figure 1d, e), evidencing the effectiveness of the

electrostatic adsorption-assisted nucleation and growth strategy. High-resolution TEM (HRTEM) of pure Bi_2Te_3 reveals well-defined lattice fringes with an interplanar spacing of 0.323 nm (Figure 1g), corresponding to the (015) plane of rhombohedral Bi_2Te_3 (PDF#08-0027) [26, 27]. In comparison, the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ composite (Figure 1f) exhibits a slightly expanded lattice spacing of 0.326 nm for the same plane, indicative of lattice dilation induced by Te vacancy formation. More importantly, the corresponding 3D surface-intensity reconstruction further reveals pronounced lattice fluctuations and enhanced

local structural disorder in $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ relative to pure Bi_2Te_3 , indicating the presence of abundant defect sites and significant lattice distortion, which are expected to contribute to modulate the local electronic environment and accelerated charge transfer. The high-angle annular darkfield scanning TEM (HAADF-STEM) image and corresponding energy dispersive spectroscopy (EDS) elemental mappings clearly demonstrate the presence and uniform distribution of Ti, C, O, Bi, and Te elements within the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ (Figure 1h-m).

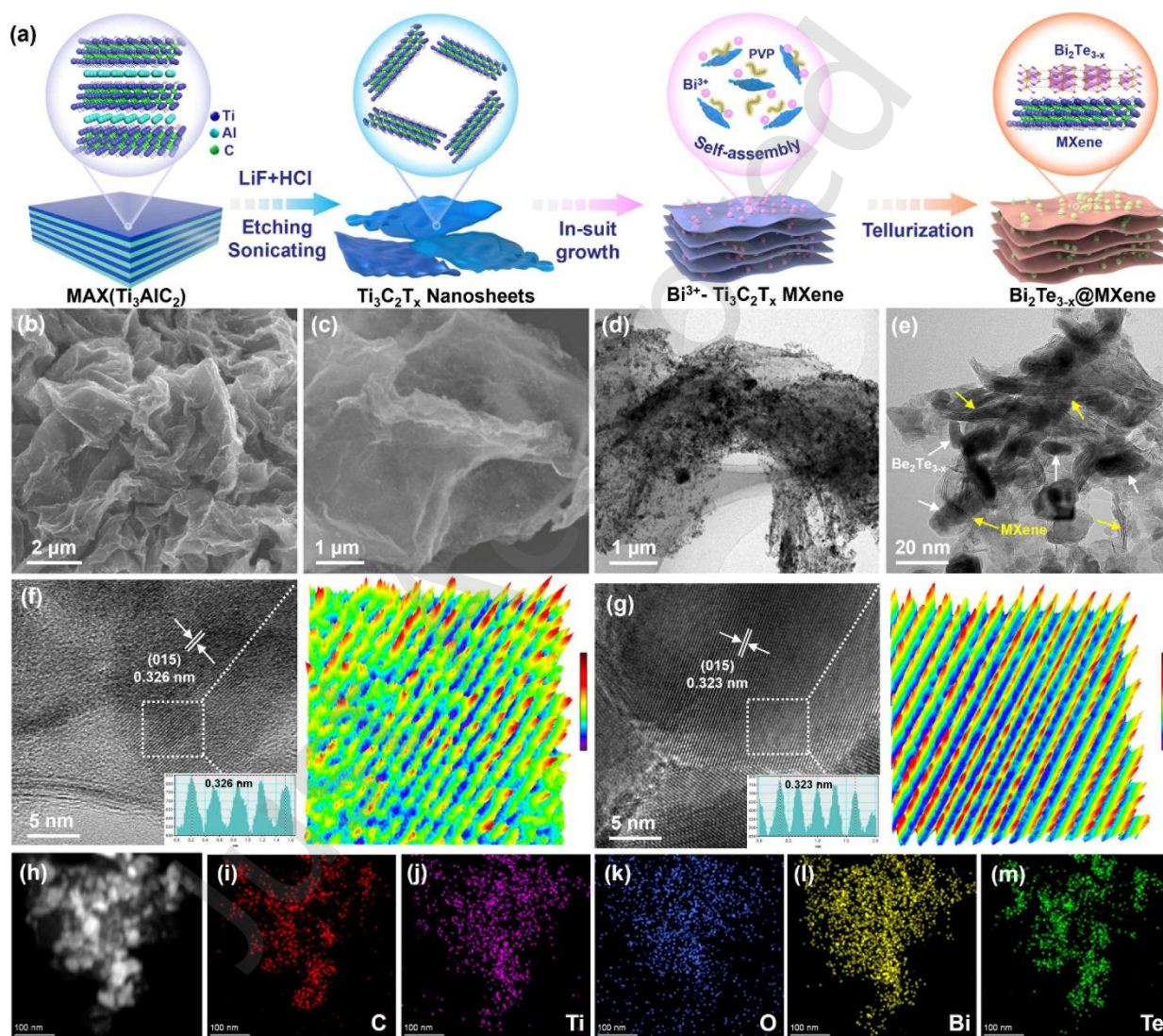


Figure 1. Synthesis and morphology characteristics. (a) Schematic illustration of the synthesis process. (b, c) FESEM images and (d, e) TEM images of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ composite. (f) HRTEM image and 3D Surface Plots of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ composite. (g) HRTEM image and 3D Surface Plots of the pure Bi_2Te_3 . (h) HAADF-STEM image and (i-m) corresponding elemental mappings of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ composite.

The crystal structure and phase composition of the $\text{Bi}_2\text{Te}_3\text{@MXene}$ composite were investigated by X-ray diffraction (XRD). As shown in Figure 2a, all diffraction peaks of both pure Bi_2Te_3 and $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ can be

unambiguously indexed to rhombohedral Bi_2Te_3 phase (JCPDS no. 08-0027), with no detectable impurity peaks, confirming the successful formation of highly crystalline and phase-pure Bi_2Te_3 [28]. The characteristic reflection located below 10° is assigned to the (002) plane of $\text{Ti}_3\text{C}_2\text{Tx}$

MXene, consistent with its typical layered structure. Notably, compared with pure MXene, the (002) peak of $\text{Bi}_2\text{Te}_3/\text{MXene}$ shifts toward lower diffraction angles, indicating an increased interlayer spacing after the incorporation of Bi_2Te_3 nanostructures. This enlarged spacing not only mitigates nanosheet restacking but also facilitates electrolyte infiltration and shortens ion transport pathways, thereby promoting faster charge transfer and improved electrochemical kinetics. Moreover, the magnified XRD pattern (Figure 2b) reveals subtle shifts of selected Bi_2Te_3 reflections, indicative of slight lattice distortion while preserving the rhombohedral phase, which can be reasonably associated with Te-defect formation and interfacial coupling with MXene. Electron paramagnetic resonance (EPR) spectroscopy was further

employed to probe the defect chemistry of the obtained samples. As displayed in Figure 2c, $\text{Bi}_2\text{Te}_3/\text{MXene}$ exhibits a pronounced resonance signal centered at 2.003, whereas pure Bi_2Te_3 shows only a much weaker response. This signal is characteristic of unpaired electrons trapped at Te-vacancy-related defect centers, demonstrating a markedly higher defect concentration in the hybrid [29, 30]. The increased defect density is attributed to the strong interfacial coupling between Bi_2Te_3 and MXene, which promotes the generation and stabilization of vacancies. Such abundant vacancy defects can serve as additional electrochemically active sites and modulate the local electronic structure, thereby enhancing charge transfer and accelerating ion-storage kinetics.

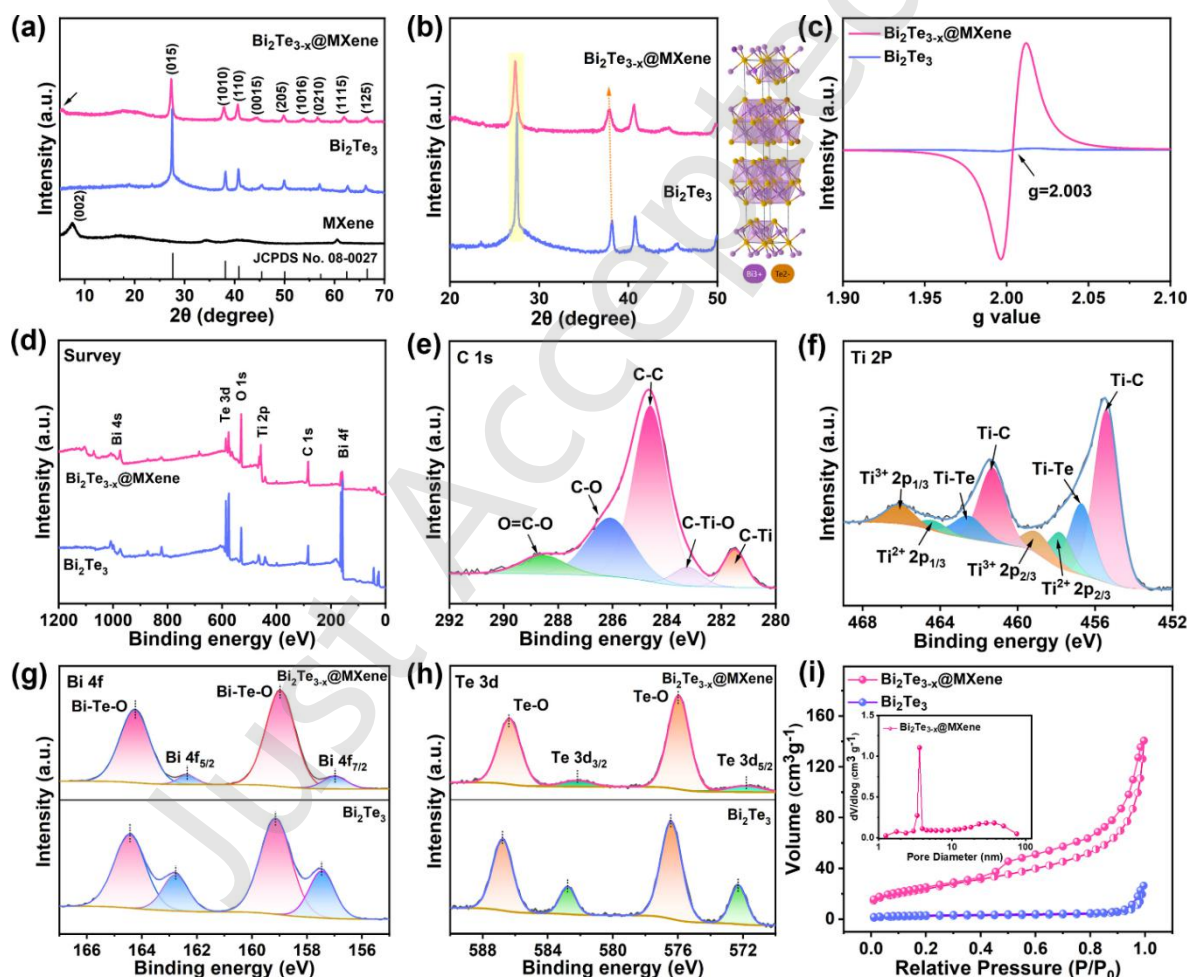


Figure 2. Structural characterization. (a, b) XRD pattern of MXene, pure Bi_2Te_3 and $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$. (c) EPR spectra and (d) XPS panoramic spectra of pure Bi_2Te_3 and $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$. High-resolution XPS spectra of (e) C 1s and (f) Ti 2p for $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$. High-resolution XPS spectra of (g) Bi 4f, (h) Te 3d and (i) BET analysis for pure Bi_2Te_3 and $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$ (inset: pore size distribution).

The surface chemical composition and electronic structure evolution of the $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$ hybrid were systematically investigated by X-ray photoelectron spectroscopy (XPS). In the survey spectra (Figure 2d),

both pure Bi_2Te_3 and $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$ exhibit characteristic Bi and Te signals, while the emergence of distinct Ti-related peaks in the $\text{Bi}_2\text{Te}_{3-x}/\text{MXene}$ composite confirms the successful integration of the MXene framework into the hybrid architecture. The

high-resolution C 1s spectrum of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ (Figure 2e) can be deconvoluted into five components centered at 281.5, 283.2, 284.6, 286.1, and 288.6 eV, corresponding to C-Ti, C-Ti-O, C-C, C-O, and O-C=O species, respectively.[18, 25] The retained C-Ti and C-Ti-O components verify that the carbide backbone of MXene is preserved after hybrid formation, whereas the oxygen-containing species arise from surface terminations and slight surface oxidation during etching and exfoliation. More importantly, the Ti 2p spectrum can be fitted into four pairs of spin-orbit doublets located at 455.4/461.3, 456.7/462.2, 457.8/464.4, and 459.2/466.1 eV (Figure 2f), corresponding to Ti-C, Ti-Te, $\text{Ti}^{2+} 2\text{P}_{2/3}$, and $\text{Ti}^{3+} 2\text{P}_{2/3}$ species, respectively [18, 31, 32]. Notably, the appearance of the Ti-Te component suggests the formation of strongly chemical bonding between Ti atoms of MXene and Te atoms in $\text{Bi}_2\text{Te}_{3-x}$, rather than simple physical contact. Such interfacial Ti-Te bonding not only anchors $\text{Bi}_2\text{Te}_{3-x}$ nanocrystals onto the conductive MXene scaffold but also establishes an efficient electronic communication pathway across the heterointerface. The high-resolution Bi 4f spectrum of pure Bi_2Te_3 (Figure 2g) displays two characteristic peaks located at 157.5 and 162.7 eV, assigned to Bi 4f_{7/2} and Bi 4f_{5/2}, respectively [26, 33]. Additional peaks at 159.1 and 164.4 eV are attributed to oxidized Bi-Te-O species, indicating partial surface oxidation [34]. Similarly, the Te 3d spectrum of pure Bi_2Te_3 (Figure 2h) exhibits Te 3d_{3/2} and 3d_{5/2} peaks at 572.3 and 582.8 eV, accompanied by Te-O signals at 576.4 and 586.8 eV.[18] Compared with pure Bi_2Te_3 , both Bi 4f and Te 3d peaks of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ exhibit obvious shifts toward lower binding energies, accompanied by a noticeable suppression of the Bi-Te-O and Te-O components. The negative shifts reveal an increased electron density around both Bi and Te atoms, suggesting substantial electronic reconstruction within the $\text{Bi}_2\text{Te}_{3-x}$ lattice. This phenomenon can be attributed to the synergistic effect of Te-vacancy-induced charge redistribution and interfacial electron transfer from MXene to $\text{Bi}_2\text{Te}_{3-x}$. The strong electronic coupling at the heterointerface effectively alters the local electronic environment of Bi and Te atoms, confirming the formation of a defect-rich electronically coupled heterostructure. Nitrogen adsorption-desorption measurements were further carried out to elucidate the porous characteristics. As shown in Figure 2i, the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ exhibits a typical type IV isotherm with a pronounced hysteresis loop, indicative of a mesoporous architecture. The Brunauer-Emmett-Teller (BET) specific surface area of $\text{Bi}_2\text{Te}_3\text{@MXene}$ reaches $92.7 \text{ m}^2 \text{ g}^{-1}$, which is much higher than that of the pure Bi_2Te_3 ($11.4 \text{ m}^2 \text{ g}^{-1}$), demonstrating that the integration of $\text{Bi}_2\text{Te}_{3-x}$ with the two-dimensional MXene framework substantially increases the exposed surface area and accessible interface. The pore-size distribution (inset of Figure 2i) further suggests the presence of hierarchical pores dominated by mesopores together with larger transport voids. Such a multiscale

porous network provides abundant electrochemically active sites, facilitates electrolyte infiltration and ion diffusion, and effectively buffers the volume variation of $\text{Bi}_2\text{Te}_{3-x}$ during repeated charge/discharge processes.

The sodium-storage behavior of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ composite was investigated by cyclic voltammetry (CV) at a scanning rate of 0.1 mV s^{-1} (Figure 3a). During the initial three cycles, the CV profiles exhibit highly overlapped cathodic and anodic peaks, indicating excellent electrochemical reversibility and structural stability upon repeated sodiation/desodiation. In the first cathodic scan, several distinct reduction peaks located at approximately 1.41, 1.13, 0.62, and 0.35 V versus Na^+/Na , are observed, suggesting a multistep sodium-storage mechanism. The broad peak centered at $\sim 1.13 \text{ V}$ is primarily associated with the formation of a solid-electrolyte interphase (SEI) layer together with the conversion reaction of Bi_2Te_3 to metallic Bi and Na_2Te [34]. Subsequently, the reduction peaks at 0.62 and 0.35 V can be assigned to the sequential alloying reactions between Bi and Na, leading to the formation of NaBi and Na_3Bi phases, respectively [33]. During the anodic sweep, the corresponding oxidation peaks arise from the reversible dealloying of Na_3Bi and the reconstruction of the Bi-Te framework. Notably, the CV response of pure Bi_2Te_3 exhibits similar redox features (Figure S4), confirming the preservation of the intrinsic sodium-storage chemistry after MXene incorporation and Te-defect engineering. The galvanostatic charge-discharge (GCD) profiles recorded at 0.2 A g^{-1} for the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode display well-defined voltage plateaus that closely correspond to the redox peaks observed in the CV curves, further verifying the proposed reaction mechanism (Figure 3b). The $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode delivers an initial discharge and charge capacity of 504.1 and 439.3 mAh g^{-1} , respectively, corresponding to a high initial Coulombic efficiency (ICE) of 87.1%, which is higher than that of pure Bi_2Te_3 (76.8%, Figure S5). The irreversible capacity loss in the first cycle can be mainly attributed to SEI formation and irreversible electrolyte decomposition. Despite these irreversible processes, the ICE of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ compares favorably with those of representative metal-chalcogenide anodes reported in the recent literature (Table S1). Encouragingly, the Coulombic efficiency rapidly increases and stabilizes at nearly 100% in subsequent cycles, indicating highly reversible electrochemical reactions and excellent interfacial stability.

The cycling performance was further evaluated at 0.2 A g^{-1} (Figure 3c). Remarkably, the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode retains a reversible capacity of 383.2 mAh g^{-1} after 200 cycles, substantially outperforming pure Bi_2Te_3 electrode, which only maintains 219.4 mAh g^{-1} under identical conditions. The rate capability of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode was subsequently examined over a wide range of current densities (Figure 3d). The electrode delivers reversible capacities of 451.3, 419.4, 396.7, 374.8, 353.1, and 336.5 mAh g^{-1} at 0.1, 0.2, 0.5, 1, 2 and 5 A g^{-1} ,

respectively. Even under an ultrahigh current density of 10 A g^{-1} , the capacity (317.9 mAh g^{-1}) of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ remains significantly higher than that of pure Bi_2Te_3 (114.2 mAh g^{-1}), highlighting the superior reaction kinetics of the hybrid architecture. Notably, the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode maintains 70.4% of its initial capacity despite a 100-fold increase in current density, whereas pure Bi_2Te_3 retains only 33.1%, underscoring the remarkable rate tolerance of the composite. These results demonstrate that an appropriate amount of MXene not only synergistically enhances electronic conductivity but also stabilizes the overall electrode architecture during repeated (de)sodiation. The corresponding GCD curves at different current densities of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ exhibit highly reversible charge/discharge characteristics with only a slight increase in polarization as the current density increases compared to pure Bi_2Te_3 (Figure 3e and S6), suggesting fast charge-transfer kinetics and efficient Na^+ diffusion within the electrode. Such behavior can be attributed to the synergistic effects of Te-vacancy engineering and the highly conductive MXene framework, which collectively accelerate electron transport, expose additional electrochemically active sites, and buffer the volume variations associated with repeated alloying/dealloying reactions. When the current density is restored to 0.1 A g^{-1} , the capacity of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$

rapidly recovers to 446.3 mAh g^{-1} , corresponding to 98.9% of its initial value, whereas pure Bi_2Te_3 electrode recovers only 295.1 mAh g^{-1} , further demonstrating the excellent structural robustness and electrochemical reversibility of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode. To further benchmark its high-rate performance, the electrochemical properties of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ were compared with previously reported Bi_2Te_3 and Bi_2Se_3 based anodes for SIBs (Figure 3f) [28, 33-39]. The $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode exhibits one of the highest reversible capacities across a broad current-density range, highlighting the effectiveness of the integrated defect-engineering and MXene-coupling strategy. To further evaluate the electrolyte compatibility of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$, its electrochemical performance was also examined in a conventional carbonate-based electrolyte of 1 M NaClO_4 in EC/DMC (1:1, v/v). As shown in Figure S7, $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ exhibits slightly lower capacity and stability in the carbonate-based electrolyte than in the diglyme-based electrolyte, while still outperforming pristine Bi_2Te_3 . The improved performance in diglyme can be attributed to the more favorable interfacial chemistry and Na^+ transport characteristics of the ether-based electrolyte, which are better suited to the repeated conversion/alloying reactions and associated structural evolution of telluride anodes.

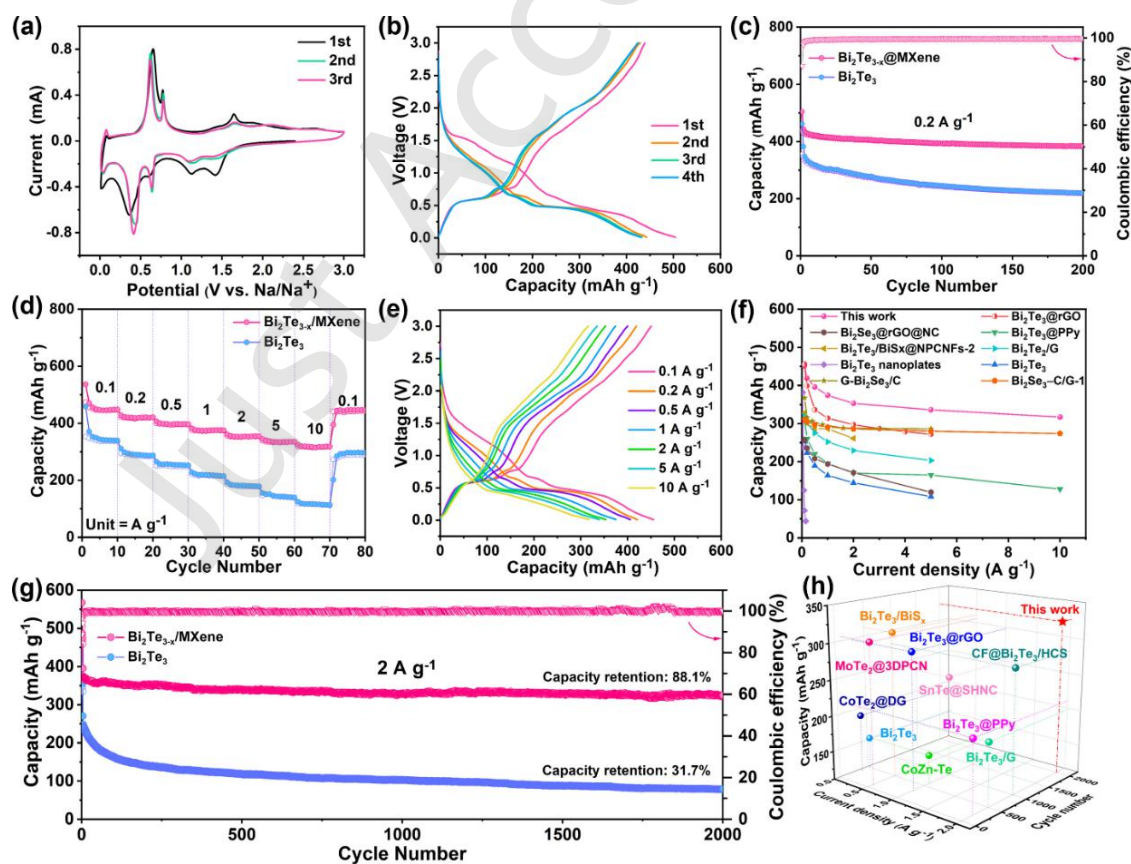


Figure 3. Electrochemical performance. (a) CV curves at a scan rate of 0.1 mV s^{-1} and (b) galvanostatic charge/discharge voltage profiles of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode at 0.2 A g^{-1} . (a) Cycling stability at 0.2 A g^{-1} , (d) rate performance and (e) charge/discharge profiles of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ at different current densities. (f) Rate capability comparison with previously

reported Bi_2Te_3 and Bi_2Se_3 based anodes. (g) Long-term cycling performance of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Be_2Te_3 at 2.0 A g^{-1} . (h) Comparison of long-term cycling stability with other reported metal telluride anodes for SIBs.

More importantly, the long-term cycling stability was evaluated at a high current density of 2 A g^{-1} (Figure 3g). The $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode maintains a reversible capacity of 324.8 mAh g^{-1} after 2000 cycles, with an impressive capacity retention of 88.1%, evidencing its excellent cycling robustness under high-rate operation. Ex situ structural characterization reveals that, after prolonged cycling, the $\text{Bi}_2\text{Te}_{3-x}$ nanoparticles remain uniformly anchored on the crumpled MXene nanosheet framework, without pronounced pulverization or aggregation (Figure S8 a, b). Moreover, the HRTEM and EPR results confirm that the Te-vacancy-related defects are substantially retained after prolonged cycling (Figure S8c, d). This preserved architecture verifies the key role of MXene in accommodating the volume variation of $\text{Bi}_2\text{Te}_{3-x}$, restraining the migration/agglomeration of active species,

and sustaining continuous charge-transport pathways during repeated sodiation/desodiation. Notably, the Coulombic efficiency remains nearly 100% over the entire cycling process, suggesting highly reversible Na^+ storage reactions and a stable electrode/electrolyte interface. In sharp contrast, pure Be_2Te_3 retains only 31.7% of its initial capacity after 2000 cycles, highlighting the synergistic effect of MXene integration and Te-vacancy engineering in enhancing structural stability and electrochemical reversibility. Furthermore, benchmarking against recently reported Bi-based and metal telluride anodes for SIBs confirms that $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ offers a competitive combination of high reversible capacity, excellent rate performance, and outstanding long-term cycling durability. (Figure 3h) [26, 28, 33-35, 37, 40-43].

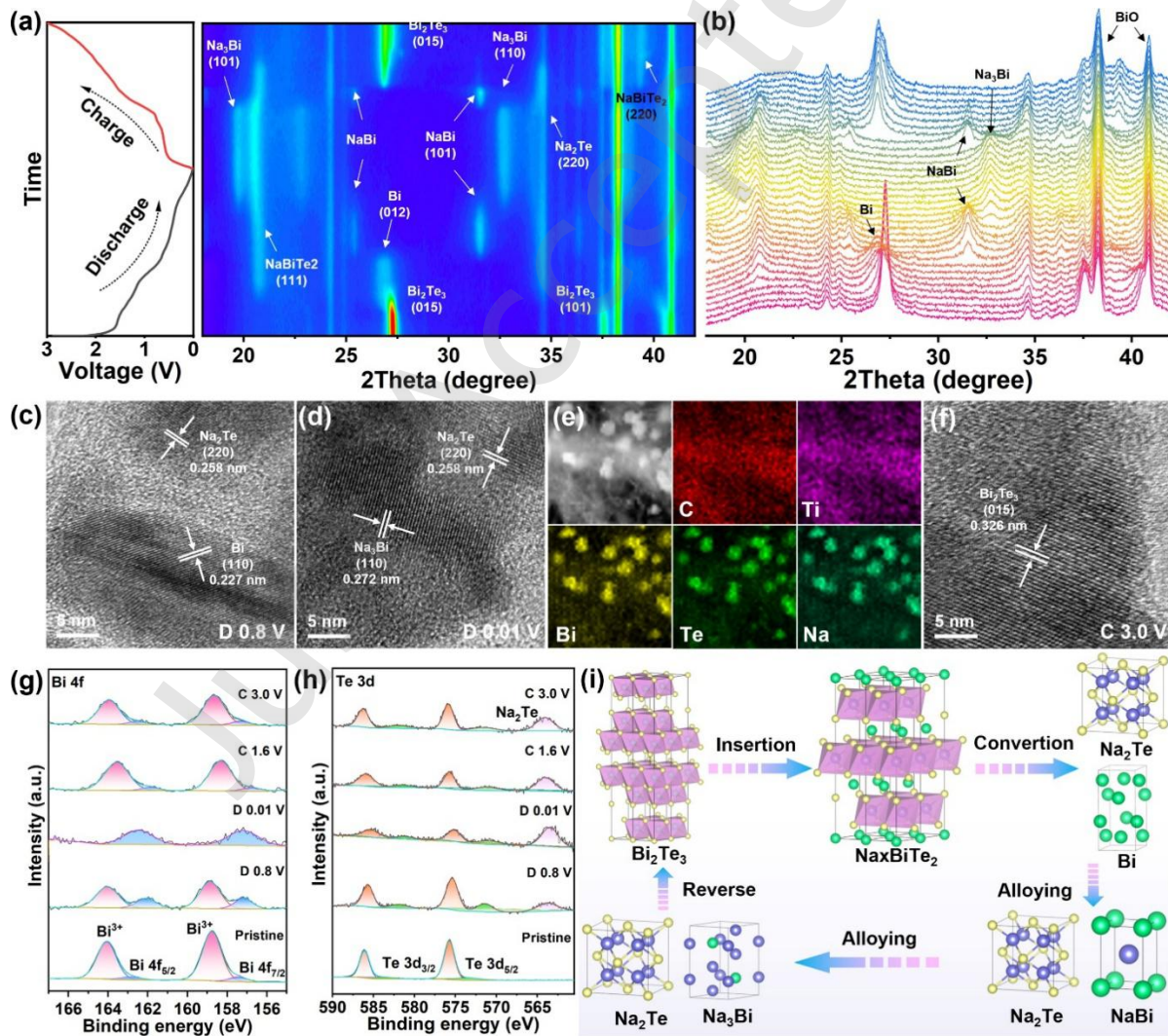


Figure 4. Elucidation of the Na-storage mechanism in $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode. (a, b) Galvanostatic discharge/charge curve and corresponding operando XRD patterns. Ex situ HRTEM images acquired at (c) 0.8 V and (d) 0.01 V during discharge, (e) HAADF-STEM image with elemental mappings at 0.01 V, and (f) 3.0 V after charge. Ex situ XPS spectra of (g) Bi 4f and (h) Te 3d at selected electrochemical states. (i) Schematic illustration of the coupled

insertion-conversion-alloying mechanism during Na^+ storage.

To elucidate the sodium-storage mechanism of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode, in-situ XRD measurements were carried out during the discharge/charge process (Figure 4a). At open-circuit voltage, the diffraction peaks located at 27.2° , 37.5° , and 40.4° can be assigned to crystalline Bi_2Te_3 . Upon sodiation, these characteristic peaks progressively weaken, accompanied by the emergence of new reflections at 26.9° and 20.9° , which can be indexed to the (012) plane of metallic Bi (JCPDS No. 85-1329) and the (111) plane of NaBiTe_2 (JCPDS card no. 65-6863), respectively [34, 37]. This evolution indicates that the pristine Bi_2Te_3 phase undergoes a conversion reaction with Na^+ , generating intermediate NaBiTe_2 together with Bi. As the discharge proceeds to below 1.0 V, additional diffraction signals corresponding to Na_2Te and NaBi become discernible, suggesting a sequential multistep conversion process. With further sodiation from 0.6 to 0.01 V, new peaks appear at 32.7° and 19.9° , assignable to the (101) and (110) planes of Na_3Bi (JCPDS card no. 04-0351), respectively [18]. The formation of Na_3Bi demonstrates that the Bi species generated during the conversion process subsequently undergo alloying with sodium, leading to the fully sodiated state. During desodiation, the Na_3Bi -related peaks gradually vanish when the cell is charged to 0.8 V, accompanied by the reappearance of the NaBi phase, indicative of the stepwise dealloying of Na_3Bi . Upon further charging to 1.6 V, the reflections associated with Bi and NaBiTe_2 re-emerge, implying the reversibility of the conversion reaction between sodium and the telluride framework. When the potential reaches 3.0 V, the diffraction features of Bi_2Te_3 become detectable again, although with relatively weakened intensity, suggesting the reformation of Bi_2Te_3 with reduced crystallinity after desodiation.

The ex-situ TEM characterization of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode at different (dis)charge states further provide direct visualization of the phase evolution. At 0.8 V discharge (Figure 4c), lattice fringes with spacings of 0.227 nm and 0.258 nm are observed, corresponding to the (110) plane of Bi and the (220) plane of Na_2Te , confirming the initial conversion of Bi_2Te_3 into Bi and Na_2Te [33]. Upon deep discharge to 0.01 V (Figure 4d), additional fringes at 0.272 nm, assignable to the (110) plane of Na_3Bi , appear alongside Na_2Te , indicating subsequent alloying of Bi to form Na_3Bi phase inferred from the XRD patterns. Elemental mapping at full discharge (Figure 4e) reveals uniform distribution of C, Ti, Bi, Te, and Na, demonstrating intimate integration of MXene with active phases, which facilitates electron transport and accommodates volumetric changes. During the subsequent charge to 3.0 V (Figure 4f), the lattice fringes corresponding to the (015) plane of Bi_2Te_3 reappear, evidencing reversible reconstruction of the Bi_2Te_3 phase, although reduced contrast and partial lattice

disorder suggest lower crystallinity and nanoscale structural features, consistent with the weakened XRD reflections after charging.

To further verify the phase evolution and valence-state variation during the sodiation/desodiation process, ex situ XPS measurements were conducted at representative electrochemical states. For the pristine electrode, the Bi 4f spectrum shows peaks corresponding to Bi^{3+} in Bi_2Te_3 , along with higher-binding-energy components from surface-oxidized species (Figure 4g). Upon discharge to 0.8 V, all Bi 4f peaks shift to lower binding energies, indicating partial reduction to metallic Bi and the onset of the conversion reaction. Further sodiation to 0.01 V induces a more pronounced shift, consistent with formation of Na-Bi alloy species, confirming the progression from conversion to alloying [44]. During charging, the alloy-related peaks gradually decrease, while the Bi^{3+} and oxidized peaks recover. At 3.0 V, the Bi 4f spectrum nearly returns to its original state, evidencing the reversible regeneration of the Bi_2Te_3 framework. A similar evolution is observed in the Te 3d spectra (Figure 4h). The pristine electrode displays the characteristic Te $3d_{5/2}$ and Te $3d_{3/2}$ peaks of Bi_2Te_3 . Upon sodiation, new components associated with Na_2Te emerge, accompanied by a decrease in the intensity of the original Te signals, demonstrating the conversion of Te species into sodium tellurides. At the fully discharged state, the Na_2Te -related peaks become dominant, corroborating the formation of Na_2Te identified by operando XRD and HRTEM. Upon subsequent charging, the Na_2Te signals gradually diminish, while the Te peaks characteristic of Bi_2Te_3 reappear, evidencing the reversible reconstruction of the telluride framework. Based on the above analyses results, the sodium-storage mechanism of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode can be summarized as a coupled insertion-conversion-alloying process (Figure 4i) [16, 33]. During this process, Na^+ is initially inserted into the Bi_2Te_3 lattice to form an intermediate NaBiTe_2 phase, which subsequently undergoes a conversion reaction to generate Bi and Na_2Te . The resulting Bi species further react with Na^+ through a stepwise alloying process to form NaBi and ultimately Na_3Bi . Upon desodiation, the reverse dealloying and conversion reactions occur, leading to the regeneration of the Bi_2Te_3 framework.

To gain deeper insight into the superior Na^+ storage kinetics of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode, cyclic voltammetry (CV), galvanostatic intermittent titration technique (GITT), and electrochemical impedance spectroscopy (EIS) analyses were systematically performed. As shown in Figure 5a, the CV curves of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ retain nearly identical shapes with increasing scan rates from 0.2 to 1.2 mV s^{-1} , indicating good reversibility and limited polarization during the sodiation/desodiation processes. The charge-storage kinetics were further investigated to elucidate the Na^+

storage mechanism (Figure 5b). The calculated b values for the four representative redox peaks of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ range from 0.717 to 0.859, which are significantly higher than those of pure Be_2Te_3 (0.413-0.611, Figure S9a, b). These results suggest that Na^+ storage in $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ is predominantly governed by surface-controlled pseudocapacitive processes, whereas the pure Be_2Te_3 electrode is more diffusion-limited [45]. To quantitatively distinguish the capacitive and diffusion-controlled contributions, the current response was analyzed according to Figure 5d. The capacitive-controlled contribution of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ reaches 81.6% at 1.0 mV s^{-1}

s^{-1} and continuously increases from 67.4% to 84.3% with increasing scan rate from 0.2 to 1.2 mV s^{-1} (Figure 5c). In comparison, the pure Be_2Te_3 electrode exhibits a considerably lower capacitive contribution of only 61.8% at 1.0 mV s^{-1} (Figure S9c), together with lower capacitive fractions over the entire scan-rate range. The significantly enhanced pseudocapacitive behavior indicates that Te-defect engineering coupled with the highly conductive MXene network facilitates rapid charge transfer and surface-induced Na^+ storage, thereby contributing to the superior rate capability.

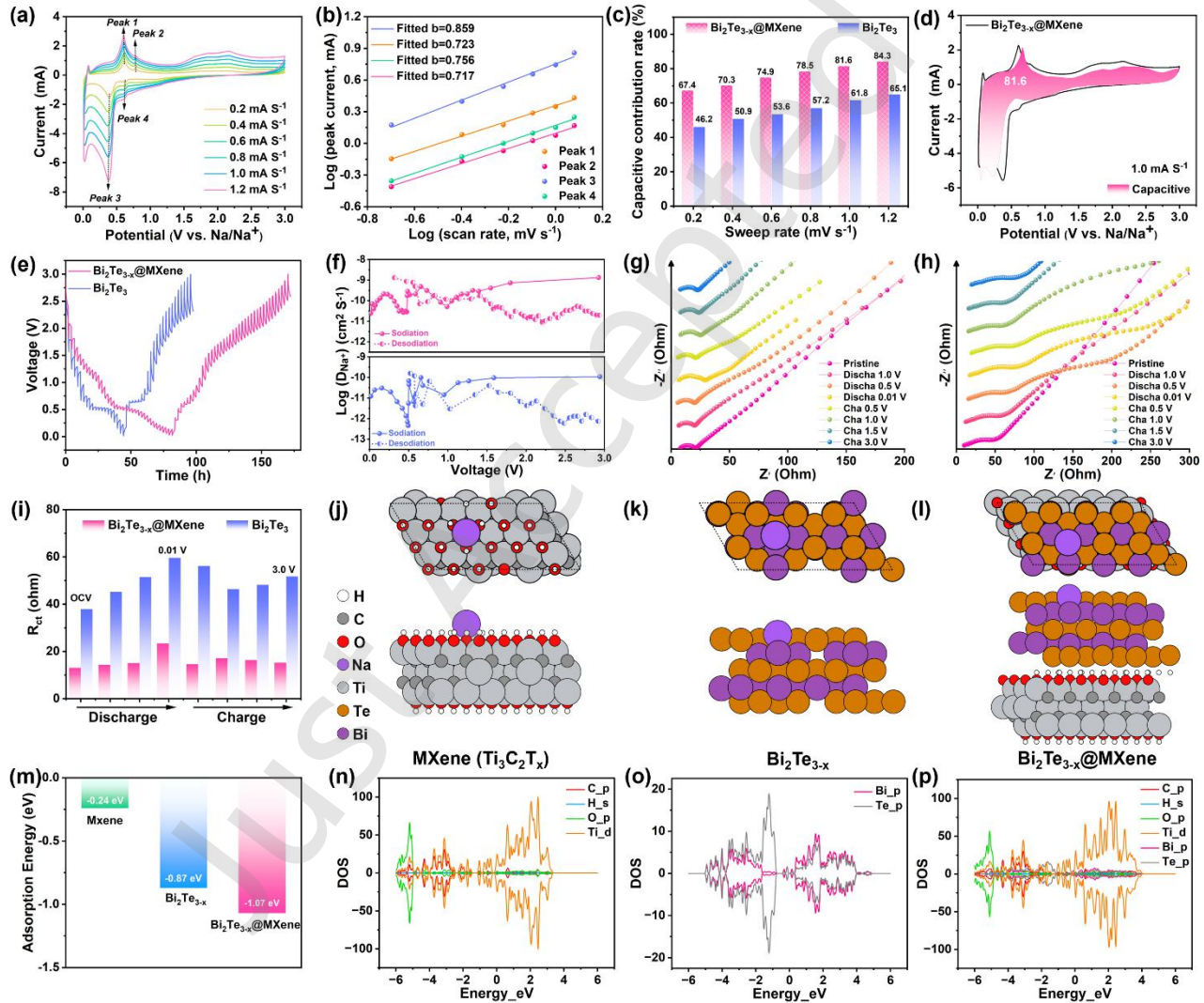


Figure 5. Kinetic analysis. (a) CV curves at various scan rates from 0.2 to 2.0 mV s^{-1} and (b) corresponding $\log(i)$ - $\log(v)$ plots for $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrodes. (c) Calculated capacitive contribution ratios of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Be_2Te_3 at different sweep rate. (d) Capacitive contribution of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode at 1.0 mV s^{-1} . (e, f) GITT profiles and corresponding Na^+ diffusion coefficients of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Be_2Te_3 after 50 cycles at 0.2 A g^{-1} . (g, h) Ex situ EIS spectra of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Be_2Te_3 collected during the initial discharge and charge processes, respectively. (i) Evolution of the fitted R_{ct} values of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Be_2Te_3 during the initial discharge/charge process. (j-l) Structure diagram of Na adsorption on MXene, $\text{Be}_2\text{Te}_{3-x}$, and $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$. (m) The corresponding Na adsorption energies. (n-p) DOS of MXene, $\text{Be}_2\text{Te}_{3-x}$, and $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$.

The Na^+ diffusion kinetics were further investigated by GITT measurements (Figure 5e and S10). Compared with pure Be_2Te_3 , the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode exhibits markedly smaller voltage polarization during both sodiation and desodiation processes, indicative of reduced reaction barriers and faster electrochemical kinetics. The corresponding Na^+ diffusion coefficients (D_{Na^+}) calculated from GITT profiles are shown in Figure 5f. Throughout the entire sodiation/desodiation process, $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ maintains consistently higher D_{Na^+} values, typically in the range of 10^{-11} to $10^{-9} \text{ cm}^2 \text{ s}^{-1}$, whereas the pure Be_2Te_3 electrode shows lower diffusion coefficients accompanied by pronounced fluctuations. The accelerated Na^+ transport kinetics are attributed to the shortened ion diffusion pathways and abundant active sites introduced by Te vacancies, together with the efficient electron-conduction channels provided by the MXene framework [46]. To gain further insight into the interfacial charge-transfer behavior, EIS measurements were performed at different states of charge and discharge (Figure 5g, h). Both electrodes exhibit typical Nyquist plots consisting of a depressed semicircle in the high-frequency region and an inclined line in the low-frequency region, corresponding to the charge-transfer process and Na^+ diffusion behavior, respectively. Notably, the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ electrode displays consistently smaller semicircle diameters and lower Warburg factors (σ) than pure Be_2Te_3 throughout the entire electrochemical process (Figure S11), indicating facilitated charge-transfer kinetics and accelerated solid-state Na^+ diffusion. More importantly, the fitted charge-transfer resistance (R_{ct}) of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ remains relatively stable with negligible fluctuation upon cycling, suggesting the formation of a robust and dynamically stable electrode/electrolyte interface that effectively suppresses interfacial polarization and sustains rapid charge transport. In contrast, the larger and more variable impedance response of pure Be_2Te_3 reflects sluggish reaction kinetics and inferior interfacial stability. The corresponding DRT curves and contour plots are presented in Figure S12. As shown in Figure S12a,b, three characteristic relaxation processes, denoted as τ_1 , τ_2 , and τ_3 , can be distinguished based on their characteristic relaxation-time regions. The τ_1 process, located in the long-relaxation-time region, is associated with the ion-diffusion impedance in the low-frequency regime, reflecting the relatively slow diffusion of Na^+ into the bulk electrode. The τ_2 process in the intermediate-relaxation-time region is mainly related to interfacial film/SEI processes and Na^+ transport across the interfacial layer, whereas the τ_3 process at shorter relaxation times is associated with rapid interfacial charge-transfer and surface-related ion-transport processes. Notably, compared with pure Bi_2Te_3 , $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ exhibits substantially weaker τ_1 and τ_2 responses and smaller variations in DRT intensity during charge/discharge (Figure S12a,c), indicating more favorable and stable ion-transport and interfacial kinetics.

In contrast, pure Bi_2Te_3 shows pronounced evolution of the τ_1 and τ_2 processes (Figure S12b,d), suggesting stronger interfacial polarization and progressive kinetic deterioration. These results further demonstrate that the introduction of MXene and defect engineering effectively regulates the electrode/electrolyte interface and facilitates Na^+ transport during cycling. Moreover, even after prolonged cycling, $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ retains a substantially lower R_{ct} than pristine Bi_2Te_3 (Figure S13), further confirming its superior interfacial stability and sustained charge-transfer capability. These results collectively demonstrate that the defect-engineered $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ heterostructure establishes a kinetically favorable ion/electron transport network and a stable interfacial environment, thereby enabling highly reversible and ultrafast sodium-storage reactions.

To further elucidate the respective roles of Te vacancies and MXene in enhancing the electrochemical performance of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$, density functional theory (DFT) calculations were performed. As shown in Figures S14 and 5j–l, the structural models and corresponding Na adsorption configurations of MXene, $\text{Be}_2\text{Te}_{3-x}$, and $\text{Be}_2\text{Te}_{3-x}\text{@MXene}$ were constructed. The calculated Na adsorption energies are -0.24, -0.87, and -1.07 eV for MXene, $\text{Be}_2\text{Te}_{3-x}$, and $\text{Be}_2\text{Te}_{3-x}\text{@MXene}$, respectively (Figure 5m). The stronger Na adsorption of $\text{Be}_2\text{Te}_{3-x}$ compared with MXene indicates that Te vacancies provide favorable active sites for Na^+ adsorption, which can facilitate Na^+ storage and stabilize the electrode during cycling. The further enhanced adsorption in $\text{Be}_2\text{Te}_{3-x}\text{@MXene}$ suggests a synergistic effect between the Te-vacancy-rich $\text{Be}_2\text{Te}_{3-x}$ and MXene substrate. Furthermore, the density of states (DOS) was analyzed to clarify the electronic effects of MXene incorporation (Figures 5n–p). MXene exhibits a pronounced metallic character, with abundant Ti 3d states near the Fermi level, whereas $\text{Be}_2\text{Te}_{3-x}$ shows a relatively lower density of states around the Fermi level, mainly contributed by Bi and Te orbitals. After forming the $\text{Be}_2\text{Te}_{3-x}\text{@MXene}$ heterostructure, the Ti 3d, Bi, and Te states show evident overlap and redistribution near the Fermi level, indicating strong interfacial orbital hybridization and electronic coupling accompanied by charge redistribution. Meanwhile, the composite maintains a high DOS near the Fermi level, suggesting enhanced electronic conductivity. Overall, the DFT results demonstrate that Te vacancies facilitate Na^+ adsorption, whereas MXene enhances interfacial electronic coupling and electron transport, together accounting for the improved electrochemical performance of $\text{Be}_2\text{Te}_{3-x}\text{@MXene}$.

Encouraged by the outstanding Na^+ storage performance of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ anode in half cells, sodium-ion full cells were further assembled using $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ (NVP) as the cathode to evaluate the practical feasibility of the proposed electrode system. Prior to full-cell assembly, the morphology, crystal structure, and electrochemical properties of the NVP cathode were

systematically investigated. As shown in Figure S15a, the as-prepared NVP consists of densely packed nanoparticles assembled from numerous nanosized primary grains, forming a rough and porous surface that is beneficial for electrolyte penetration and rapid Na^+ transport. The XRD pattern can be well indexed to the rhombohedral NASICON-type $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ phase without detectable impurities (Figure S15b), indicating the successful formation of highly crystalline NVP [22, 47, 48]. The Na-storage properties of the NVP cathode were first evaluated in half cells (Figure S16). Typical charge/discharge profiles exhibit characteristic voltage plateaus associated with the reversible $\text{V}^{3+}/\text{V}^{4+}$ redox reaction, demonstrating highly reversible Na^+ insertion/extraction processes. Benefiting from the intrinsically open three-dimensional NASICON framework, the NVP cathode delivers excellent rate capability, retaining considerable capacities even at high current densities up to 6.4 A g^{-1} , and rapidly recovering its initial capacity when the current density is switched back to 0.1 A g^{-1} (Figure S16a, b). Moreover, the NVP electrode exhibits remarkable long-term cyclability over 1000 cycles with nearly unchanged Coulombic efficiency at 1 A g^{-1} (Figure S16c), highlighting its robust structural stability and highly reversible electrochemical reaction. Therefore, considering the capacity matching between the cathode and anode, the active mass ratio of NVP to $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ was optimized to approximately 5:1 for the subsequent

full-cell assembly.

The corresponding Na^+ storage mechanism of the NVP// $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ full cell during the discharge process is schematically illustrated in Figure 6a. Benefiting from the favorable voltage matching between the high-voltage NVP cathode and the low-potential $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ anode, the assembled full cell exhibits a broad operating voltage window with average charge and discharge voltages close to 2.8 V, as evidenced by the voltage profiles of the individual electrodes and the full cell plotted against normalized capacity (Figure 6b). Such a large voltage output is advantageous for maximizing the energy density of the full-cell system. Figure 6c displays the cycling performance of the NVP// $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ full cell at 0.1 A g^{-1} . Based on the total mass of both electrodes, the full cell delivers an initial reversible capacity of approximately 85 mAh g^{-1} and maintains a highly stable capacity upon prolonged cycling, accompanied by nearly 100% Coulombic efficiency. The excellent reversibility demonstrates the high compatibility between the NVP cathode and $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ anode as well as the robust electrode/electrolyte interfaces inherited from both electrodes. More importantly, a single coin-type full cell is capable of powering a commercial LED display (inset of Figure 6c), directly demonstrating its feasibility for practical energy-storage applications.

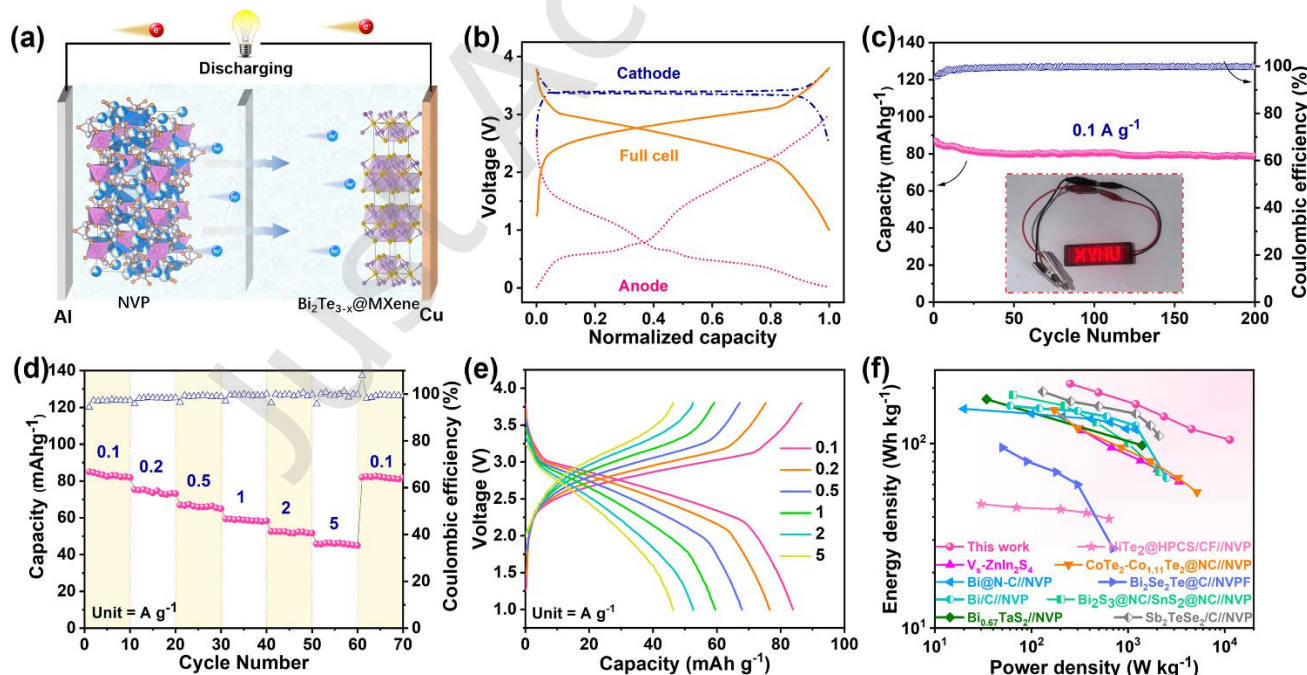


Figure 6. Sodium-ion full-cell performance. (a) Schematic illustration of the NVP// $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ full cel. (b) Charge and discharge curves, (c) cycling performance at 0.1 A g^{-1} , (d) rate capability, and (e) charge/discharge voltage profiles at different current densities. (f) Ragone plots of the NVP// $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ full cell in comparison with previously reported sodium-ion full cells. Inset in (c): photographs of LED lights with different colors powered by the full cell.

The rate capability of the NVP// $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ full cell

was further investigated (Figure 6d). As the current density increased from 0.1 to 5 A g⁻¹, the device delivered reversible capacities of 83.8, 76.6, 67.9, 59.5, 52.6, and 46.2 mAh g⁻¹, respectively, demonstrating favorable rate capability. Notably, when the current density was restored to 0.1 A g⁻¹, the reversible capacity rapidly recovered to 83.1 mAh g⁻¹, evidencing highly reversible electrochemical processes and robust structural stability under high-rate operation. Meanwhile, the charge/discharge curves at various current densities exhibit well-preserved voltage plateaus and only slight polarization even under high-current conditions (Figure 6e and S17), confirming the rapid reaction kinetics and efficient Na⁺ transport within the full-cell configuration. Such superior rate performance can be attributed to the synergistic combination of the fast Na⁺ diffusion and dominant pseudocapacitive behavior of the defect-engineered Bi₂Te_{3-x}@MXene anode together with the intrinsically open NASICON framework of the NVP cathode. In addition, the NVP//Bi₂Te_{3-x}@MXene full cell delivered an initial capacity of 44 mAh g⁻¹ at 5.0 A g⁻¹ and retained 36 mAh g⁻¹ after 200 cycles, corresponding to 82% capacity retention (Figure S18). In contrast, the NVP//Bi₂Te₃ full cell exhibited severe capacity decay under the same conditions, retaining only ~3–4 mAh g⁻¹ after 200 cycles. Furthermore, the Ragone plot in Figure 6f reveals that the NVP//Bi₂Te_{3-x}@MXene full cell delivers a high energy density while simultaneously maintaining excellent power capability. It can deliver a maximum energy density of 210.6 Wh kg⁻¹ at a power density of 251 W Kg⁻¹. Even at ultrahigh power densities of 11300 W Kg⁻¹, the device still retains considerable energy output of 104.7 Wh Kg⁻¹, outperforming many previously reported sodium-ion full-cell systems [49–57]. These results demonstrate that the NVP//Bi₂Te_{3-x}@MXene full cell successfully translates the superior half-cell kinetics into practical device-level performance, offering great promise for high-energy and high-power SIBs in the future.

3 Conclusion

In summary, we have successfully fabricated Te-vacancy-rich Bi₂Te_{3-x}@MXene with strong interface bonding as the fast-charging anode for SIBs. The uniformly distributed Bi₂Te_{3-x} nanoparticles are chemically anchored on conductive MXene nanosheets through strong Ti–Te interfacial interactions, forming an integrated conductive framework that facilitates rapid electron/Na⁺ transport, accommodates volume fluctuations, and suppresses active-species aggregation during prolonged cycling. Meanwhile, Te-vacancy engineering modulates the electronic structure, creates abundant Na⁺-accessible active sites, and accelerates charge-transfer kinetics. Combined in situ XRD and ex situ XPS/HRTEM analyses reveal a highly reversible insertion-conversion-alloying sodium-storage mechanism with stabilized phase evolution. Benefiting from this synergistic defect-interface-structure engineering, the Bi₂Te_{3-x}@MXene anode exhibits a high reversible capacity

of 383.2 mAh g⁻¹ after 200 cycles at 0.2 A g⁻¹, excellent rate capability of 317.9 mAh g⁻¹ at 10 A g⁻¹, and remarkable long-term cycling stability with 324.8 mAh g⁻¹ retained after 2000 cycles at 2 A g⁻¹. More importantly, when paired with a Na₃V₂(PO₄)₃ cathode, the assembled full cell achieves a high energy density of 210.6 Wh kg⁻¹ and retains 104.7 Wh kg⁻¹ at an ultrahigh power density of 11.3 kW kg⁻¹, demonstrating excellent energy-power characteristics and practical feasibility. This work highlights a powerful strategy based on vacancy engineering and MXene-coupled interfacial stabilization for developing advanced metal chalcogenide anodes toward high-energy and high-power SIBs.

Acknowledgements

This work was financially supported by the Key Science and Technology Program of Henan Province (262102240074), National Natural Science Foundation of China (22409171, 22579166), Support Program for Innovative Talents in Higher Education Institutions of Henan Province (26HASTIT039), the Postdoctoral Fellowship Program of CPSF (No. 2025M771107), Natural Science Foundation of Fujian Province (2025J09055), the Self-deployment Project Research Program of Haixi Institutes, Chinese Academy of Sciences (CXZX-2023-JQ08).

Declaration of conflicting interests

The authors declare no conflicting interests regarding the content of this article.

Data availability

All data needed to support the conclusions in the paper are presented in the manuscript and/or the Supplementary Materials. Additional data related to this paper may be requested from the corresponding author upon request.

Electronic Supplementary Material: Supplementary material (e.g., experimental details, characterizations including SEM, TEM images, XRD spectra, as well as corresponding electrochemical tests for the prepared samples, etc.) is available in the online version of this article at <https://doi.org/10.26599/NRE.2026.9120289>.

References

- [1] Zhao, C.; Wang, Q.; Yao, Z.; Wang, J.; Sanchez-Lengeling, B.; Ding, F.; Qi, X.; Lu, Y.; Bai, X.; Li, B.; Li, H.; Aspuru-Guzik, A.; Huang, X.; Delmas, C.; Wagemaker, M.; Chen, L.; Hu, Y. S. Rational design of layered oxide materials for sodium-ion batteries. *Science* **2020**, *370*, 708–711.
- [2] Wang, Q.; Zhou, D.; Zhao, C.; Wang, J.; Guo, H.; Wang, L.; Yao, Z.; Wong, D.; Schuck, G.; Bai, X.; Lu, J.; Wagemaker, M. Fast-charge high-voltage layered cathodes for sodium-ion batteries. *Nat. Sustain.* **2024**, *7*, 338–347.
- [3] Yabuuchi, N.; Kubota, K.; Dahbi, M.; Komaba, S. Research development on sodium-ion batteries. *Chem. Rev.* **2014**, *114*, 11636–11682.
- [4] Hwang, J. Y.; Myung, S. T.; Sun, Y. K. Sodium-ion batteries: present and future. *Chem. Soc. Rev.* **2017**, *46*, 3529–3614.
- [5] Yuan, J.; Pan, D.; Chen, J.; Liu, Y.; Yu, J.; Hu, X.; Zhan, H.; Wen, Z.

- Ultrafast Na-Ion Storage in Amorphization Engineered Hollow Vanadium Oxide/MXene Nanohybrids for High-Performance Sodium-Ion Hybrid Capacitors. *Adv. Mater.* **2024**, *36*, e2408923.
- [6] Wu, C.; Huang, W.; Zhang, Y.; Chen, Q.; Li, L.; Zhang, Y.; Wu, X.; Chou, S.-L. Revisiting the critical role of metallic ash elements in the development of hard carbon for advancing sodium-ion battery applications. *eScience* **2025**, *5*, 100371.
- [7] Ding, X.; Yuan, W.; Lin, J.; Li, H.; Yang, X.; Liu, L.; Xiao, Y.; Chen, F.; Han, L. In-situ surface coating and subsurface gradient doping contrives $P_2\text{-Na}_{0.67}\text{Ni}_{0.33}\text{Mn}_{0.67}\text{O}_2$ single crystal with highly stable interface and structure. *Nano Research Energy* **2025**, *4*, e9120203.
- [8] Zhao, W.; Ma, X.; Gao, L.; Wang, X.; Luo, Y.; Wang, Y.; Li, T.; Ying, B.; Zheng, D.; Sun, S.; Liu, Q.; Zheng, Y.; Sun, X.; Feng, W. Hierarchical Architecture Engineering of Branch-Leaf-Shaped Cobalt Phosphosulfide Quantum Dots: Enabling Multi-Dimensional Ion-Transport Channels for High-Efficiency Sodium Storage. *Adv. Mater.* **2024**, *36*, e2305190.
- [9] Li, S.; Zhang, J.; Li, Y.; Fan, P.; Wu, M. Revisiting N, S co-doped carbon materials with boosted electrochemical performance in sodium-ion capacitors: The manipulation of internal electric field. *Nano Research Energy* **2024**, *3*, e9120098.
- [10] Liu, Y.; Guo, Y.; Zhang, Y.; Xu, L.; Chen, J.; Hu, X.; Wen, Z. Orchestrating Penta-Element Interplay in Gradient-Porous Carbons for Advanced Sodium-Ion Hybrid Capacitors. *Angew. Chem., Int. Ed.* **2025**, *64*, e202505469.
- [11] Liu, Q.; Li, Y.; Su, Y.; Fan, Y.; Hu, F.; Li, C.; Tian, L.; Luo, Y.; Cao, B.; Xu, L.; Meng, Q.; Dong, P. Challenges and strategic approaches to constructing the full life cycle value chain of layered cathode materials for sodium-ion batteries. *Nano Research Energy* **2026**, *5*, e9120177.
- [12] Zhong, Y.; Zheng, H.; Guo, Z.; Gao, J.; Ma, X.; Sun, X.; Zhao, W. Synergistic selenium substitution and interfacial confinement in indium-based chalcogenide anodes enabling rapid and stable sodium storage. *Nano Research Energy* **2026**, *5*, e9120244.
- [13] Pan, J.; Sun, Z.; Wu, X.; Liu, T.; Xing, Y.; Chen, J.; Xue, Z.; Tang, D.; Dong, X.; Zhang, H.; Liu, H.; Wei, Q.; Peng, D. L.; Amine, K.; Zhang, Q. Mechanically Robust Bismuth-Embedded Carbon Microspheres for Ultrafast Charging and Ultrastable Sodium-Ion Batteries. *J. Am. Chem. Soc.* **2025**, *147*, 3047-3061.
- [14] Long, H.; Wang, J.; Zhao, S.; Zou, B.; Yan, L.; Huang, Q.; Zhao, Y. Enable the Domino-Like Structural Recovering in Bismuth Anode to Achieve Fast and Durable Na/K Storages. *Angew. Chem., Int. Ed.* **2024**, *63*, e202406513.
- [15] Fang, Z.; Fan, S.; Yan, Z.; Tang, D.; Gao, X.; Huang, X.; Zheng, H.; Wang, B.; Jiang, Q.; Han, J.; Lin, J.; Xie, Q.; Peng, D. L.; Wei, Q. Root-Growth-Inspired Self-Morphology-Evolution of Microsized Bismuth Surrounded by Microsized Hard Carbon for Stabilized Sodium-Ion Storage. *Adv. Mater.* **2025**, *37*, e2412636.
- [16] Cui, J.; Zheng, H.; Zhang, Z.; Hwang, S.; Yang, X.-Q.; He, K. Origin of anomalous high-rate Na-ion electrochemistry in layered bismuth telluride anodes. *Matter* **2021**, *4*, 1335-1351.
- [17] Ko, J. K.; Jo, J. H.; Kim, H. J.; Park, J. S.; Yashiro, H.; Voronina, N.; Myung, S.-T. Bismuth telluride anode boosting highly reversible electrochemical activity for potassium storage. *Energy Storage Mater.* **2021**, *43*, 411-421.
- [18] Cheng, Z. Y.; Cui, F. H.; Yao, Y. W.; Ke, Y. C.; Cao, D. X.; Yan, J.; Zhu, C. Y.; Zhu, K. Design of Soft/Hard Interfaces with Stress Variation for Improved Sodium Ion Storage. *Adv. Funct. Mater.* **2025**, *35*, 2424000.
- [19] Zhao, M. Q.; Xie, X.; Ren, C. E.; Makaryan, T.; Anasori, B.; Wang, G.; Gogotsi, Y. Hollow MXene Spheres and 3D Macroporous MXene Frameworks for Na-Ion Storage. *Adv. Mater.* **2017**, *29*, 1702410.
- [20] Ghidui, M.; Lukatskaya, M. R.; Zhao, M. Q.; Gogotsi, Y.; Barsoum, M. W. Growth of two-dimensional titanium carbide 'clay' with high volumetric capacitance. *Nature* **2014**, *516*, 78-81.
- [21] Ge, W. Preparation of MXene Modified by Vanadium Ion and Their Application in Lithium-Sulfur Batteries. *Journal of Xinyang Normal University (Natural Science Edition)*, **2024**, *37*, 147-153.
- [22] Zhang, J.; Yu, Z.; Tian, L.; Zhu, Y.; Wang, M.; Gao, P.; Zhang, Y.; Zhang, N.; Wang, D.; Shen, Y.; Wang, M. Orbital modulation to restrain anti-site defects in NASICON cathode for high-performance sodium-ion batteries. *Mater. Futures* **2026**, *5*, 025104.
- [23] Chen, H.; Wang, Y.-Q.; Zhang, D.-T.; Zhao, B.; Li, M.-P.; Li, C.-Y.; Xu, T.-P.; Liu, M.-C. Enhanced rate capability and cycle stability of Ti₂C MXene for sodium storage through an aniline molecules welding strategy. *Tungsten* **2024**, *7*, 161-171.
- [24] Xu, X.; Feng, D.; You, L.; Xie, Y.; Wu, F.; Zhu, Y.; Mei, Y.; Xie, D. Carbon-Encrusted SnS₂ Decorated on MXene Nanosheets for Advanced Li-Ion Battery Anodes. *Energy Material Advances* **2024**, *5*, 0146.
- [25] Hu, X.; Ma, P.; Sun, Z.; Zhang, Z.; Sun, J.; Li, H.; Yang, H. Y. Ultrafast Na⁺ Diffusion Enabled by Defective 3D In₂S₃/MXene Nanostructure toward High - Rate Sodium Ion Batteries. *Adv. Energy Mater.* **2025**, *15*, 2500443.
- [26] Cheng, Y.; Xu, L.; Zhang, D.; Yang, J.; Chen, Y.; Yuan, Y.; Guo, S. Bismuth telluride nanoparticles@hollow carbon sphere encapsulated in one-dimensional carbon fibers for durable fast sodium-ion storage. *Journal of Power Sources* **2025**, *645*, 237248.
- [27] Wang, G.; Li, Q.; Zhang, W.; Wu, J.; Fan, W.; Wang, L.; Liang, Z.; Huang, Z.; Lin, Z.; Wang, G.; Wang, J.; Huang, S. Unveiling the Synergy of Architecture and Anion Vacancy on Bi₂Te_{3-x}@NPCNFs for Fast and Stable Potassium Ion Storage. *ACS Appl. Mater. Interfaces* **2024**, *16*, 13858-13868.
- [28] Wang, J.; Wang, M.; Yang, H.; Wang, Z.; Wang, Y.; Liu, G.; Yong, Y.; Liu, B.; Zhou, X.; He, H.; Wang, H.; Yin, Z. Chalcogen-Directed Dual-Heterointerfaced Bi(2)Te(3)/BiS(x) in N-Doped Carbon Nanofibers for Sodium Storage. *Small* **2026**, *22*, e73235.
- [29] Zong, J.; Liang, Y.; Liu, F.; Zhang, M.; Song, K.; Feng, J.; Xi, B.; Xiong, S. Engineering twin structures and substitutional dopants in ZnSe_{0.7}Te_{0.3} anode material for enhanced sodium storage performance. *Nat. Commun.* **2025**, *16*, 4406.
- [30] Xu, X.; Zhang, Y.; Sun, H.; Zhou, J.; Liu, Z.; Qiu, Z.; Wang, D.; Yang, C.; Zeng, Q.; Peng, Z.; Guo, S. Orthorhombic Cobalt Ditelluride with Te Vacancy Defects Anchoring on Elastic MXene Enables Efficient Potassium-Ion Storage. *Adv. Mater.* **2021**, *33*, e2100272.
- [31] Ma, G.; Luo, Z.; Shao, H.; Shen, Y.; Lin, Z.; Simon, P. Tellurium-Terminated MXene Synthesis via One-Step Tellurium Etching. *Nano-Micro Lett.* **2025**, *18*, 28.
- [32] Ma, H.; Li, J.; Yang, J.; Wang, N.; Liu, Z.; Wang, T.; Su, D.; Wang, C.; Wang, G. Bismuth Nanoparticles Anchored on Ti₃C₂T_x MXene Nanosheets for High - Performance Sodium - Ion Batteries. *Chem. Asian J.* **2021**, *16*, 3774-3780.
- [33] Liu, X.; Si, Y.; Li, K.; Xu, Y.; Zhao, Z.; Li, C.; Fu, Y.; Li, D. Exploring sodium storage mechanism of topological insulator Bi₂Te₃ nanosheets encapsulated in conductive polymer. *Energy Storage Mater.* **2021**, *41*, 255-263.
- [34] Lee, S. Y.; Kang, S. W.; Yu, H. J.; Lim, H.-K.; Park, Y. I.; Lee, J. E. Nano-Sized Bi₂Te₃@Reduced graphene oxide for enhanced sodium-ion storage: Insight into the electrochemical mechanism through in situ analysis. *Chem. Eng. J.* **2024**, *491*, 151784.
- [35] Chong, S.; Qiao, S.; Wang, Z.; Chen, B.; Yuan, B.; Huang, W.; Cao, G. Tuning the electrochemical kinetics of bismuth-based conversion-alloying anodes with anion modulation for sodium-ion storage. *Nano Energy* **2024**, *130*, 110097.
- [36] Abzal, S. M.; Janga, S. L.; Bhaskara Rao, Y.; Khatua, S.; Kalyan, K.; Maiti, P.; Patel, R.; Patro, L. N.; Dash, J. K. Solvothermally synthesized bismuth telluride hexagonal platelets as an efficient anode material for lithium- and sodium-ion batteries. *J. Mater. Sci.* **2024**, *59*, 6879-6893.
- [37] Sun, D.; Zhang, G.; Li, D.; Liu, S.; Jia, X.; Zhou, J. A layered Bi₂Te₃ nanoplates/graphene composite with high gravimetric and volumetric performance for Na-ion storage. *Sustain. Energy Fuels* **2019**, *3*, 3163-3171.
- [38] Chong, S.; Yuan, L.; Qiao, S.; Ma, M.; Li, T.; Huang, X. L.; Zhou, Q.; Wang, Y.; Huang, W. Chemical bonding in multiple encapsulation geometry of Bi₂Se₃-based conversion-alloying anode materials for superior sodium-ion storage. *Sci. China Mater.* **2023**, *66*, 2641-2651.
- [39] He, B.; Cunha, J.; Hou, Z.; Li, G.; Yin, H. 3D hierarchical self-supporting Bi₂Se₃-based anode for high-performance lithium/sodium-ion batteries. *J. Colloid Interface Sci.* **2023**, *650*, 857-864.
- [40] Liang, M.; Ma, L.; Chen, B.; Liu, E.; Shi, C.; He, C.; Zhao, N. Two

Birds with One Stone: A NaCl-Assisted Strategy toward MoTe₂ Nanosheets Nanoconfined in 3D Porous Carbon Network for Sodium-Ion Battery Anode. *Energy Storage Mater.* **2022**, *47*, 591-601.

[41] Jiang, Y.; Wu, F.; Ye, Z.; Zhou, Y.; Chen, Y.; Zhang, Y.; Lv, Z.; Li, L.; Xie, M.; Chen, R. Confining CoTe₂-ZnTe heterostructures on petal-like nitrogen-doped carbon for fast and robust sodium storage. *Chem. Eng. J.* **2023**, *451*, 138430.

[42] Jiang, Y.; Wu, F.; Ye, Z.; Zhou, Y.; Chen, Y.; Zhang, Y.; Lv, Z.; Li, L.; Xie, M.; Chen, R. Superimposed effect of hollow carbon polyhedron and interconnected graphene network to achieve CoTe₂ anode for fast and ultralong sodium storage. *J. Power Sources* **2023**, *554*, 232174.

[43] Liang, Z.; Huang, J.; Zhang, W.; Chu, H.; Li, Q.; Lu, H.; Lin, Z.; Wang, J.; Lin, H.; Chen, Y.; Xiong, S.; Huang, S. Uncovering and preventing polytellurides dissolution enables stable sodium-ion storage: A case study of SnTe. *Chem. Eng. J.* **2024**, *498*, 154873.

[44] Zou, Z.; Yu, Z.; Chen, C.; Wang, Q.; Zhu, K.; Ye, K.; Wang, G.; Cao, D.; Yan, J. High-Performance Alkali Metal Ion Storage in Bi₂Se₃ Enabled by Suppression of Polyselenide Shuttling Through Intrinsic Sb-Substitution Engineering. *ACS Nano* **2023**, *17*, 13769-13783.

[45] Wang, J.; Zhao, P.; Yang, Q.; Yang, C.; Zhang, Y.; Lu, P.; Jiang, N.; Hao, Y.; Shang, Z.; Ren, Z.; Hou, Y.; Huang, P.; Lu, X.; Huang, Z.; Qiu, J. Confined interfacial microenvironment design of hard carbon anodes for wide-temperature sodium-ion batteries. *Nano Research Energy* **2026**, *5*, e9120235.

[46] Duan, Z.; Zhou, W.; Mo, Y.; Tang, R.; Duan, Y.; Hu, A.; Liu, J. Tuning hard carbon pore structure via water vapor activation for enhanced sodium-ion storage. *Green Energy Environ.* **2026**, *11*, 1096-1107.

[47] Fan, D.; Shen, Q.; Li, H.; Qu, X.; Jiao, L.; Liu, Y. Redox Couple Modulation in NASICON Phosphates toward High-Performance Cathodes for Na-Ion Batteries. *Energy Material Advances* **2024**, *5*, 0073.

[48] Hu, J.; Li, X.; Liang, Q.; Xu, L.; Ding, C.; Liu, Y.; Gao, Y. Optimization Strategies of Na₃V₂(PO₄)₃ Cathode Materials for Sodium-Ion Batteries. *Nano-Micro Lett.* **2024**, *17*, 33.

[49] Wang, C.; Yuan, Y.; Yan, W.; Shen, S.; Zhu, M.; Cai, G.; Wang, B. Nickel telluride nanoparticles@hollow porous carbon sphere confined

within carbon fibers for fast stable sodium storage. *J. Colloid Interface Sci.* **2025**, *686*, 151-162.

[50] Wang, Y.; Zhang, H. H.; Wen, Z.; Sun, C. N.; Wang, G. Y.; Wang, M. S.; Yang, C. C.; Jiang, Q. ZnIn₂S₄ with a hybrid reaction mechanism and sulfur vacancies for sustainable sodium storage. *Carbon Energy* **2025**, *7*, e654.

[51] Chen, W.; Wang, Z.; Huang, Z.; Xie, W.; Zhao, J.; Xiao, Y.; Lei, S.; Huang, B.; Cheng, B. Mixed-dimensional van der Waals heterostructure of Bi₂S₃ nanorods and SnS₂ nanosheets bridged with N-doped carbon interlayer for enhanced sodium-ion batteries. *Energy Storage Mater.* **2024**, *73*, 103880.

[52] Hao, Y.; Xu, H.; Lv, Z.; Tu, X.; Xu, W.; Dong, W.; Qin, P.; Huang, F. Lattice-confined localized alloying of Bi_{0.67}TaS₂ anode enabling ultrafast and stable sodium storage up to 150 °C. *Chem. Eng. J.* **2024**, *496*, 153876.

[53] Hu, L.; Liu, C.; Zhang, F.; Wang, H.; Wang, B. Vacancy-Defect Ternary Topological Insulators Bi₂Se₂Te Encapsulated in Mesoporous Carbon Spheres for High Performance Sodium Ion Batteries and Hybrid Capacitors. *Small* **2024**, *20*, e2311079.

[54] Yuan, H.; Ma, F.; Wei, X.; Lan, J. L.; Liu, Y.; Yu, Y.; Yang, X.; Park, H. S. Ionic-Conducting and Robust Multilayered Solid Electrolyte Interphases for Greatly Improved Rate and Cycling Capabilities of Sodium Ion Full Cells. *Adv. Energy Mater.* **2020**, *10*, 2001418.

[55] Xue, P.; Wang, N.; Fang, Z.; Lu, Z.; Xu, X.; Wang, L.; Du, Y.; Ren, X.; Bai, Z.; Dou, S.; Yu, G. Rayleigh-Instability-Induced Bismuth Nanorod@Nitrogen-Doped Carbon Nanotubes as A Long Cycling and High Rate Anode for Sodium-Ion Batteries. *Nano Lett.* **2019**, *19*, 1998-2004.

[56] Muhammad, M. A.; Li, J.; Abdel - aziz, A.; Liu, Y.; Haruna, B.; Yu, J.; Liang, P.; Wang, P.; Hu, X.; Wen, Z. Crystallochemical Tailoring of Ternary Sb₂TeSe₂ Anodes Enables Fast and Durable Sodium - Ion Storage. *Adv. Funct. Mater.* **2026**, *36*, e74887.

[57] Luo, J.; Bo, S.; Park, S.; Park, B. K.; Li, O. L. Spatial confinement and interfacial electron regulation in N-doped carbon-encapsulated CoTe₂/Co_{1.11}Te₂ heterostructure with enhanced kinetics for robust sodium-ion storage. *J. Colloid Interface Sci.* **2026**, *707*, 139640.



Qian Sun obtained her PhD degree in Chemistry from the University of New South Wales (UNSW) in 2023, under the supervision of Prof. Chuan Zhao. She then did postdoctoral research in Prof. Chuan Zhao's group, focusing on single atom catalysts for electroreduction of CO₂ and CO (2023–2024). After that, she joined Prof. David Sinton's group as a postdoctoral fellow at the University of Toronto in Canada. Her current research is production of multi-carbon species from CO₂ and CO electroreduction, and CO₂ capture.



Yu Zhang is an associate professor at Xinyang Normal University. She received her Ph. D. degree from Northwest University in 2016. After graduation, she joined Xinyang Normal University as a faculty member. Her primary research focuses on the design and synthesis of functional nanomaterials for energy storage and conversion, with particular emphasis on their applications in electrochemical energy.

Electronic Supplementary Material

Defect-Interface Synergistic Engineering of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ Anodes toward Fast-Charging and Durable Sodium Storage

Minghui Ma¹, Manyu Zhang², Chao Li², Mingyuan Wang¹, Jin'an Wang³, Xiang Hu⁴, Qian Sun⁵ (✉), and Yu Zhang² (✉)

1 School of Vehicle and Traffic Engineering, Zhengzhou University of Science and Technology, Zhengzhou, Henan, 450064, China

2 College of Chemistry and Chemical Engineering, Xinyang Normal University, Xinyang, Henan, 464000, China

3 National Polytechnic Institute of Mexico, Higher School of Chemical Engineering and Metallurgical Industry, Mexico City, 07736 Mexico

4 State Key Laboratory of Structural Chemistry, and Fujian Provincial Key Laboratory of Materials and Techniques toward Hydrogen Energy, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002 China

5 Department of Mechanical & Industrial Engineering, University of Toronto, Toronto, ON M5S 3G8, Canada

Supporting information to <https://doi.org/10.26599/NRE.2026.9120289>.

Address correspondence to Qian Sun, qian.sun@utoronto.ca; Yu Zhang, zhangyu@xynu.edu.cn

Experimental Procedures

Synthesis of MXene: Briefly, 20 mL of 9 M HCl solution was prepared, followed by the addition of 1 g LiF under continuous stirring for 20 min. Subsequently, 1 g of Ti_3AlC_2 (400 mesh) was slowly introduced into the above solution to avoid excessive reaction. The etching process was conducted at 40 °C under stirring (300 rpm) for 96 h. Afterward, the obtained suspension was repeatedly washed with deionized water until the supernatant became dark green. The resulting product was further sonicated in an ice-water bath for 2 h and centrifuged at 3500 rpm for 10 min. Finally, the collected supernatant was freeze-dried for 48 h to obtain few-layer $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanosheets.

Synthesis of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$: Few-layer MXene nanosheets (20 mg) were first dispersed in 20 mL deionized water via ultrasonication in an ice-water bath for 1 h to form a homogeneous suspension. Separately, 1 mmol of $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ and 100 mg Polyvinyl pyrrolidone (PVP) was dissolved in 10 mL of ethylene glycol under magnetic stirring. The obtained Bi^{3+} -containing solution was then slowly introduced into the MXene dispersion and continuously stirred at room temperature for 6 h to ensure sufficient adsorption of Bi^{3+} species on the MXene surface. The resulting precursor was collected by freeze-drying for 48 h. Subsequently, the as-prepared Bi^{3+} /MXene precursor was thoroughly mixed with Te powder at a mass ratio of 1:2 and transferred into a porcelain boat for thermal treatment. The tellurization process was carried out in a tube furnace at 500 °C for 1 h under a flowing 5% H_2 /Ar atmosphere with a heating rate of 5 °C min^{-1} , yielding the final product $\text{Bi}_2\text{Te}_{3-x}$ /MXene composite. For comparison, pure Bi_2Te_3 was synthesized under identical conditions in the absence of MXene nanosheets.

Synthesis of nanosized $\text{Na}_3\text{V}_2(\text{PO}_4)_3$: The nano $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ (NVP) was synthesized via a hydrothermal-assisted sol-gel route. Briefly, V_2O_5 (4 mmol), $\text{NH}_4\text{H}_2\text{PO}_4$ (12 mmol), and Na_2CO_3 (6 mmol) were dissolved in deionized water under continuous stirring, followed by the addition of ascorbic acid (6 mmol) and polyethylene glycol (6 mL) to form a homogeneous blue suspension. After further stirring, the mixture was transferred into a Teflon-lined autoclave and subjected to hydrothermal treatment at 180 °C for 40 h. Upon cooling, the obtained suspension was ultrasonically dispersed and concentrated through solvent evaporation to yield a brown sol, which was subsequently dried at 120 °C overnight. The resulting precursor was ground thoroughly and annealed at 750 °C for 4 h under an Ar atmosphere,

affording nano-sized NVP powders.

Characterization: The microstructures and morphologies of the obtained samples were characterized by field-emission scanning electron microscopy (FESEM, Hitachi SU-8020) and high-resolution transmission electron microscopy (HRTEM, Tecnai F20). Elemental distribution and composition were further analyzed using an energy-dispersive X-ray (EDX) spectrometer attached to the HRTEM system. Phase identification was carried out by X-ray diffraction (XRD, Miniflex 600) with Cu K α radiation. Electron paramagnetic resonance (EPR, Bruker-550) spectroscopy was employed to probe the defect characteristics of the materials. The specific surface area and pore structure were evaluated from N₂ adsorption/desorption measurements using an Intelligent Gravimetric Sorption Analyzer (Hiden IGA100B). The MXene content of the composites was determined through thermogravimetric analysis (TGA, NETZSCH STA449F3) under an air atmosphere at a heating rate of 10 °C min⁻¹. In addition, surface elemental composition and valence states were investigated by X-ray photoelectron spectroscopy (XPS, ESCALAB 250).

Electrochemical Characterizations: The sodium-storage properties of the prepared samples were evaluated using CR2032 coin-type half-cells assembled in an argon-filled glovebox with oxygen and moisture levels strictly controlled below trace amounts. The working electrodes were fabricated by mixing the active material, Super P conductive carbon, and carboxymethyl cellulose (CMC) binder at a mass ratio of 8:1:1. After dispersing the mixture in deionized water, the resulting slurry was uniformly coated onto Cu foil and subsequently dried under vacuum. The average active material loading was maintained at approximately 1.5 mg cm⁻². Sodium metal was employed as both the counter and reference electrode. The electrolyte consisted of 1 M NaPF₆ dissolved in diglyme (DEGLYME), while Whatman glass fiber membranes were used as separators. Galvanostatic charge/discharge (GCD) measurements and galvanostatic intermittent titration technique (GITT) tests were conducted on a LAND multichannel battery testing system at room temperature within a voltage range of 0.01-3.0 V versus Na⁺/Na. For the GITT measurements, the cells were tested after the fifth cycle using current pulses of 0.2 A g⁻¹ for 20 minutes, followed by relaxation periods of 2 h to evaluate the Na⁺ diffusion kinetics. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) analyses were carried out on a CHI660E electrochemical workstation to investigate the electrochemical reaction behavior, charge-transfer characteristics, and ion-transport kinetics. For post-cycling characterization, the cells were disassembled inside the glovebox, and the harvested electrodes were carefully rinsed with DEGLYME to remove residual electrolyte species prior to in situ and ex situ analyses.

To further assess the practical sodium-storage capability, full cells were assembled using Na₃V₂(PO₄)₃ (NVP) as the cathode and pre-sodiated Bi₂Te_{3-x}/MXene as the anode. The pre-sodiation treatment was applied to compensate for the initial irreversible sodium loss of the anode. The cathode slurry was prepared by dispersing 80 wt.% Na₃V₂(PO₄)₃, 10 wt.% acetylene black, and 10 wt.% polyvinylidene fluoride (PVDF) in N-methyl-2-pyrrolidone (NMP), followed by coating onto Al foil. After vacuum drying at 100 °C overnight, the cathode was paired with the Bi₂Te_{3-x}/MXene anode to assemble full cells. The same electrolyte and separator used in the half-cells were adopted for full-cell testing. Electrochemical measurements were performed on a LAND multichannel battery testing system at room temperature over a voltage window of 1.0-3.8 V.

The energy (E, Wh kg⁻¹) and power densities (P, W kg⁻¹) of sodium ion full-cells were calculated based on the following equations:

$$E = \frac{CV^2}{2} = \frac{It(V_{\max} - V_{\min})}{2 \times 3.6 \times m} \quad (\text{Equation S1})$$

$$P = \frac{E \times 3600}{t} \quad (\text{Equation S2})$$

where I (A) is the constant discharge current, t (s) is the discharge time, m (g) is the total mass of active materials in both the anode and cathode, $V_{\max}$ (V) is the initial discharge voltage excluding the IR drop and $V_{\min}$ (V) is the final discharge voltage.

Calculation of the b Value and Capacitive Contribution: The charge-storage behavior was evaluated by analyzing the relationship between the current response (i) and scan rate (v) obtained from cyclic voltammetry (CV) measurements according to the power-law equation:

$$i = a v^b \quad (\text{Equation S3})$$

$$\log(i) = b \log(v) + \log(a) \quad (\text{Equation S4})$$

where a and b are adjustable parameters. The b -value reflects the dominant charge-storage mechanism, with $b = 0.5$ corresponding to a diffusion-controlled intercalation process and $b = 1.0$ indicating an ideal capacitive-controlled behavior. To further quantify the relative contributions from capacitive and diffusion-controlled processes, the current response at a given potential can be separated using:

$$i(V) = k_1 v + k_2 v^{1/2} \quad (\text{Equation S5})$$

$$i(V)/v^{1/2} = k_1 v^{1/2} + k_2 \quad (\text{Equation S6})$$

where both k_1 and k_2 are fitting constants. The term $k_1 v$ represents the capacitive contribution, including surface-controlled redox reactions and electrical double-layer capacitance, whereas $k_2 v^{1/2}$ corresponds to the diffusion-limited sodium-ion storage process.

Galvanostatic intermittent titration (GITT) measurement: The sodium-ion diffusion coefficient (D_{Na^+}) was estimated from GITT measurements based on the simplified solution of Fick's second law:

$$D = \frac{4}{\pi\tau} \left(\frac{m_B V_M}{M_B S} \right)^2 \left(\frac{\Delta E_s}{\Delta E_t} \right)^2 \quad (\text{Equation S7})$$

where m_B denotes the mass loading of active material, S (cm^2) is the effective electrode area, M_B (g mol^{-1}) and V_M ($\text{cm}^3 \text{mol}^{-1}$) represent the molecular weight and molar volume of the active material, respectively, and τ is the duration of the current pulse. ΔE_s corresponds to the steady-state potential variation before and after each pulse, while ΔE_t represents the transient voltage change during the current pulse after eliminating the IR drop.

Computational details: First-principles calculations based on density functional theory (DFT) were carried out using the Vienna Ab initio Simulation Package (VASP) [1] within the projector augmented-wave (PAW) framework. The exchange-correlation energy was treated using the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional [2]. Long-range dispersion interactions were taken into account through the DFT-D3 correction [3]. A plane-wave kinetic-energy cutoff of 450 eV was employed for all calculations, while the electronic self-consistency criterion was set to 10^{-5} eV. Brillouin-zone integrations were performed using a $1 \times 3 \times 1$ Monkhorst–Pack k -point mesh. The atomic configurations were fully optimized until the residual force on each atom was below $0.05 \text{ eV}/\text{\AA}$. A vacuum spacing of $15 \text{ \AA}$ was introduced along the z direction to eliminate artificial interactions between periodically repeated slabs. Spin-polarized calculations were considered throughout.

The adsorption energy of Na was evaluated using bulk metallic Na as the reference state according to:

$$E_{\text{ads}}(\text{Na}) = E_{\text{slab+Na}} - E_{\text{slab}} - \mu_{\text{Na}}^{\text{bulk}},$$

where $E_{\text{slab+Na}}$ and E_{slab} represent the calculated total energies of the Na-adsorbed and bare surfaces, respectively, and $\mu_{\text{Na}}^{\text{bulk}}$ denotes the chemical potential of Na, which was determined from the energy per atom of bulk metallic Na.

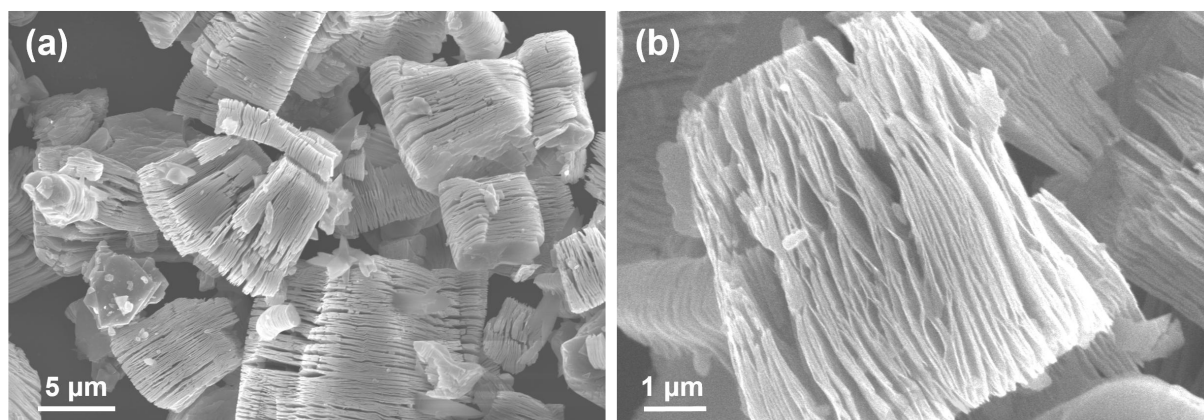


Figure S1. (a, b) SEM images of multi-layered $\text{Ti}_3\text{C}_2\text{T}_x$ MXene.

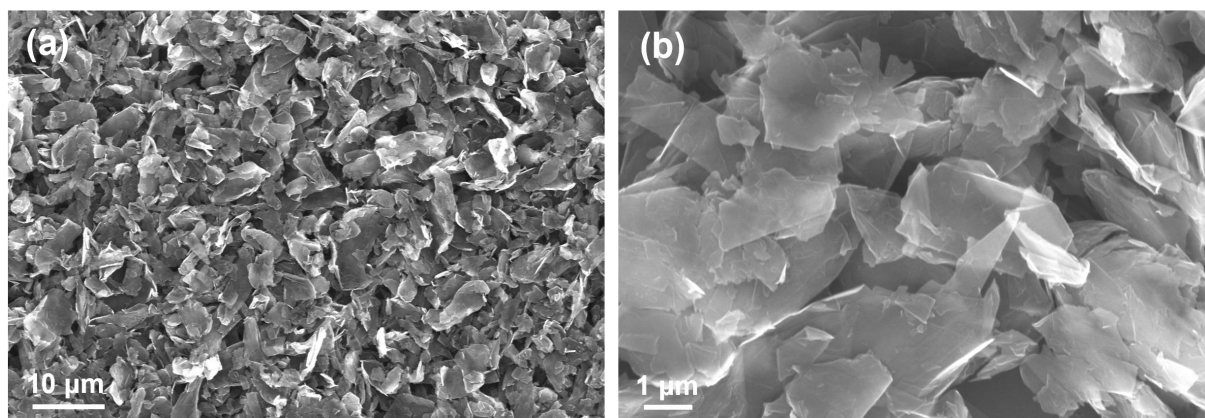


Figure S2. (a, b) SEM images of few-layered $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanosheets.

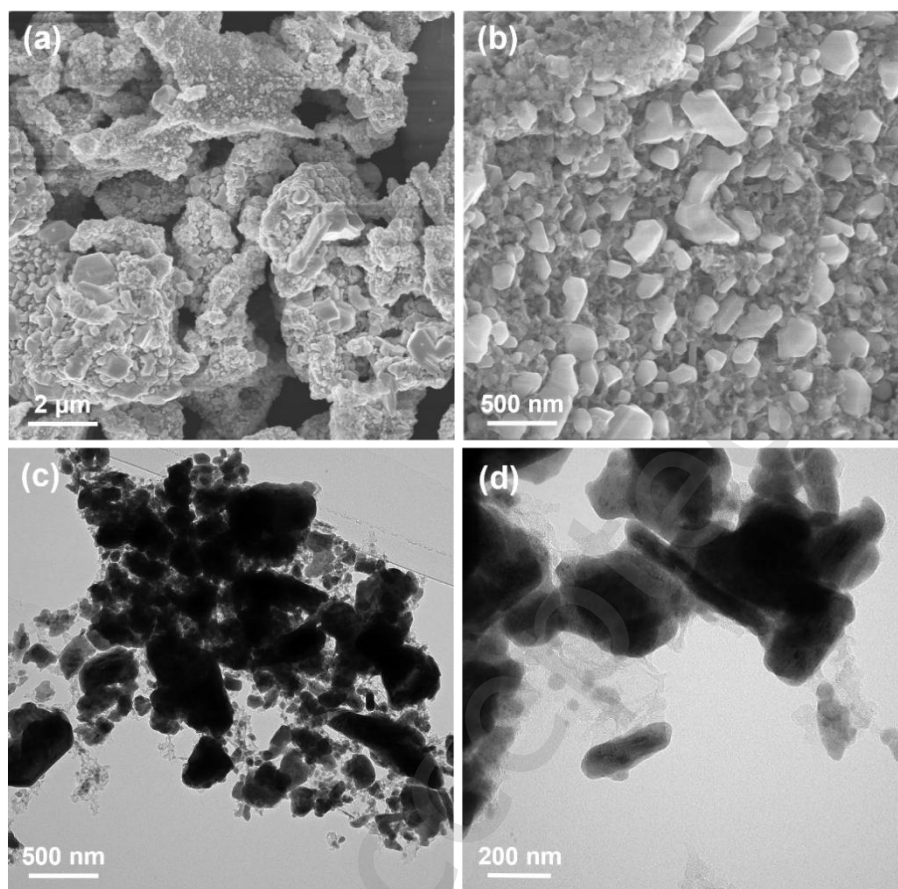


Figure S3. (a, b) FESEM and (c-e) TEM images of pure Be_2Te_3 .

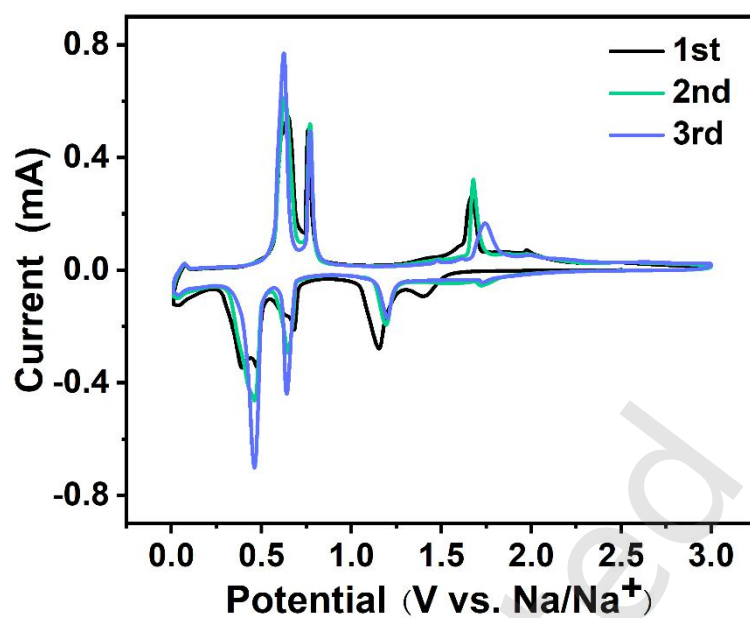


Figure S4. CV curves of the pure Be₂Te₃ electrode at a scan rate 0.1 mV s⁻¹.

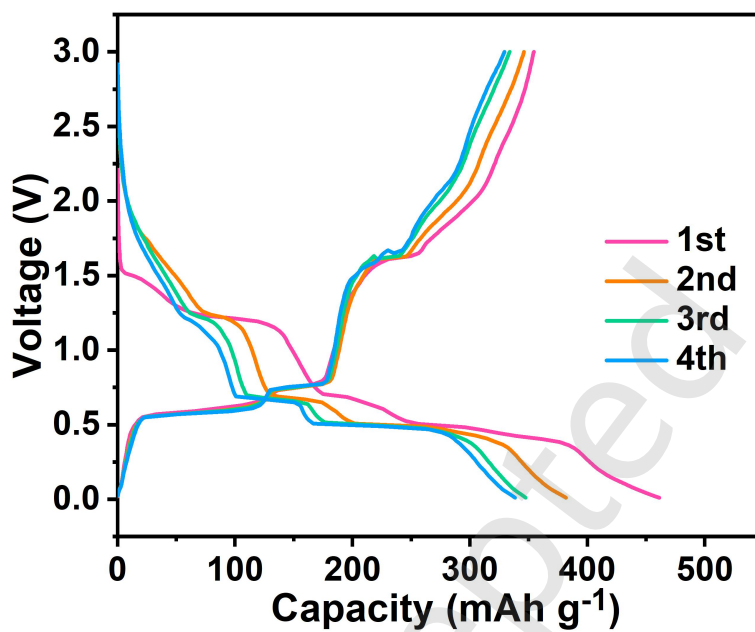


Figure S5. galvanostatic charge/discharge voltage profiles of pure Be₂Te₃ electrode at 0.2 A g⁻¹.

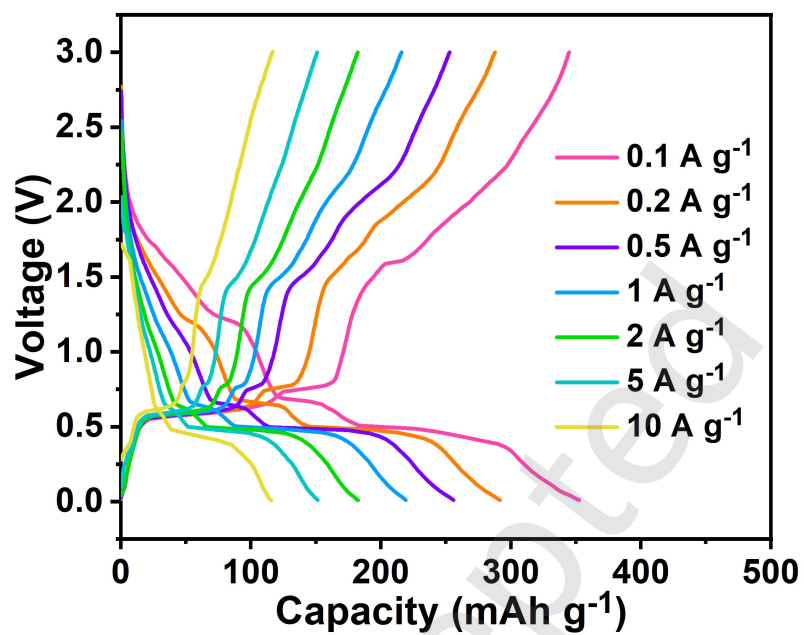


Figure S6. The GCDs curves of pure Be_2Te_3 at different current densities.

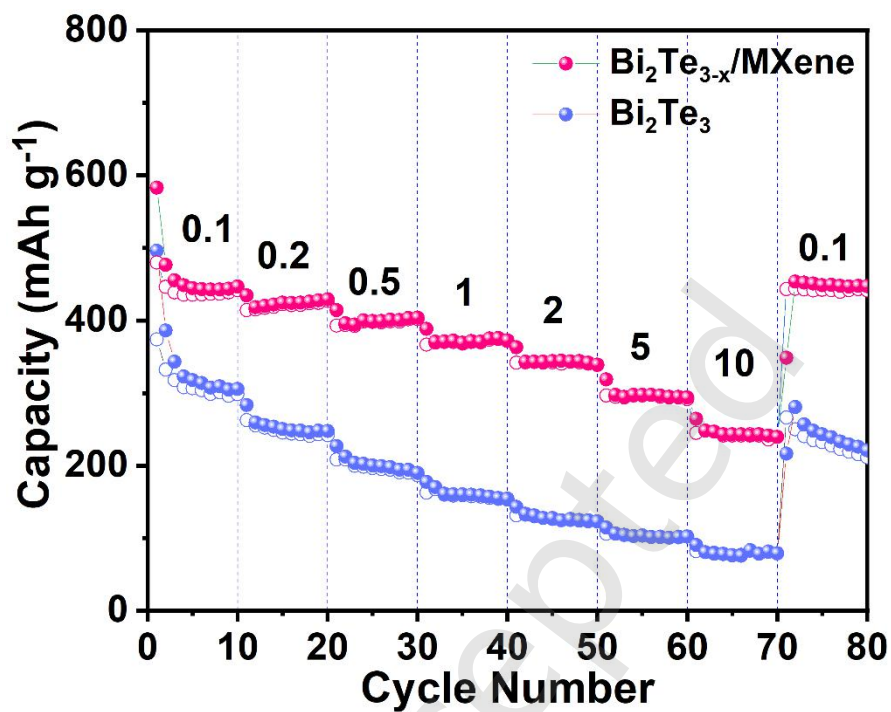


Figure S7. Rate performance of the Bi₂Te_{3-x}@MXene and pure Bi₂Te₃ electrodes in 1 M NaClO₄ electrolyte dissolved in a mixture of ethylene carbonate and dimethyl carbonate (EC/DMC, 1:1, v/v).

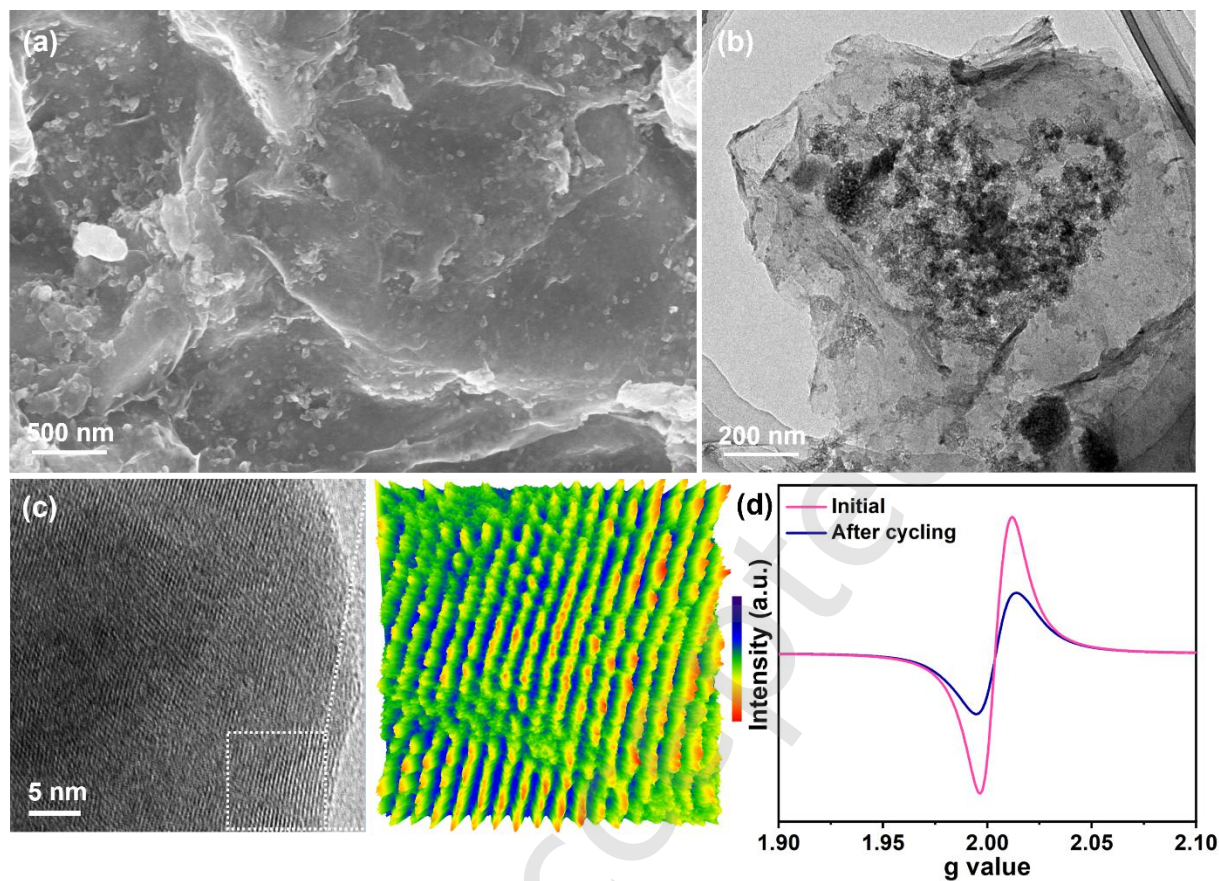


Figure S8. Structural stability and EPR characterization of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ after prolonged cycling at 2 A g^{-1} . (a) FESEM image, (b) TEM image, and (c) HRTEM image with the corresponding 3D surface plot of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ after 2000 cycles. (d) EPR spectra of $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ before and after 2000 cycles, showing the persistence of the characteristic Te-vacancy-related signal.

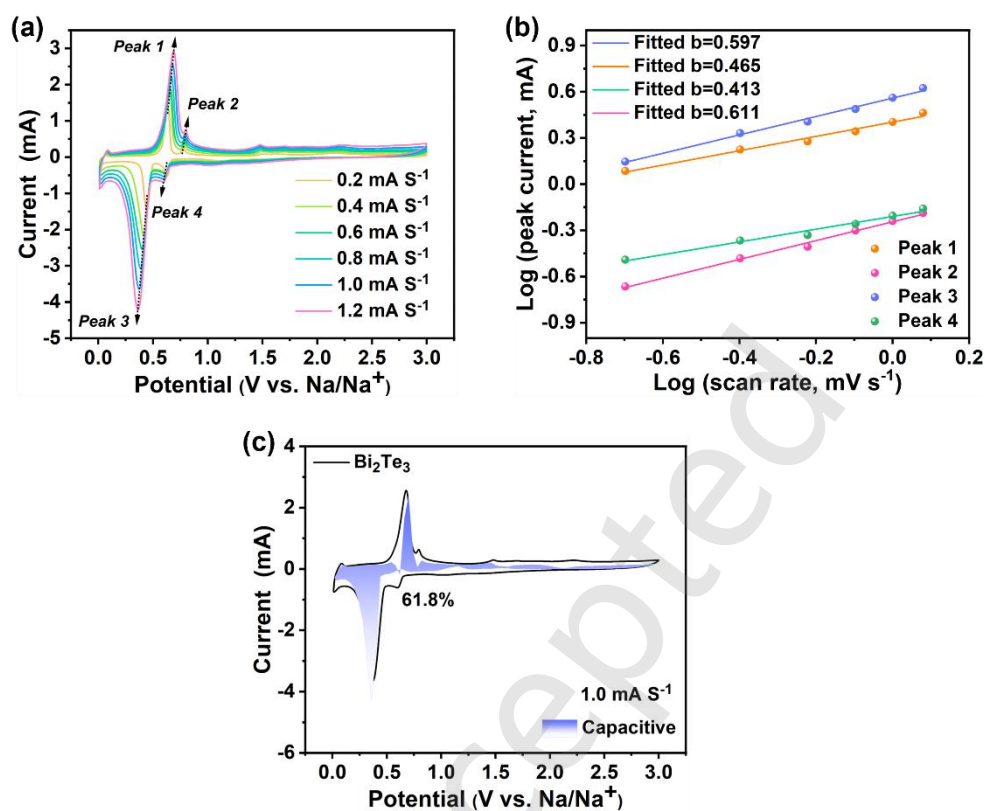


Figure S9. (a) CV curves at various scan rates from 0.2 to 1.2 mV s^{-1} , (b) Linear relationships between logarithm currents and logarithm sweep rate, (g-h) capacitive contribution at 1.0 mV s^{-1} of the pure Be_2Te_3 electrode.

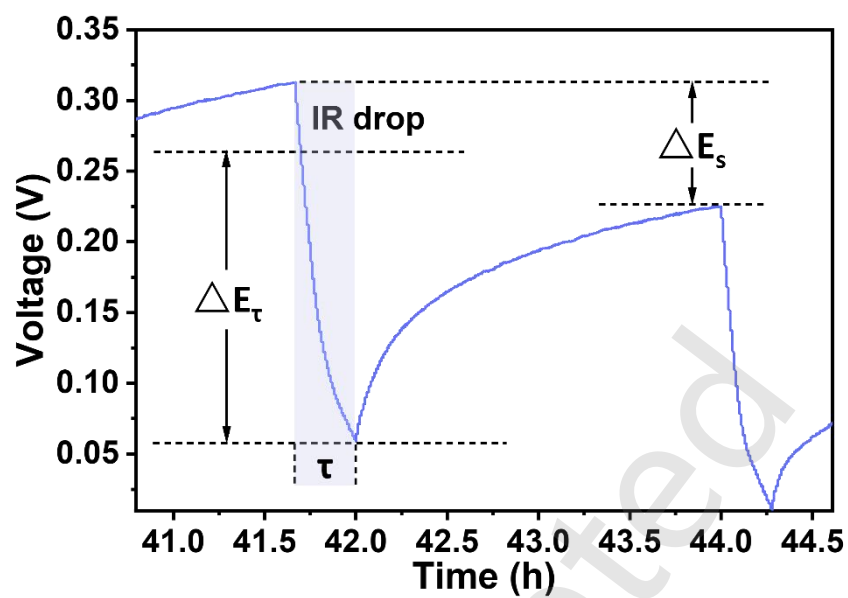


Figure S10. Representative GITT profile. Determination of ΔE_τ (voltage change during the current pulse) and ΔE_s (quasi-equilibrium voltage difference before and after the current pulse) from the measured GITT profile.

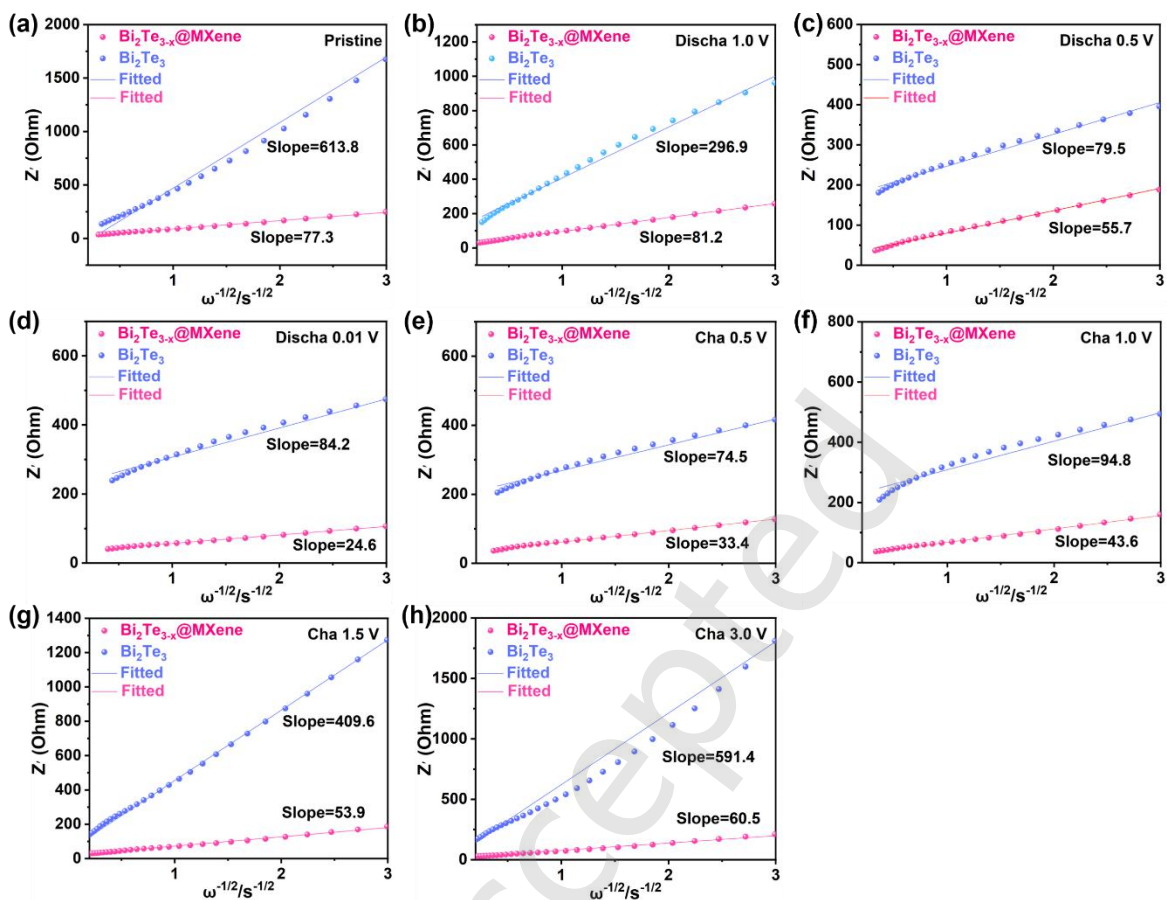


Figure S11. Z' - $\omega^{-1/2}$ plots for $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Bi_2Te_3 collected at different status. (a) pristine, discharging to (b) 1.0 V, (c) 0.5 V, (d) 0.01 V, and charging to (e) 0.5 V, (f) 1.0 V, (g) 1.5 V and (h) 3.0 V.

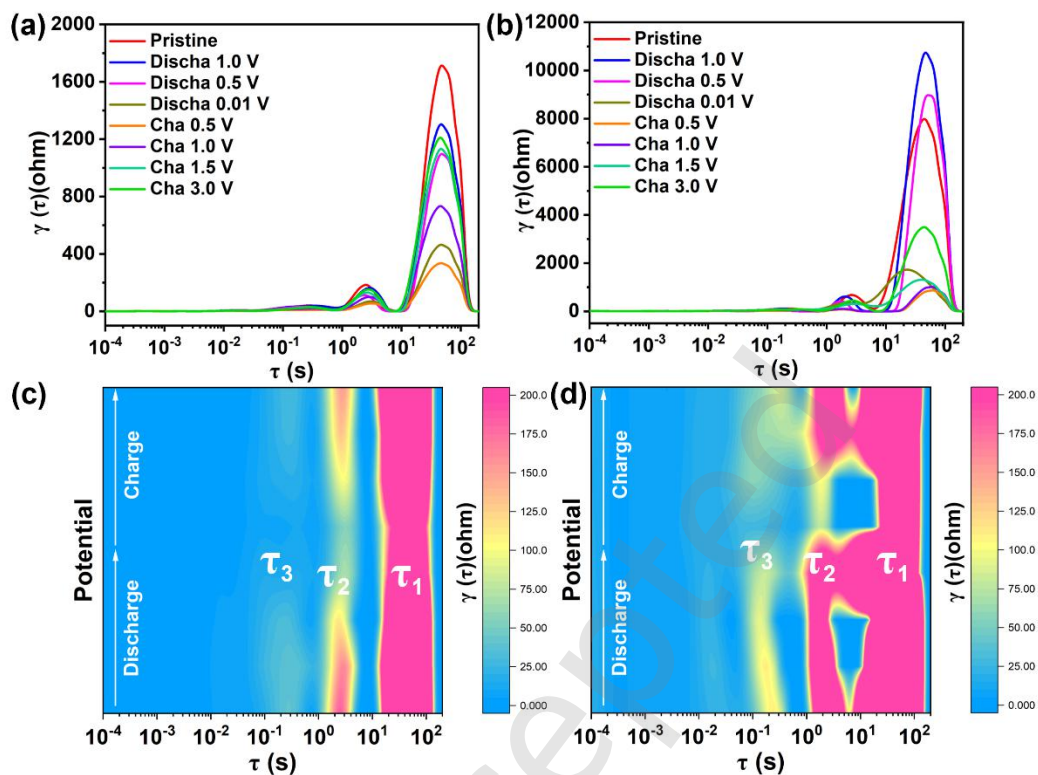


Figure S12. DRT curves obtained from EIS measurements of (a) $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and (b) pure Be_2Te_3 at different potentials, and corresponding contour plots of (c) $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and (d) pure Be_2Te_3 .

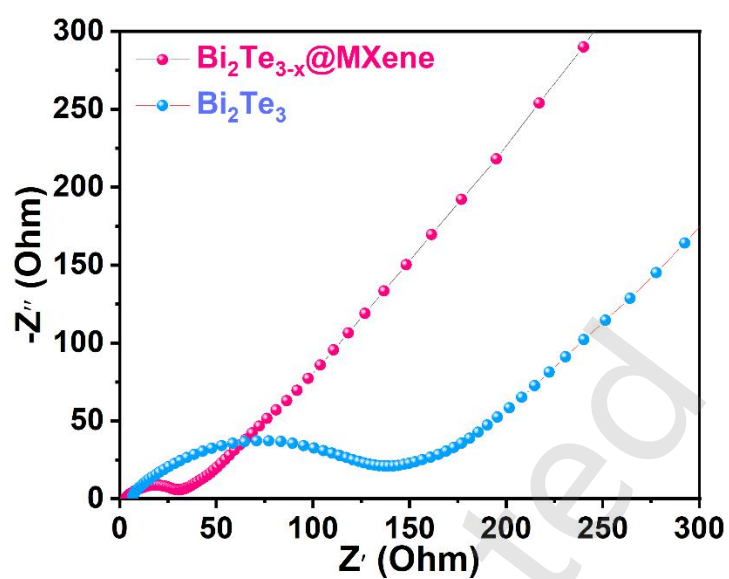


Figure S13. Electrochemical impedance spectra of the $\text{Bi}_2\text{Te}_{3-x}\text{@MXene}$ and pure Bi_2Te_3 electrodes obtained after 200 cycles at 0.2 A g^{-1} .

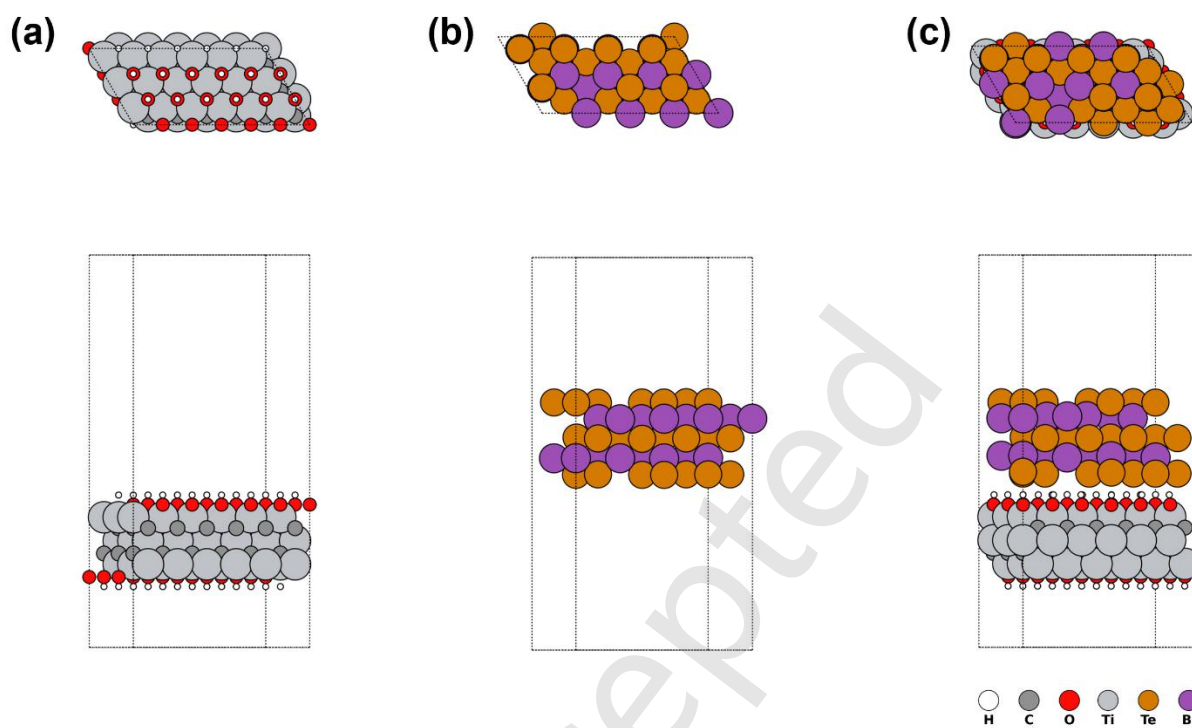


Figure S14. Top and side illustration of simulations for (a) Mxene, (b) $\text{Bi}_2\text{Te}_{3-x}$, (c) $\text{Bi}_2\text{Te}_{3-x}@\text{MXene}$.

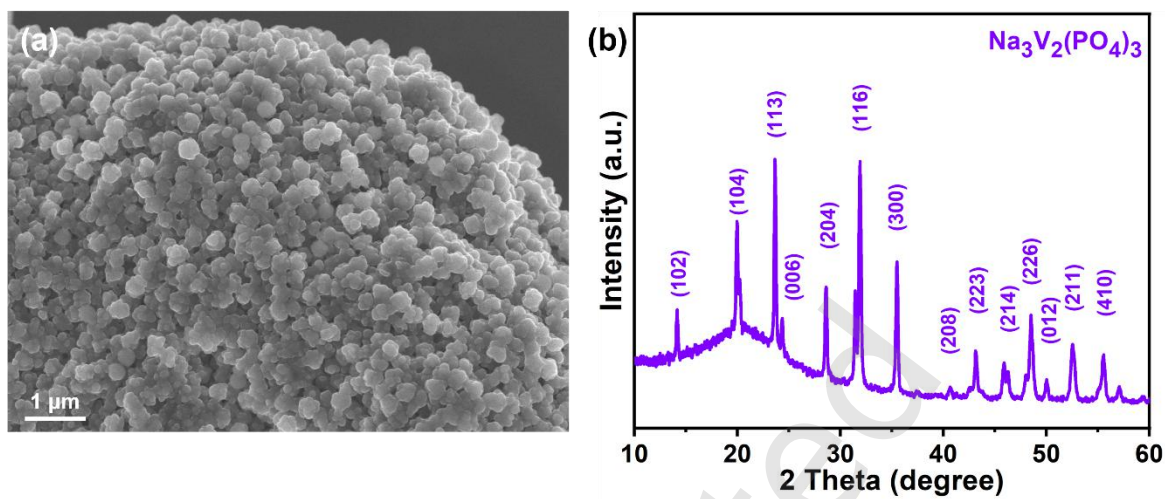


Figure S15. (a) FESEM image, (b) XRD pattern of the $\text{Na}_3\text{V}_2(\text{PO}_4)_3$.

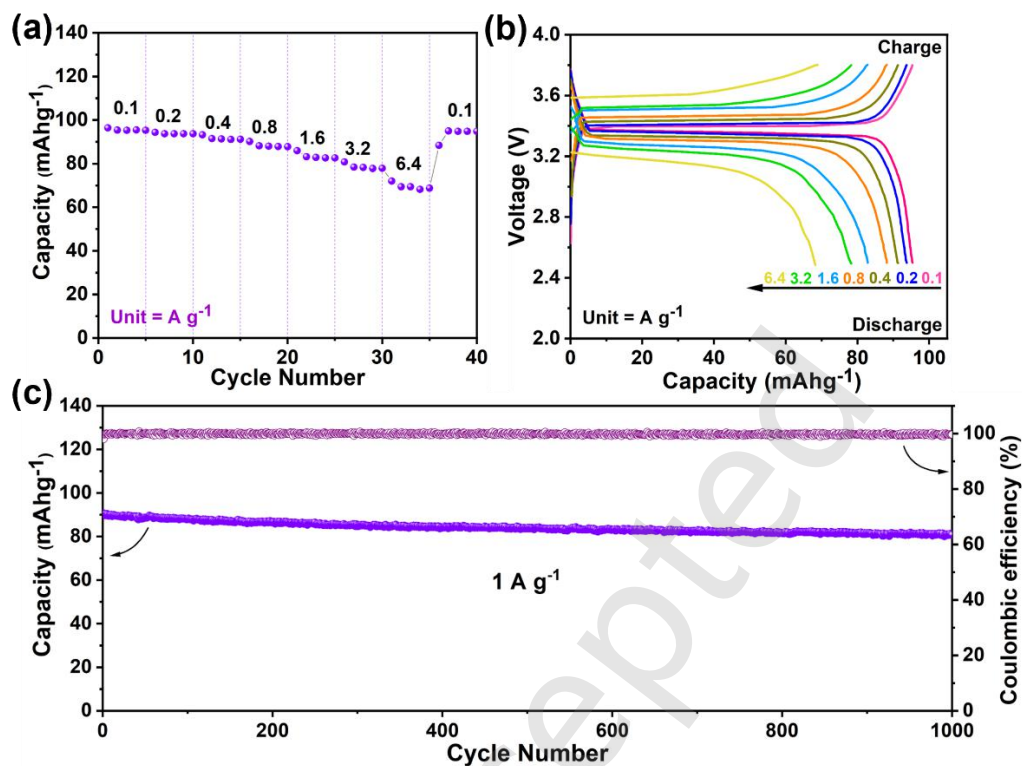


Figure S16. Electrochemical performance of $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ cathode evaluated within a voltage range of 2.5-3.8 V versus Na metal. (a) Rate capability at various current densities. (b) Representative galvanostatic charge/discharge profiles recorded at different current densities. (c) Long-term cycling stability measured at 1 A g^{-1} .

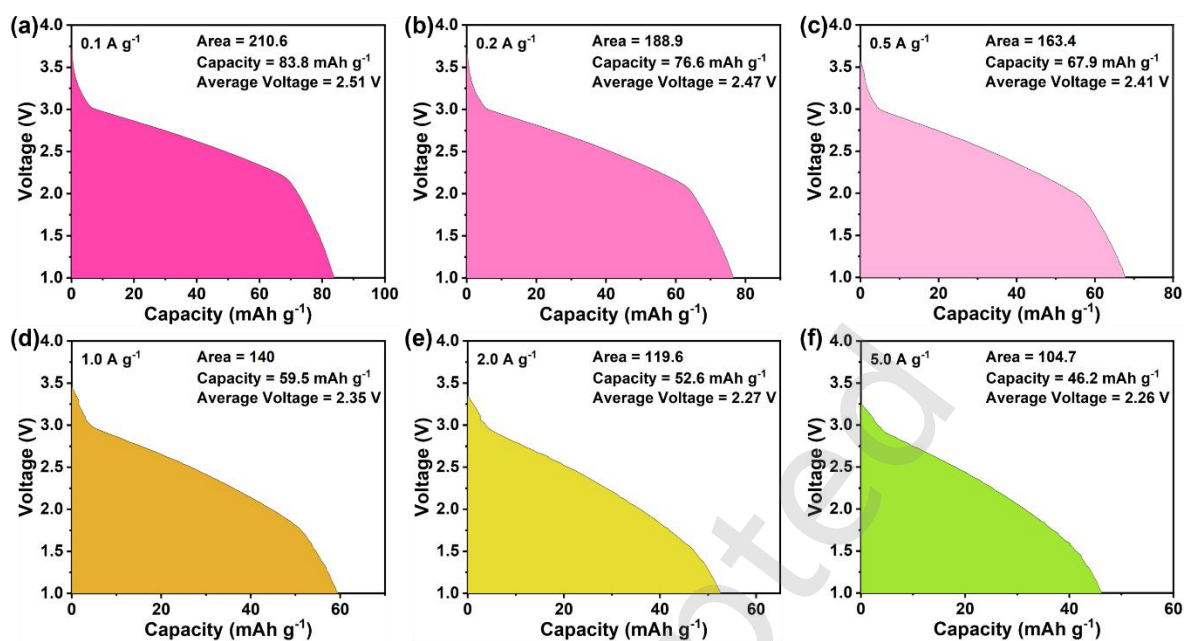


Figure S17. Average voltage calculations in discharge process at the current densities for NVP//Bi₂Te_{3-x}@MXene full cell.

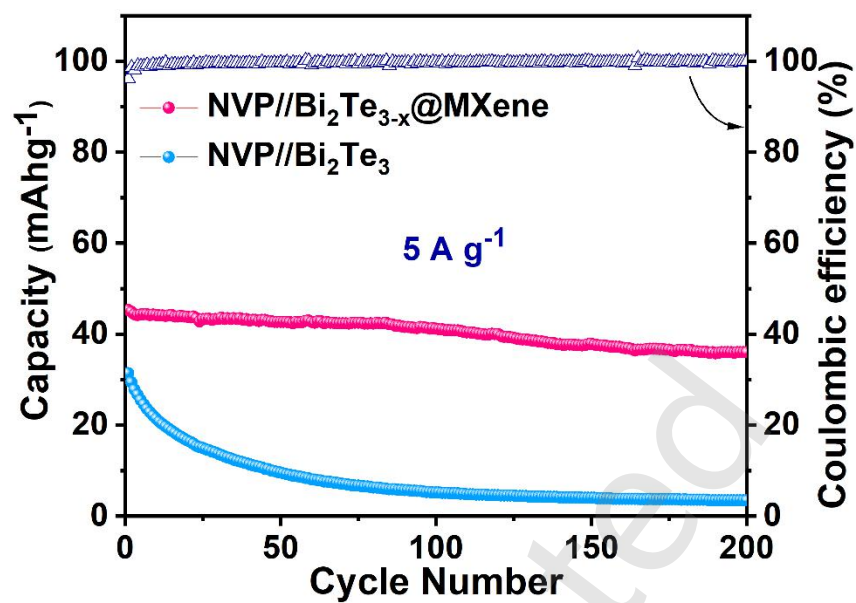


Figure S18. Cycling performance of the NVP//Bi₂Te_{3-x}@MXene and NVP//Bi₂Te₃ full cell at 5 A g⁻¹.

Table S1. The initial Coulombic efficiency comparisons for sodium ion batteries between this work and other metal chalcogenide anodes.

Sample	Current density (A g ⁻¹)	initial Coulombic efficiency (%)	References
Bi ₂ Te _{3-x} @MXene	0.2	87.1	This work
CuS@MoS ₂	0.1	78	4
2D-MoTe ₂ @3DPNCN	0.1	46.1	5
MoS _{2-x} Se _y /m-C@rGO	0.1	63	6
Vs - ZnIn ₂ S ₄	0.5	78	7
KCu ₇ S ₄	0.02	80.3	8
FePS ₃ /Ti ₃ C ₂ T _x	0.05	77.9	9
(Co,Cu)Se ₂ /NC	0.2	59.4	10
Se-CoS ₂ /CoSe ₂	0.1	80.88	11
SnTe@SHNC	0.1	58	12
W-P/WSe ₂ /C	0.1	46.7	13

References

- [1] Kresse, G.; Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. *Physical Review B* 1999, 59, 1758-1777.
- [2] Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Physical Review Letters* 1996, 77, 3865-3868.
- [3] Grimme S, Antony J, Ehrlich S and Krieg H 2010 A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu *Journal of Chemical Physics* 2010, 132, 154104.
- [4] Peng, H.;Miao, W.;Zeng, J.;Wang, Z.;Yan, C.;Ma, G.; Lei, Z. Electronic Modulation and Built-in Electric Field Strategies in Heterostructures Together Induce 1T-Rich MoS₂ Conversion for Advanced Sodium Storage. *Adv. Sci.* **2025**, 12, e2417288.
- [5] Liang, M.;Ma, L.;Chen, B.;Liu, E.;Shi, C.;He, C.; Zhao, N. Two Birds with One Stone: A NaCl-Assisted Strategy toward MoTe₂ Nanosheets Nanoconfined in 3D Porous Carbon Network for Sodium-Ion Battery Anode. *Energy Storage Mater.* **2022**, 47, 591-601.
- [6] Wu, D.;Gai, L.;Cui, D.;Wang, Q.;Yu, H.;Wong, C. P.; Lian, G. Oxygen - Doped Carbon Monolayer Intercalation and Selenization Stabilizing 1T - Rich MoS₂ to Enable Fast and Durable Sodium - Ion Storage. *Adv. Energy Mater.* **2025**, 15, e03274.
- [7] Wang, Y.;Zhang, H. H.;Wen, Z.;Sun, C. N.;Wang, G. Y.;Wang, M. S.;Yang, C. C.; Jiang, Q. ZnIn₂S₄ with a hybrid reaction mechanism and sulfur vacancies for sustainable sodium storage. *Carbon Energy* **2025**, 7, e654
- [8] Guo, Y.;Wang, H.;Yang, C.;Dai, S.;Wang, Y.; Cheng, S. High - Mobility Cu⁺ - Induced Multi - Dimensional Structured Copper - Based Sulfide Anode for Advanced Sodium Ion Batteries. *Adv. Funct. Mater.* **2025**, 35, 2510286.
- [9] Zhong, L. S.;Yue, M.;Liang, Y. Z.;Xi, B. J.;An, X. G.;Xiao, Y. H.;Cheng, B. C.;Lei, S. J.; Xiong, S. L. In Situ Universal Construction of Thiophosphite/MXene Hybrids via Lewis Acidic Etching for Superior Sodium Storage. *Adv. Funct. Mater.* **2024**, 34, 2407740.
- [10] Wang, D.;Chao, Y.;Guo, K.;Wang, Z.;Yang, M.;Zhu, J.;Cui, X.; Xu, Q. Engineering Metal Electron Spin Polarization to Regulate p - Band Center of Se for Enhanced Sodium - Ion Storage. *Adv. Funct. Mater.* **2024**, 34, 2405642.
- [11] Feng, T.;Wang, F.;Sun, Z.;Guo, F.;Xiong, Y.;Ren, F.;Tang, C.;Li, J.;Kun Liu, H.; Xue Dou, S. Cascade Selenization Regulated the Electronic Structure and Interface Effect of Transition Metal Sulfides for Enhanced Sodium Storage. *Angew. Chem. Int. Ed.* **2025**, 64, e202420504.
- [12] Liang, Z. X.;Huang, J. L.;Zhang, W.;Chu, H. Y.;Li, Q. H.;Lu, H. B.;Lin, Z. Y.;Wang, J. L.;Lin, H. P.;Chen, Y. Y.;Xiong, S. Y.; Huang, S. M. Uncovering and preventing polytellurides dissolution enables stable sodium-ion storage: A case study of SnTe. *Chem. Eng. J.* **2024**, 498, 154873.
- [13] Yu, M.;Zeng, F.;Qu, Y.;Wang, X.;Chen, S.;Hu, S.;Ma, D.;Xie, M.; Luo, S. Robust P-Se bond coupling of atomically amorphous W-P clusters to crystalline WSe₂ via dual p-band centers for enhanced sodium-ion storage. *Energy Storage Mater.* **2024**, 67, 103265.