

A scalable multifunctional Bi_2Te_3 -MXene heterostructure for energy conversion and storage

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Abstract

Topological insulators (TIs), particularly bismuth telluride (Bi_2Te_3), exhibit exceptional electronic properties but are frequently hindered by low intrinsic conductivity and structural instability in their bulk form. In this work, we report a strategic interface engineering approach to hybridize layered Bi_2Te_3 nanosheets with conductive $\text{Ti}_3\text{C}_2\text{T}_x$ MXene, creating a high-performance bifunctional heterostructure. Phase-pure Bi_2Te_3 was synthesized via a surfactant-assisted hydrothermal method and integrated into MXene matrix, which functions as both a conductive scaffold and a structural buffer. Synchrotron-based structural analysis and temperature-dependent Raman spectroscopy demonstrate that the MXene interface facilitates significant structural refinement, expanding Van der Waals gaps and reorganizing bond geometries, while effectively passivating the chalcogenide surface against oxidation. The resulting $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite exhibits superior electrocatalytic activities, delivering a low overpotential of 260 mV at $100 \text{ mA}\cdot\text{cm}^{-2}$ for the hydrogen evolution reaction (HER), 490 mV at $100 \text{ mA}\cdot\text{cm}^{-2}$ for the oxygen evolution reaction (OER), and an onset potential of 0.81 V for the oxygen reduction reaction (ORR), significantly outperforming pristine Bi_2Te_3 . Mechanistic study probes indicate HER proceeds predominantly at Bi sites enabled by partial Bi-O surface termination while MXene supplies rapid electron conduction and defect sinks that stabilize catalytic centers. These results suggest that engineered 2D/2D heterojunctions provide a versatile platform for optimizing charge transport and ion kinetics in next-generation energy conversion and storage systems.

Introduction

Layered materials ignited a significant interest with intriguing properties that are observed when single- or multiple-layer thick sheets produced which can diverge from bulk multilayered material. Amongst this phenomena graphene is the best example which has laid a pathway in scientific research towards several 2D materials, such as transition metal dichalcogenides (TMDs), black phosphorous, graphitic-carbon nitrides ($\text{g-C}_3\text{N}_4$), boron nitride, MXenes, and transition metal borides (MBenes), etc. The topological insulators (TIs) are indeed another class of materials which exhibit remarkable thermal, optical, spectroscopical, and electrical properties when they are reduced to single- or multiple-layer like sheets. In the bulk state, these materials demonstrate anisotropic electrical properties along the c-axis acting as an insulator in bulk state but with a metallic phase along the surface of the layer. In the A_2B_3 family of TIs ($\text{A} = \text{Bi, Sb, Cr}$ pnictogen; $\text{B} = \text{Se, Te}$ chalcogenide), the single-crystal structures are the most explored materials as they are the best thermoelectric materials and the various synthesis routes and protocols were proposed to fabricate the single-phase with single-sheets to investigate their physio-electro properties [1–6]. Due to the large intrinsic electronic band gap of these materials, which contain a singular Dirac-cone-like topologically protected metallic surface state within the bulk energy gap, they function as prototypical TIs with massless fermions, leading to high carrier mobility, structural stability, nano-structuring with confinement effect and quantum transport properties. Various methods were proposed for synthesizing single-crystal TIs, including molecular beam epitaxy (MBE), metal-organic chemical vapor deposition (MO-CVD), electro-chemical deposition (ECD), wet-chemical methods,

solvothermal and hydrothermal methods [7–10]. The optimization and preparation of single-crystal TIs represent a pivotal strategy; however, comprehensive studies of their physicochemical properties remain insufficient. Despite their attractive electrical properties, TIs are hindered by low thermal conductivity and limited transport efficiency due to their crystalline structures. Integrating them into nanocomposites helps overcome the alloy limit by modulating phonon behavior, which enhances electron transport and boosts stability for enhanced electrocatalytic performance. To achieve this, transition-metal carbides known as MAX phases ($M_{n+1}AX_n$) were employed. These materials consist of a transition metal (M), an A-group element (A), and carbon or nitrogen (X). Through selective etching, the MXenes are derived from the MAX phase without compromising the M-X bonds. The resulting MXene structure features M atoms in an hcp pattern inherited from the parent phase with X atoms situated in octahedral interstices to form the $M_{n+1}X_n$ sheets. These sheets are stabilized by surface-terminating species (T) bonded to the outermost M atoms [11–13]. Consequently, integrating TIs into a nanocomposite with MXenes significantly enhances intercalation mobility, electronic conductivity, and surface termination effects.

As the electronegativity of chalcogen atoms decreases down the group ($O > S > Se > Te$), the covalent character of metal-chalcogen bonds progressively increases. Previous studies have demonstrated that such enhanced covalency in metal-anion bonds significantly boost the catalytic efficiency of the oxygen evolution reaction (OER) [14, 15]. Consequently, a systematic improvement in catalytic performance is expected across the chalcogenide series. Among these, tellurides, possessing the lowest electronegativity, exhibit the strongest covalent interactions and favorable band alignment with the water oxidation potential, making them promising candidates for water splitting [16]. These materials emerge as viable alternatives to noble-metal catalysts including Pt, IrO_2 , and RuO_2 . While these noble-metal catalysts show exceptional HER and OER activities, their high cost, scarcity, and instability in alkaline media limit their large-scale application [17, 18]. For the sustainable hydrogen generation, it is essential to develop such telluride-based systems which can effectively lower kinetic barriers and improve the efficiency of electrochemical water splitting. While research has predominantly focused on Co- and Ni-based tellurides [19–21], the broader class of tellurides has gained attention as bifunctional electrocatalysts for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER).

In this work, we employed interface engineering by hybridizing layered bismuth telluride (Bi_2Te_3) with $Ti_3C_2T_x$ MXene to overcome the inherent limitations of bulk tellurides. Bi_2Te_3 serves as a versatile template owing to its anisotropic transport properties and quintuple-layer architecture. These layered structures feature the Van der Waals gaps that promote rapid ion/electron kinetics and allow for the formation of stable heterojunctions with 2D MXenes. We achieved high-quality, phase-pure Bi_2Te_3 through surfactant-assisted hydrothermal methods, utilizing time-resolved growth to control structural defects. By hybridizing Bi_2Te_3 with the conductive $Ti_3C_2T_x$ MXene, we developed a bifunctional heterostructure optimized for both water splitting and Li-/Na-ion batteries. The relationship between the engineered interfaces and their catalytic activity was further elucidated through a combination of synchrotron-based structural analysis and temperature dependent Raman analysis. Our strategy

highlights the potential of layered chalcogenide-MXene composites as high-performance, multifunctional energy materials.

Results and Discussion

Characterization of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite

The synthesis of Bi_2Te_3 was systematically optimized through surfactant-assisted hydrothermal routes using cetyltrimethylammonium bromide (CTAB), polyvinylpyrrolidone (PVP), and sodium dodecyl sulfate (SDS), and further optimized with time-resolved PVP-mediated growth (4–32 h) (Scheme 1). The synthesized Bi_2Te_3 was characterized with XRD analysis and their results are depicted in **Fig. S1a-b** and **Note S1.1–S1.2**. In addition, the formation of Ti_3AlC_2 MAX and its etched $\text{Ti}_3\text{C}_2\text{T}_x$ MXene phase was confirmed by XRD (**Note S1.3**) and illustrated in **Fig. S2a**. These studies establish the structural foundation for achieving phase-pure Bi_2Te_3 and a well-defined $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite.

The synchrotron diffraction profile of pristine Bi_2Te_3 , refined within the $R\bar{3}m$ space group, reveals a phase-pure rhombohedral crystal with no detectable secondary phases. The quintuple-layer stacking sequence $-\text{Te1}-\text{Bi}-\text{Te2}-\text{Bi}-\text{Te1}-$ is clearly resolved in the refinement with strong covalent Bi–Te bonding within each quintuple and weak Van der Waals interactions across the Te1–Te1 interface (Fig. 1a). This layered topology results in an inter-quintuple spacing of 3.730(14) Å, which is consistent with the Van der Waals gap reported in Bi_2Te_3 [22, 23]. The dominant reflection at $2\theta = 27.7^\circ$ corresponds to the (015) plane, while higher-order basal reflections confirm preferential c-axis alignment. No residual signals from precursor phases (Bi, Te) are observed. Refined bond lengths and angles in **Table S1** reveals a symmetric coordination of Bi between Te1 and Te2 sites with Bi–Te1 = 3.026(8) Å, Bi–Te2 = 3.267(6) Å, and nearly ideal angular geometries (Te1–Bi–Te2 = 91.2° , Bi–Te1–Bi = 93.3°). The Williamson-Hall (W–H) analysis identifies compressive residual strain (negative slope), relatively small crystallite size, and elevated dislocation density, reflecting the strain-limited crystallinity intrinsic of Bi_2Te_3 by the hydrothermal synthesis routes (**Fig. S3a**). The 2D synchrotron image of Bi_2Te_3 exhibits concentric and isotropic Debye-Scherrer rings (**inset of Fig. 1a**), indicating uniform grain orientation and the absence of significant texture or anisotropic strain. The crystal structure of Bi_2Te_3 is illustrated after the Rietveld Refinement using VESTA software and presented in Fig. 1c. The schematic sketch of Van der Waals gap of Bi_2Te_3 is shown in Fig. 1d and the polyhedral formation of Bi-Te atoms in Bi_2Te_3 was illustrated in Fig. 1e. Taken together, the 1D refinement and 2D synchrotron establish the pristine Bi_2Te_3 as a well-ordered Van der Waals layered system with compressive microstrain and isotropic polycrystallinity. In the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite, the refined Bi_2Te_3 phase remains intact with lattice constants nearly identical to the pristine Bi_2Te_3 , but the subtle perturbations reveal the fingerprints of MXene incorporation (Fig. 1b). The Van der Waals gap of Bi_2Te_3 expands to 3.735(9) Å, a seemingly modest shift that nevertheless indicates weak interfacial coupling between Bi_2Te_3 quintuple layers and $\text{Ti}_3\text{C}_2\text{T}_x$ MXene sheets. The bond lengths deviate systematically where Bi–Te1 elongates to

3.039(7) Å, while Bi–Te₂ contracts to 3.249(6) Å, and bond angles adjust accordingly, suggesting the interfacial strain transfer within composite. The intensity and broadening in the main peaks of Bi₂Te₃ shows the decreased crystallinity, which is consistent with the structural disorder induced by heterointerfacing. Importantly, the characteristic reflections of MXene, notably the basal (002) and high-order (600), are visible in the composite, though their intensity and fitting deviate from the pristine Ti₃C₂, confirming the presence of terminated MXene (T_x = –O, –OH, –F) rather than bare carbide (**Fig. S2b**) [24]. The 2D synchrotron image of the Bi₂Te₃/Ti₃C₂T_x composite reveals arc-like intensity distributions and anisotropic ring broadening in stark contrast to the pristine isotropic pattern (**inset of Fig. 1b**). These features are attributed to grain texturing, orientation alignment with MXene surfaces, and anisotropic strain fields. The W–H analysis shows that the evolution of the microstrain is accompanied by crystallite growth and a decline in dislocation density (**Fig. S3b**), indicating that MXene sheets act as stress-relief buffers and defect sinks. This dual-mode mechanism of MXene in the composite, which couples the introduction of anisotropic interfacial strain with the elimination of structural defects, provides a robust framework for enhancing the intrinsic properties of the heterostructure. Comparing pristine Bi₂Te₃ with the Bi₂Te₃/Ti₃C₂T_x composite reveals how MXene integration drives structural refinement. Although the quintuple-layer rhombohedral symmetry remains intact, the MXene interface triggers a sophisticated structural response with expanding the Van der Waals gaps, reorganizing Bi–Te bond geometries, and facilitating specific crystallographic orientations evident in the 2D synchrotron data. Remarkably, the composite exhibits reduced dislocation density even under enhanced strain anisotropy. This demonstrates that the Bi₂Te₃/Ti₃C₂T_x system is a model van der Waals heterostructure where structural properties are dictated by precisely engineered interfaces rather than traditional chemical doping.

Raman spectroscopy was employed to investigate the vibrational characteristics of pristine Bi₂Te₃ and Bi₂Te₃/Ti₃C₂T_x composite with particular emphasis on temperature-dependent phonon behavior and surface/interface modifications. Also, the detailed Raman analysis for different Bi₂Te₃ products using different surfactants and different synthesis time with PVP surfactant is provided in **Note S2.1-2.2** and **Fig. S4**. The obtained results show the role of surfactants and growth time in modulating crystallinity, stacking faults, and interfacial strain. The Raman spectra of pristine Bi₂Te₃ and Bi₂Te₃/Ti₃C₂T_x composite were recorded in the range 80-1000 cm^{–1} with fitting carried out using multi-peak Lorentzian functions (**Fig. 2a-b and Table S2**). The synthesized Bi₂Te₃ crystallizes in the rhombohedral *R*-3*m* space group, and group theory predicts 15 vibrational modes at the Brillouin zone center:

$$\Gamma = 2\Gamma_1^+ (A_{1g}) + 2\Gamma_3^+ (E_g) + 3\Gamma_2^- (A_{2u}) + 3\Gamma_3^- (E_u)$$

Of these, the acoustic $\Gamma_2^-(A_{2u})$ and $\Gamma_3^-(E_u)$ modes leave four Raman-active vibrations: E_g^1 , A_1g^1 , E_g^2 , and A_1g^2 , expected near 36.5, 62.0, 102.3, and 134.0 cm^{–1}, respectively [25–27]. In our measurements, two prominent modes were observed at ~ 122 cm^{–1} (A_1u^1 , nominally infrared-active but Raman-allowed under broken symmetry) and 148 cm^{–1} (A_1g^2), consistent with prior reports. The absence of low-frequency E_g modes is attributed to the experimental cutoff (> 100 cm^{–1}). The A_1u^1 mode, forbidden in

bulk but activated in thin flakes and defect-rich systems, arises due to loss of translational symmetry and surface disorder, implying nanoscale structural inhomogeneity. Upon the MXene incorporation, this mode exhibits a distinct blue shift, indicating the interface-induced local strain and charge redistribution. The A_{1g}^2 mode, which is associated with out-of-plane vibrations of Bi and Te atoms along [111], also shows a blue shift and narrowing of FWHM in the composite, accompanied by enhanced intensity. These features signify phonon hardening and reduced scattering, attributed to compressive interfacial strain and strong $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ coupling. Two additional high-frequency bands at ~ 652 and 748 cm^{-1} are observed in the pristine Bi_2Te_3 , which is commonly associated with surface oxides such as Bi_2O_3 or TeO_2 . Their intensities are drastically suppressed ($> 50\%$) in the composite, indicating that MXene effectively mitigates surface oxidation by stabilizing Bi_2Te_3 against ambient degradation. Collectively, the room-temperature Raman results reveal that the MXene incorporation modifies vibrational symmetry through strain and disorder, enhances lattice coherence, and passivates surface oxidation, resulting in tailoring the local phonon environment for improved stability and electronic coupling.

Temperature-dependent Raman spectra were acquired to probe phonon dynamics and thermal stability. The Raman spectra for the pristine Bi_2Te_3 in Fig. 2c reveal that low-frequency modes exhibit phonon softening and merging above 380 K, reflecting the enhanced phonon-phonon scattering and diminished vibrational coherence. Concurrently, the high-frequency oxide-related band at $\sim 680\text{ cm}^{-1}$ broadens and vanishes beyond 400 K, which is consistent with the surface disordering. The intense A_{1g}^2 peak progressively broadens and weakens its intensity with the increase of temperature, indicating typical anharmonic effects and reduced phonon lifetime. In contrast, the Raman spectra of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite in Fig. 2d exhibits superior phonon stability. The A_{1g}^2 mode at 148 cm^{-1} remains the most intense across the entire temperature window with only a mild blue shift on the increase of temperature, which is consistent with residual compressive strain and interfacial phonon stiffening. Notably, the higher-order bands at ~ 650 and 748 cm^{-1} display unconventional behaviour, where the 650 cm^{-1} mode intensifies up to 385K before plateauing, while the 748 cm^{-1} mode remains nearly constant, both maintaining higher stability than in pristine Bi_2Te_3 . This anomalous enhancement suggests the temperature-activated interfacial coupling, where MXene facilitates charge redistribution that selectively modulates Raman activity. The comparative analysis thus demonstrates that the MXene incorporation suppresses the anharmonic phonon softening, stabilizes Raman-active modes against thermal disorder, and sustains phonon coherence over an extended temperature range. Functionally, these effects imply the improved electron-phonon coupling, lower non-radiative recombination losses, and enhanced vibrational resilience under catalytic and thermoelectric operating conditions. The temperature-dependent Raman response therefore provides compelling indirect evidence of MXene-mediated structural stabilization and interfacial charge transfer in the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite. A comprehensive Raman analysis is further provided in **Note S2.3-2.4**, including symmetry assignments, forbidden mode activation, surface oxide contributions, and detailed temperature-dependent phonon evolution of both Bi_2Te_3 and $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites. These extended discussions further elaborate on interfacial

strain effects, defect-induced vibrational activity, and correlations to catalytic and electronic functionality.

Magnetic measurements are crucial for understanding the presence of defect-induced or interface-driven magnetic ordering, which can influence the electronic structure, spin-dependent transport, and potentially enhance performance in electrocatalytic applications such as HER and OER. Room-temperature magnetization (M-H) measurements were performed in the field range of ± 70 kOe for both pristine Bi_2Te_3 and the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites. In both products, the magnetic response is predominantly diamagnetic due to the linear decrease in magnetization with increasing field (**Fig. S5a**). However, a small hysteresis loop centered at the origin is clearly observed, which shows the presence of a weak ferromagnetic (FM) contribution superimposed on the diamagnetic background. To isolate this ferromagnetic component, a diamagnetic correction was carried out by subtracting a linear fit for the pure diamagnetic response from the high-field regions of the M-H curve. This method effectively reveals the intrinsic magnetic contribution arising from non-linear components. The obtained results reveal that the estimated saturation magnetization (M_s) values are 0.007 emu/g for Bi_2Te_3 and 0.0044 emu/g for the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites (**Fig. S5b**). The origin of the weak ferromagnetism in Bi_2Te_3 is likely defect-induced, arising from antisite disorder, vacancies, or surface states that locally break time-reversal symmetry and introduce uncompensated magnetic moments [28]. In nanostructured or few-layered forms of Bi_2Te_3 , these effects are often amplified due to increased surface-to-volume ratio and reduced symmetry, enabling spin polarization even in otherwise nonmagnetic matrices. In the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite, although a slight reduction in M_2 is observed, the persistence of ferromagnetic character suggests an interfacial role possibly from strain, charge transfer, or orbital overlap between Bi_2Te_3 and $\text{Ti}_3\text{C}_2\text{T}_x$ MXene layers. The observed suppression could also be from screening effects due to the high electrical conductivity and strong diamagnetism of the MXene phase. These findings show the delicate interplay between structural defects, dimensionality, and interfacial effects in tuning magnetic behavior.

X-ray photoelectron spectroscopy (XPS) studies were performed to identify the individual elements and their oxidation states of prepared products. The survey XPS spectra (0 to 1100 eV) present the individual elements whereas the detailed study of individual elemental peaks shows the oxidation states and the involved bonds within the atoms/ions on fitting by Gaussian-Lorentzian components and the carbon standard (C1s) taken at 284.6 eV was adopted to calibrate the data (**Table S3**). The survey XPS spectra of pristine Bi_2Te_3 shows the existence of Bi 4f, Te 3d, and its $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite shows additional C 1s, O 1s, F 1s, and Ti 2p peaks (**Fig. S6a**). The high resolution XPS spectra of Bi 4f and Te 3d for Bi_2Te_3 are presented in Fig. 3a-b, respectively. The peak atomic % for Bi and Te elements are obtained to be 37.7 and 63.7% that agrees with the Bi_2Te_3 phase. The narrow range XPS spectra of Bi 4f is fitted to a doublet (7/2 and 5/2) at 5.4 eV apart. The peaks at 157.6 eV and 163.0 eV correspond to the +3-oxidation state which corresponds to the Bi_2Te_3 phase and the pre-peaks within the 7/2 and 5/2 could be attributed to surface defects during sample processing [29, 30]. The Te 3d spectra for Bi_2Te_3 is fitted to two sub peaks where one of them represents the Bi_2Te_3 phase, centered at 571.3 eV and 581.3 eV,

corresponding to $\text{Te}^{2-} 3d_{5/2}$ and $\text{Te}^{2-} 3d_{3/2}$, respectively, while additional peaks around 574 and 585 eV indicate surface oxidation that becomes unavoidable during sample treatment during analysis [31–34]. Additionally, the doublets of Bi 5d and Te 4d peaks are also observed at lower energy regions (**Fig. S6b**). The Bi 4f peaks for $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite shift towards higher binding energy to an extent of 0.1 eV along with rise of an additional Bi-O peak which obviously appears due to the interaction with MXene. A similar shift of core Te 3d peaks is observed along with the intense Te-O as the result of composite formation. The corresponding Ti 2p, O 1s, C 1s, and F 1s peaks for $\text{Ti}_3\text{C}_2\text{T}_x$ MXene and $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite are fitted to corresponding spin coupled doublets as shown in Fig. 3c-f. Due to variation of electronic environment of the attached atoms by the composite formation, the peak position and FWHM of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite differ from pristine $\text{Ti}_3\text{C}_2\text{T}_x$. This interaction between Bi_2Te_3 and $\text{Ti}_3\text{C}_2\text{T}_x$ phase explains the distortion of Van der Waals gaps of Bi_2Te_3 phase the composite. The distortion of Bi_2Te_3 in composite is further understood from the growth pattern of the composite where the material surface is etched till 20th level with 100 nm interval (**Fig. S7**). Depth XPS profiles for Bi_2Te_3 and $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite were further measured and the results are presented in **Fig. S7 and S8**. The XPS depth profile survey spectrum (atomic %) of Bi_2Te_3 shows the core level peaks of Bi 4f (158.8 eV, $\Delta E = 5.3$ eV) and Te 3d (572.2 and 576.0 eV, $\Delta E = 12.5$) which did not vary drastically with increase of the depth etching time. The intensity of Te 3d emission gradually increases at the beginning of the sputtering, and then it does not change much as the sputtering time goes. However, the peak intensities in Bi 4f spectra decreases after initial few etchings indicating Bi to be more exposed at the surface than Te, which is also evident as the metal center acted as redox active sites. On the other hand, the spectra of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite shows a drastic shift in peak position as well as peak intensity of Bi 4f and Te 3d from surface to bulk. It is observed that with the increase in etching level, the Bi 4f and Te 3d peak positions in the composite aligned with that of pristine Bi_2Te_3 . **Note S3** briefs high-resolution XPS analysis of Bi_2Te_3 and $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites, including oxidation state assignments, binding energy shifts, peak broadening mechanisms (Franck-Condon effects, frozen orbital approximation), and ligand-field-induced orbital mixing. These results demonstrate the defect-induced perturbations in pristine Bi_2Te_3 and the enhanced covalency and Bi-O hybridization upon composite formation.

Transmission electron microscopy (TEM) images of pristine Bi_2Te_3 in Fig. 4a exhibit the uniform rhombohedral nanosheets structure with sharp hexagonal faceting. Statistical evaluation of lateral dimensions of pristine Bi_2Te_3 indicates a narrow distribution between 400–550 nm, centered at ~ 480 nm, while thickness remains below 35–40 nm, consistent with quasi-2D platelets. High-resolution TEM (HRTEM) image reveals the single-crystalline nature of pristine Bi_2Te_3 with the clear lattice fringes of $d = 0.32$ nm (015) and $d = 0.22$ nm (110), indexed to rhombohedral Bi_2Te_3 ($R\bar{3}m$). The lattice fringes are also observed in coherently across large domains with minimal evidence of defects. These results are consistent with the sharp and spot-like SAED patterns, indexed to (110), (015), and (202) planes, which indicates the phase purity and highly ordered long-range stacking of synthesized Bi_2Te_3 . Also, this

defect-scarce nanosheets of Bi_2Te_3 are expected to exhibit low surface reactivity but superior thermoelectric transport due to minimal scattering.

In contrast, TEM images of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite in Fig. 4b reveal a distinct nucleation and growth pathway. It can be evident that Bi_2Te_3 nanosheets with the reduced lateral size to 200–350 nm are uniformly anchored on the $\text{Ti}_3\text{C}_2\text{T}_x$ nanosheets and frequently appear as secondary nanocrystallites decorating the sheet edges. This anchoring is driven by the surface terminations ($-\text{O}$, $-\text{OH}$, $-\text{F}$) of the MXene, which strongly chelate Bi^{3+} ions during hydrothermal synthesis. This coordination effectively lowers the nucleation barrier and pins the crystal growth to the 2D substrate, preventing excessive grain growth. HRTEM imaging of the interface reveals maintained lattice continuity within the Bi_2Te_3 domains, although marked by local distortions and strain fields at the junction with $\text{Ti}_3\text{C}_2\text{T}_x$. While the measured d -spacings are consistent with the rhombohedral Bi_2Te_3 phase, the presence of localized bending and edge dislocations provides clear evidence of epitaxial mismatch-induced strain. Furthermore, the SAED patterns of the composite exhibit overlapping features of sharp spots and diffuse rings, attributed to the superposition of highly crystalline Bi_2Te_3 domains and the surrounding nanocrystalline decorations. The TEM analysis confirms that the Bi_2Te_3 nanosheets are not merely surface-adsorbed, instead, they are embedded and conformally wrapped across the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene terraces, establishing intimate 3D interfacial contact. In addition, the field emission scanning electron microscope (FE-SEM) measurement shows a clear morphological evolution from pristine Bi_2Te_3 hexagonal nanosheets of 450–600 nm with smooth basal planes to $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites characterized by reduced platelet sizes of 200–450 nm and robust sheet-on-sheet anchoring (**Fig. S9 and Note S4**). From the corresponding elemental mapping analysis, the uniform distribution of Bi, Te, Ti, C, O, and F elements verifies the strong interfacial integration within the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite (**Fig. S10 and S11**). This morphological refinement optimizes interfacial contact and prevents restacking, facilitating the formation of defect-rich sites without compromising phase purity. The resulting interfacial strain and structural defects in the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites are essential for multi-functional enhancement. On one hand, the elevated density of edge dislocations and grain boundaries provides unsaturated coordination sites, acting as potent active centers for redox reactions. Simultaneously, the junction-induced lattice strain modulates the local electronic environment, fostering superior charge carrier mobility and efficient phonon scattering. Beyond these structural benefits, the direct anchoring of Bi_2Te_3 on MXene sheets enables optimal orbital overlap and accelerated interfacial charge transfer, which can significantly improve conductivity while mitigating nanoparticle aggregation. Ultimately, this integrated anchoring-decoration synergy of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite provides a robust foundation for both structural integrity and enhanced functional performance. The time-of-flight secondary ion mass spectrometry (TOF-SIMS) analysis was further performed for surface and depth-resolved ion spectra, oxidation layer estimation, quintuple-layer modulation signatures, and 2D chemical mapping of Bi_2Te_3 and $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites (**Note S5, Fig. S12, and Table S4**). The obtained TOF-SIMS results demonstrate that the incorporation of MXene effectively suppresses surface oxidation while improving both Bi/Te stoichiometric uniformity and overall chemical homogeneity.

Electrocatalytic measurements

The electrocatalytic activity of the synthesized $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composites was explored toward the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR). The electrocatalytic measurements were carried out using a typical three-electrode system. The prepared $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ catalyst ink was drop-casted on a glassy carbon working electrode (WE) and a graphite rod and Hg/HgO were used as the counter electrode (CE) and reference electrode (RE), respectively. A commercial 20% Pt/C catalyst was also tested under identical conditions for comparison. Figure 5 presents the polarization curves and Nyquist plots of prepared catalysts for HER, OER, and ORR. While the synthesized Bi_2Te_3 exhibits notable catalytic performance owing to its layered single-crystal structure and Van der Waals gaps, it is clearly observed that the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite demonstrates improved catalytic activity (**Fig. S13a-b**). The $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite delivers an overpotential of 260 mV to achieve the current density of $100 \text{ mA}\cdot\text{cm}^{-2}$ (j_{100}), compared to 370 mV for pristine Bi_2Te_3 . The corresponding Tafel slope analysis further supported this improvement. The pristine Bi_2Te_3 showed a Tafel slope of $272 \text{ mV}\cdot\text{dec}^{-1}$, while $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite shows the Tafel slope of $127 \text{ mV}\cdot\text{dec}^{-1}$ with the increased kinetic rate due to the incorporation with $\text{Ti}_3\text{C}_2\text{T}_x$, which outperforms a commercial Pt/C catalyst ($212 \text{ mV}\cdot\text{dec}^{-1}$). The observed Tafel slopes of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite for HER suggest that the Volmer step is rate-limiting in our case, though at higher overpotentials, the contribution of the Heyrovsky step cannot be excluded due to enhanced surface coverage. Electrochemical impedance spectroscopy (EIS) provided further insight into the charge transfer properties. The $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite exhibits the lowest charge transfer resistance (R_{ct}) of 3.0Ω , compared to Bi_2Te_3 (7.7Ω) and Pt/C (14.2Ω), indicating the superior electron transport of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite at the electrode-electrolyte interface. Moreover, the composite achieves a high turnover frequency (TOF) of 0.07 s^{-1} at 100 mV (**Fig. S13c**). The mechanistic pathway of HER on $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ was investigated by monitoring the XPS analyses of post-HER. The Te-surface termination of Bi_2Te_3 is known to exhibit poor water adsorption affinity, resulting in the inherently slow HER kinetics of Bi_2Te_3 [35]. Upon the introduction of $\text{Ti}_3\text{C}_2\text{T}_x$ into the system, as observed by XPS depth profile results, the partial surface oxidation of Bi_2Te_3 occurred, resulting in a partial Bi-O surface termination. This structural modification of Bi_2Te_3 promotes the adsorption of water at the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite catalyst surface, which is a critical step for enhancing reaction kinetics. The catalytic process subsequently progresses through the simultaneous migration of intermediates across the Bi and Te surfaces. As presented in **Fig. S14**, while the unaltered elemental peaks are observed for $\text{Ti}_3\text{C}_2\text{T}_x$, the noticeable change on the Bi 4f and Te 3d peaks for Bi_2Te_3 suggests that the MXene does not participate directly in the HER process as an active site. Instead, it serves as a structural scaffold that modulates the surface environment of Bi_2Te_3 to boost electrocatalytic activity. To assess the practical applicability of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite catalyst, its long-term stability was evaluated using the chronoamperometry (CA) over a period of 100 h. As shown in **Fig. S13d**, the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite exhibits excellent stability, maintaining nearly 98% of its initial

current density at an overpotential of 100 mV after 100 h of continuous operation. Further FE-SEM and Raman analysis for post-HER also demonstrate that the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite preserved its aggregated morphology and crystalline structure (**Fig. S13e-f**), and the significant Raman characteristics peaks remain unaltered after HER test with minor peak shifts and moderate broadening, especially in the high-frequency range ($\sim 1520\text{--}1556\text{ cm}^{-1}$). These results indicate the presence of surface strain in $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite caused by hydrogen adsorption without any structural degradation for enhanced HER activities.

The electrocatalytic activities of the prepared catalysts toward the OER were evaluated using a 0.1 M KOH electrolyte. As shown in the OER polarization curves (Fig. 5d), the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite delivers an overpotential of 490 mV at current density of $100\text{ mA}\cdot\text{cm}^{-2}$, which is significantly lower than those of pristine Bi_2Te_3 (570 mV) and commercial IrO_2 (620 mV) (**Fig. S15a-b**). The relationship between overpotential and current density was further analyzed through the Tafel slope values (Fig. 5e). The composite exhibits faster reaction kinetics, yielding the Tafel slope of $112\text{ mV}\cdot\text{dec}^{-1}$, compared to $179\text{ mV}\cdot\text{dec}^{-1}$ for pristine Bi_2Te_3 and $83\text{ mV}\cdot\text{dec}^{-1}$ for commercial IrO_2 . These Tafel slope values provide insight into the electron transfer coefficient ($\alpha = \frac{2 \cdot 303RT}{bF}$) as a key descriptor for reaction kinetics [36]. This suggests that the first electron transfer step may reside at a quasi-equilibrium state for Bi_2Te_3 and composite, implying that this initial step serves as the rate-determining step. The facilitated reaction kinetics are further supported by charge transfer resistance (R_{ct}) values obtained from EIS analysis, as presented in Fig. 5f. The $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite displayed the lowest R_{ct} ($5.3\ \Omega$), followed by commercial IrO_2 ($10.2\ \Omega$) and pristine Bi_2Te_3 ($19.6\ \Omega$). Additionally, the turnover frequency (TOF) values were calculated across various overpotentials to quantify the efficiency of feed-to-product conversion. The $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite demonstrates the highest TOF values among all synthesized materials (**Fig. S15c**), confirming its superior catalytic efficiency and robust performance for oxygen evolution. To explore the reaction mechanism on the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ surface, the evolution of binding energies (BEs) during the OER process was investigated. In an alkaline medium, the OER proceeds through the transformation of OH^- to O_2 , a complex process involving the removal of eight electrons and the formation of molecular oxygen with two unpaired π -electrons. This multi-step pathway generates several adsorbed intermediates, specifically $^*\text{OH}$, $^*\text{O}$, and $^*\text{OOH}$. During the chemisorption, these electron-deficient intermediates draw electrons from the catalyst surface, consequently, the factors, including spin configuration, crystal field splitting of the active metal centers, and the local electronic structure, collectively dictate the reaction kinetics. This mechanistic shift was further validated by the XPS analysis of the Bi 4f and Te 3d regions for post-OER (**Fig. S14**). The appearance of an additional Bi-O peak in the Bi 4f spectrum and a reduced Te-C to Te-O ratio in the Te 3d spectrum points toward direct Te-O interactions. These spectral evolutions suggest that oxygen intermediates diffuse across the Bi-Te framework, inducing the localized surface oxidation during the OER process. The catalytic robustness and durability of the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite are confirmed via the chronoamperometry (CA) studies, and the obtained results demonstrate nearly 98% retention of current density over 100 h of continuous OER operation (**Fig. S15d**). The stability analysis for post-OER further verifies the preservation of both

morphological integrity and electronic structure, implying the exceptional long-term stability of the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite under demanding OER conditions (**Fig. S15e-f**). In addition, after the OER test, a noticeable increase in peak broadening and intensity is observed in the defect-related Raman bands ($\sim 1338\text{--}1421\text{ cm}^{-1}$), which can be attributed to the partial surface oxidation and the structural reconstruction of the $\text{Ti}_3\text{C}_2\text{T}_x$. Nevertheless, the persistent presence of Bi-Te and Ti-C related modes, alongside the absence of new impurity phases, confirms that the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ heterostructure successfully maintains its core structural integrity. The electrochemically active surface area (ECSA) was evaluated by estimating the double-layer capacitance (C_{dl}) and specific capacitance (C_s). The calculated ECSA values exhibit a significant increase from pristine Bi_2Te_3 to the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite (**Fig. S16a** and **Table S5**). This increase of active sites is primarily attributed to the formation of the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ heterointerface, which induces partial surface oxidation and lattice phase mismatch (**Fig. S16b**). To assess the intrinsic catalytic activity, the current densities were normalized to the ECSA. As illustrated in **Fig. S16c-d**, the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite sustains higher normalized current densities at lower overpotentials, confirming its superior intrinsic activity for both the HER and OER. These findings present the critical role of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene scaffold in promoting efficient electron transfer and significantly enhancing reaction kinetics beyond a mere increase in physical surface area. These findings demonstrate that the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite exhibits efficient bifunctional electrocatalytic activity for both HER and OER. The mechanistic analysis suggests a site-specific catalytic behavior, where the HER predominantly occurs at Bi sites, while the Bi-Te framework plays a pivotal role in driving the OER. Although the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene layer does not directly participate in redox transformations of HER, it serves as a critical functional support by significantly enhancing the electroactive surface area and facilitating accelerated mass transport. Furthermore, the MXene integration provides essential structural stability by mitigating metal leaching under highly alkaline conditions, ensuring long-term durability [38]. Upon composite formation, the Bi-Te bond distance undergoes subtle variations accompanied by increased lattice strain. This structural modulation highlights the potential for enhanced chemisorption, as it alters the orbital occupancy and electronic states relative to the Fermi level, thereby optimizing the energetics for efficient water splitting [39–41]. A detailed explanation on two electrode systems is briefed in **Note S6** and illustrated in **Fig. S17a-d** and summarized in **Table S6**.

The oxygen reduction reaction (ORR) activity of the materials was evaluated in a three-electrode setup using 0.1 M KOH as the electrolyte (**Table S7**). Figure 5g presents the LSV curves for ORR recorded at a rotation speed of 1600 rpm and a scan rate of 5 mV s^{-1} . In the initial kinetically controlled region, the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite exhibits a characteristic exponential rise in current density with potential. The onset potential (E_{onset}) for ORR was measured to be 0.81 V for the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite, which is more positive than that of pristine Bi_2Te_3 (0.78 V), though lower than the benchmark Pt/C (0.97 V). This shift toward a more positive E_{onset} suggests a more facile ORR process occurring on the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite surface. Furthermore, the half-wave potential ($E_{1/2}$), which serves as a key indicator of catalytic efficiency in the kinetic diffusion-controlled region, is 0.68 V for the composite, compared to

0.64 V for pristine Bi_2Te_3 . While Pt/C maintains a superior $E_{1/2}$ of 0.84 V, these results demonstrate that the incorporation of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene effectively enhances the ORR performance of Bi_2Te_3 by optimizing the electronic environment and increasing active site availability. The Tafel slope analysis in Fig. 5h reveals a significantly faster reaction rate for the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite compared to pristine Bi_2Te_3 , showing the enhanced catalytic activity of composite catalyst. This catalytic improvement of composite is further investigated by the electrochemical impedance spectroscopy (EIS). The calculated R_{ct} values are found to be 153 Ω for the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite, which is remarkably lower than those of pristine Bi_2Te_3 (298 Ω) and Pt/C (301 Ω) (Fig. 5i), indicating substantially improved charge transport facilitated by MXene integration. The electron transfer number (n) derived from the Koutecky–Levich (K–L) plots (**Fig. S18**) approaches 4 for the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite. These results present a dominant four-electron pathway for $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite where H_2O is the primary product, although a minor amount of H_2O_2 (up to $\sim 20\%$) is detected as a byproduct. Furthermore, the chronoamperometric ORR test for $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite conducted over 12 h exhibit the robust durability of the composite, which retains approximately 96% of its initial current density at an applied potential of 0.6 V. These findings highlight the efficient kinetic performance and exceptional stability of the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ heterostructure under ORR process. Although the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite does not exceed the ORR performance of benchmark Pt/C, the implementation of heterojunction engineering markedly enhances the catalytic activity of Bi_2Te_3 . This improvement is primarily attributed to the favorable band alignment at the interface in the composite, which facilitates efficient electron transfer and optimizes the oxygen binding energy. Additionally, the unique architecture minimizes site blockage through enhanced mass transport across the Bi-Te skeleton. Since the ORR and OER share similar active sites and oxygen intermediates, despite proceeding in opposite directions [42], it is confirmed that the Bi-Te framework serves as the primary active center for both reactions (**Fig. S19**). In addition, the robust ORR performance of the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ heterostructure further demonstrates its significant potential as a high-performance air cathode material for next-generation energy storage systems, such as lithium-ion or metal-air batteries.

Alongside the excellent electrocatalytic activities for HER, OER, and ORR, the $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite was further evaluated as an anode material for both Li-ion and Na-ion batteries. The galvanostatic charge-discharge profiles (Fig. 6a-b) reveal clear signatures of a conversion-type storage mechanism, where the telluride phase undergoes reduction into metallic Bi nanoparticles dispersed within $\text{Li}_2\text{Te}/\text{Na}_2\text{Te}$ matrices during discharge, followed by partial reformation during charging. The first discharge cycle delivers high capacity, although the Coulombic efficiency remains below 70% due to SEI formation and irreversible ion trapping. From the subsequent cycles, the voltage profiles become more stable, indicating improved reversibility and gradual stabilization of the electrode/electrolyte interface. The Li-ion system exhibits higher reversible capacity and better capacity retention than the Na-ion counterpart, mainly because of the smaller ionic radius and faster diffusion kinetics of Li^+ . In contrast, the larger Na^+ ion induces greater structural strain and volume variation during cycling. Rate capability and long-term cycling results (Fig. 6c-f) further confirm the robust electrochemical behavior of the

$\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ heterostructure, where the conductive MXene matrix enhances charge transport, buffers mechanical stress, and stabilizes the interface. Complete electrochemical interpretation and detailed reaction mechanisms are provided in **Note S7**.

Conclusion

In summary, we successfully developed a robust $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ heterostructure that overcomes the inherent limitations of bulk TIs through precise interface engineering. The incorporation of MXene not only enhances electronic conductivity and intercalation mobility but also provides a defect sink that reduces dislocation density while introducing beneficial anisotropic strain. Detailed Raman and XPS analyses confirm that the MXene phase passivates surface oxidation and stabilizes the Bi_2Te_3 lattice against thermal disorder, maintaining phonon coherence over an extended temperature range (up to 788 K). Functionally, the composite exhibits exceptional electrocatalytic activities for HER, OER, and ORR, and also high reversible capacity for Li/Na-ion batteries, supported by rapid ion/electron kinetics at the engineered interfaces. These findings demonstrate that precisely controlled 2D heterojunctions can dictate material properties more effectively than traditional chemical doping, offering a versatile framework for designing next-generation, high-efficiency energy materials.

Declarations

Author contributions

T.S.K.S: Writing – original draft, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. B.M.B: Methodology, Investigation. J.J: Validation, Investigation. L.S: Methodology, Investigation. R.K: Formal analysis. Y.L: Resources, Investigation. S.H.H: Resources, Methodology. T.J.S: Resources. J.S.C: Funding acquisition, Investigation, Writing – review & editing. W.M.C: Writing – review & editing, Supervision, Resources, Funding acquisition.

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Conflicts of interest

There are no conflicts of interest to declare.

Ethics approval and consent to participate

Not applicable

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Scheme 1

Scheme 1 is available in the Supplementary Files section.

Figures

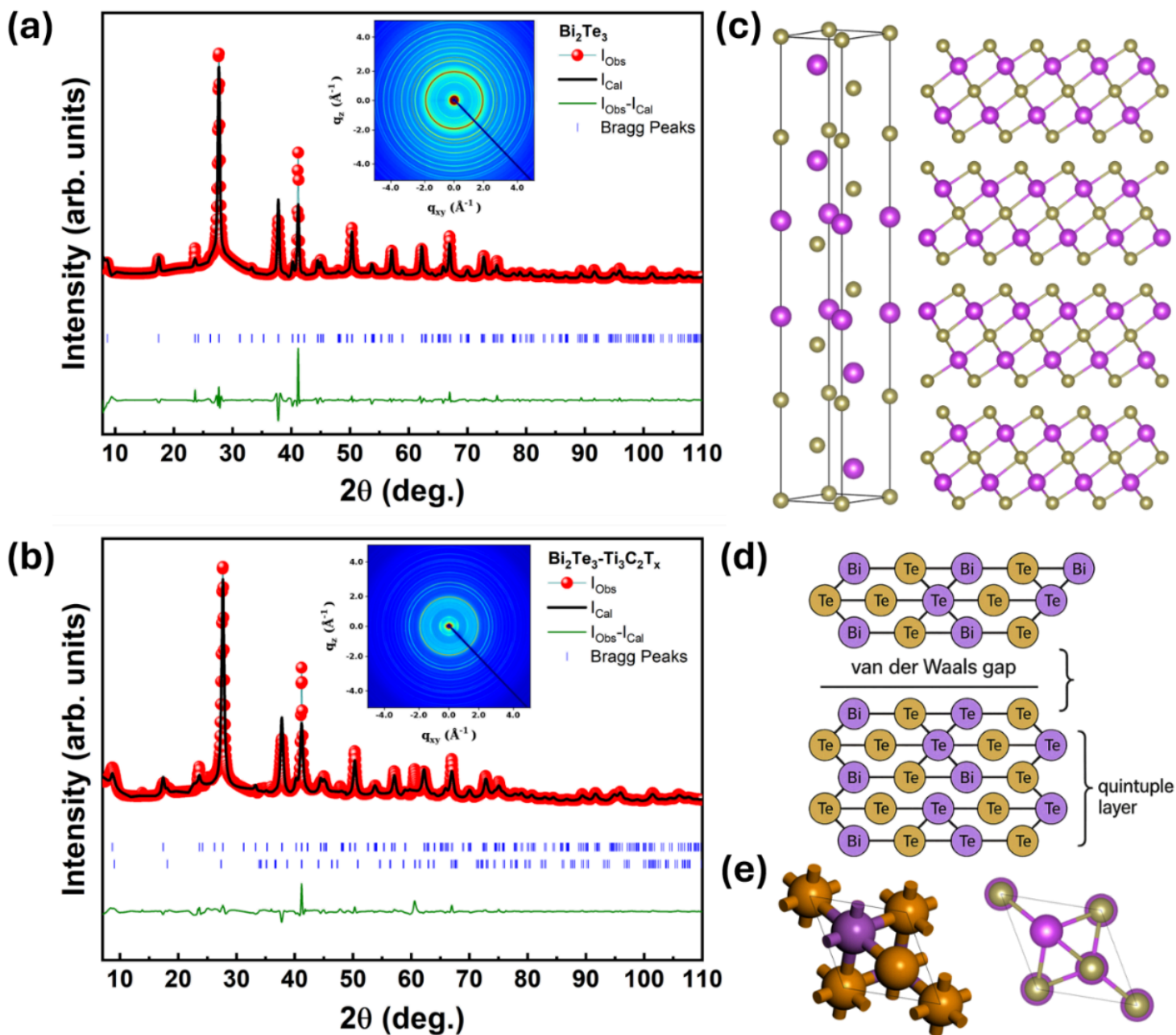


Figure 1

Rietveld refinement XRD patterns of (a) Bi_2Te_3 , (b) $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite, (c) crystal structure of Bi_2Te_3 , (d) schematic illustration of Van der Waals gap observed, and (e) polyhedral formation of Bi-Te atoms observed in Bi_2Te_3 .

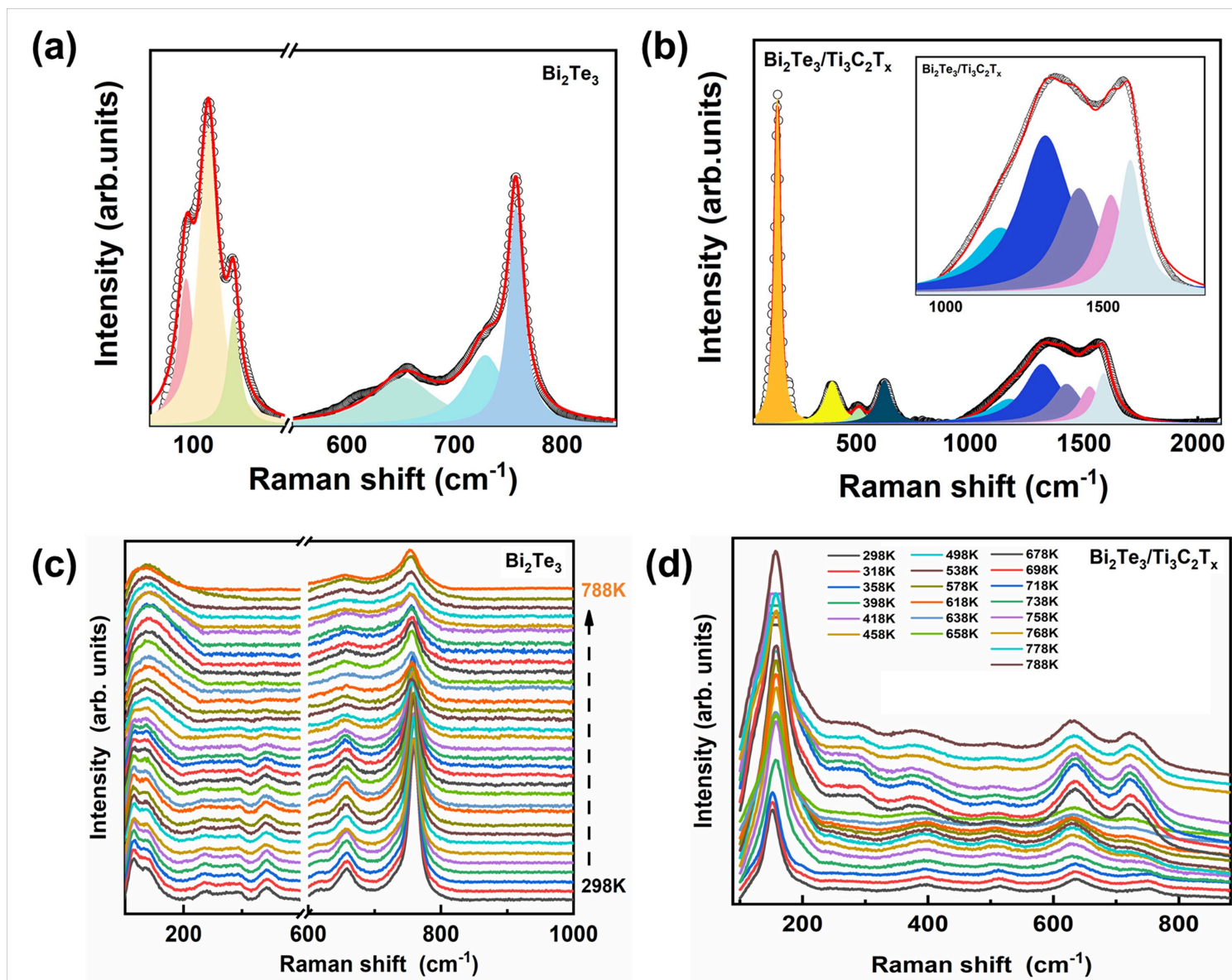


Figure 2

(a, b) Lorentzian peak-fitting of Raman spectra at room and (c, d) temperature-dependent Raman spectra from 298 to 788 K for Bi_2Te_3 and $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ composite.

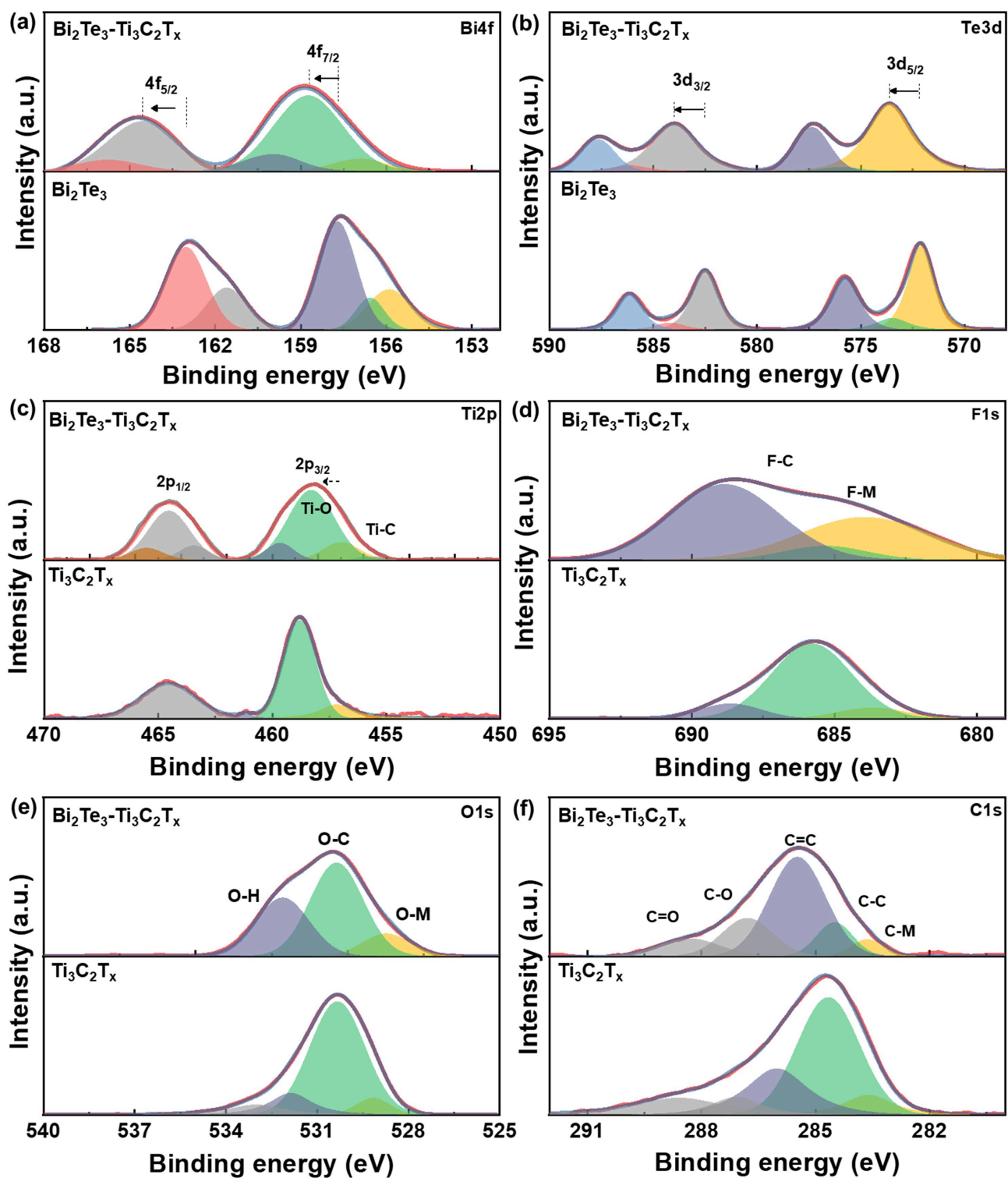


Figure 3

Narrow range comparative XPS spectra of elemental (a) Bi 4f, (b) Te 3d, (c) Ti 2p, (d) F 1s, (e) O 1s, and (f) C 1s of $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ and pristine Bi_2Te_3 as well as $\text{Ti}_3\text{C}_2\text{T}_x$.

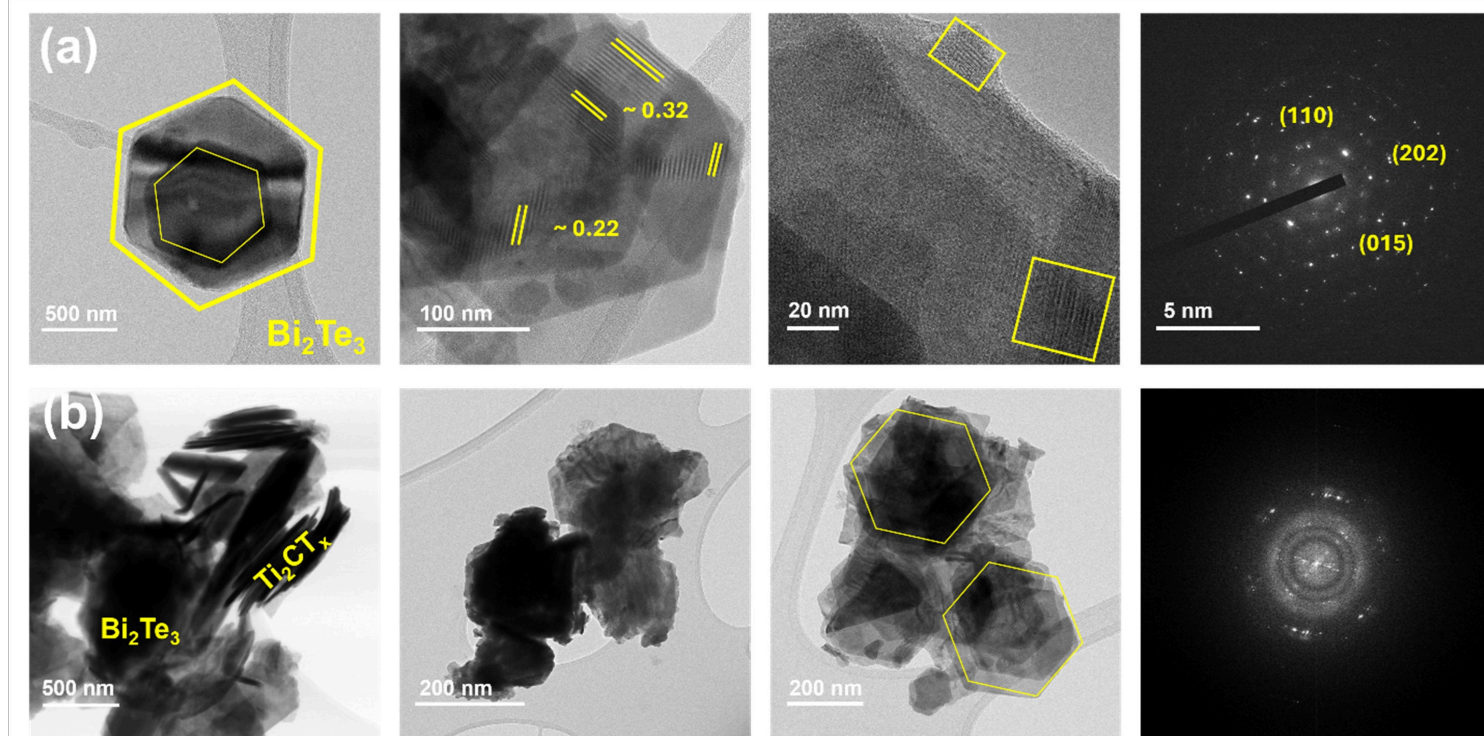


Figure 4

TEM images, lattice fringes and SAED patterns of (a) Bi_2Te_3 , and (b) $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$

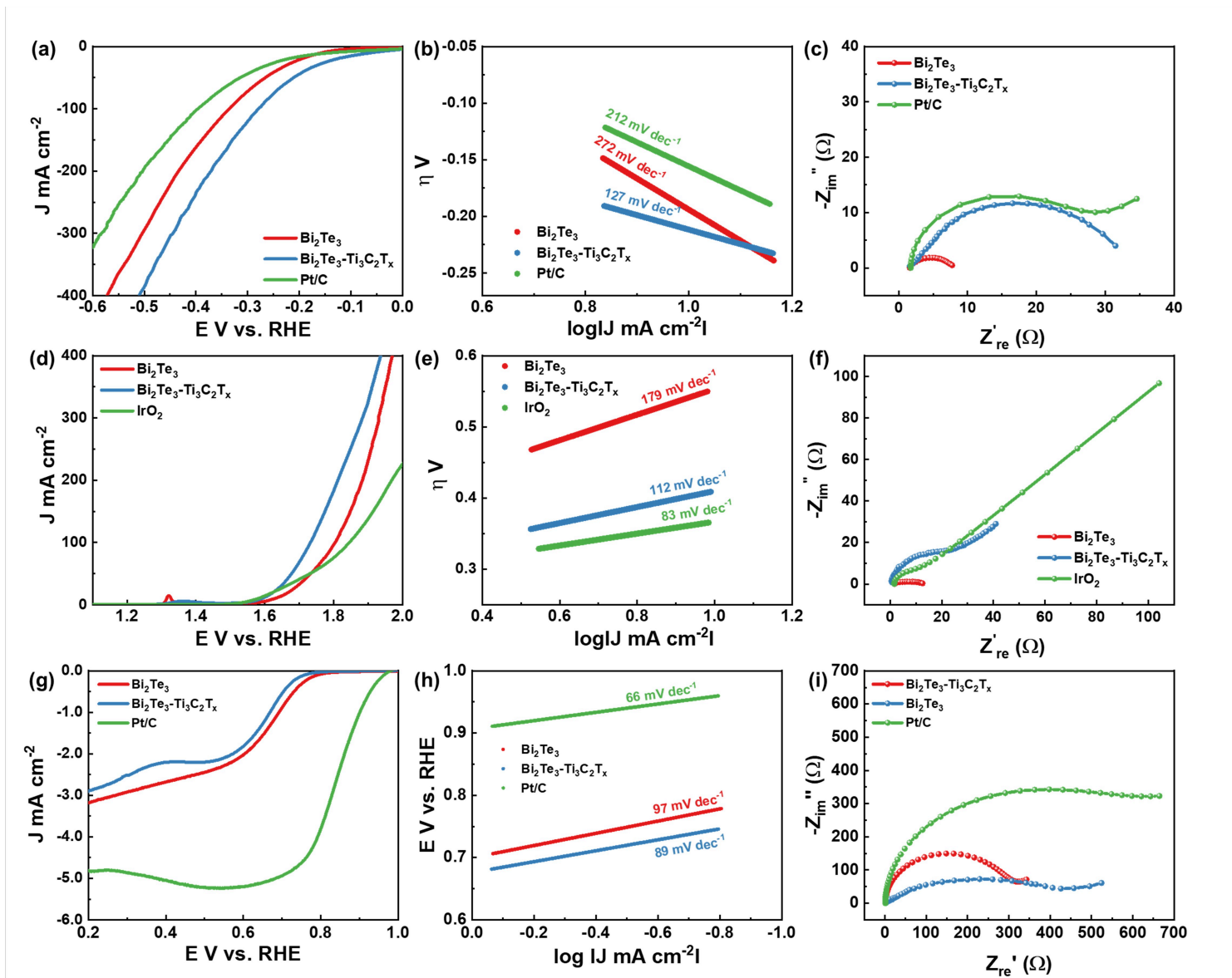


Figure 5

Polarization curves (a, d, g), Tafel slopes (b, e, h) and Nyquist plots (c, f, i) for HER, OER, and ORR on telluride materials and commercial working electrodes in a three-electrode system with graphite rod as counter and Hg/HgO as reference electrode in 0.1 M KOH electrolyte.

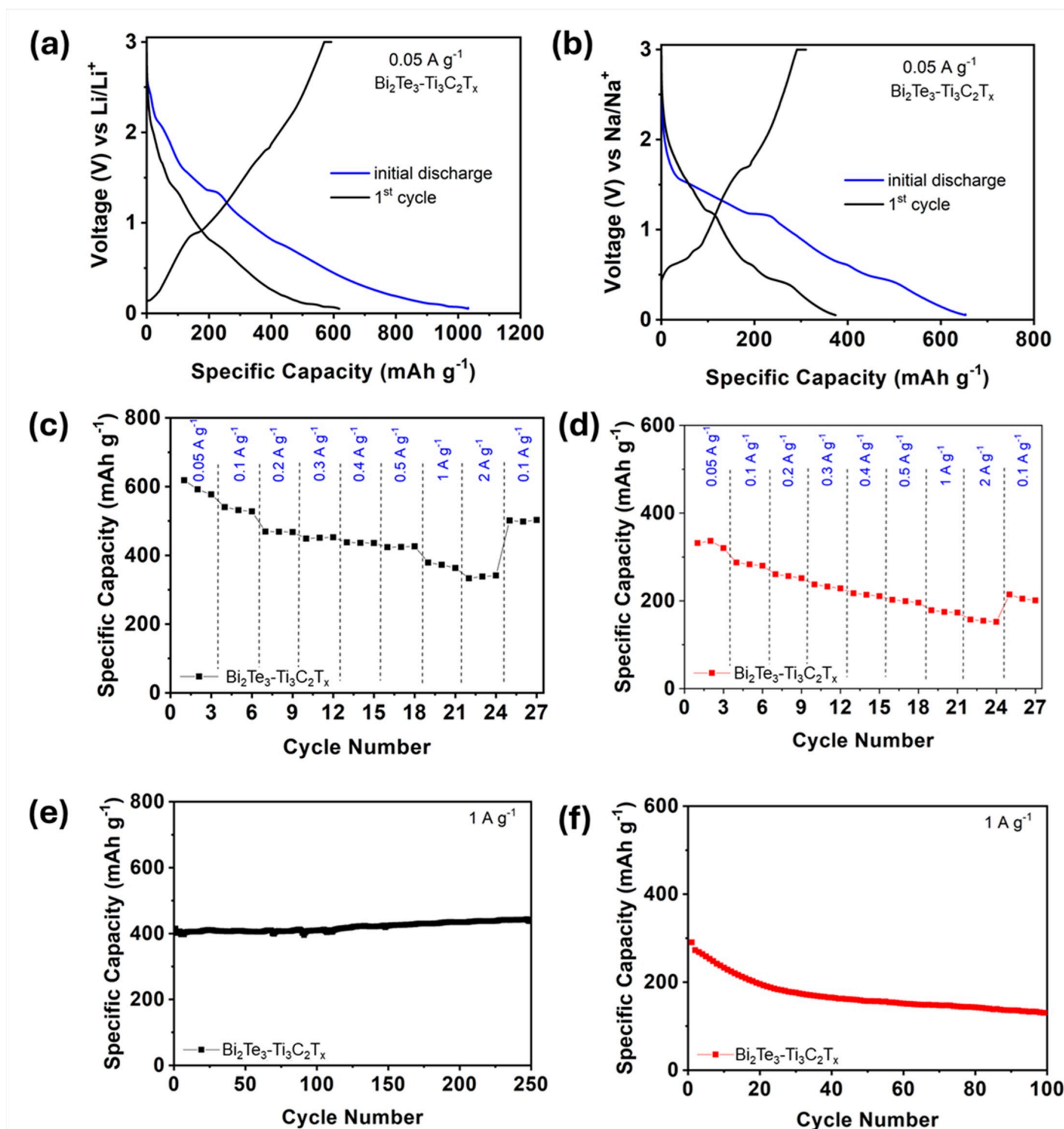


Figure 6

Galvanostatic charge/discharge profiles vs (a) Li/Li^+ and (b) vs Na/Na^+ using $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$. Rate performance for Li- and Na-ion battery using $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ for (c) Li- and (d) Na-ion batteries. Long term cycling performance of the anode materials $\text{Bi}_2\text{Te}_3/\text{Ti}_3\text{C}_2\text{T}_x$ for (e) Li-ion and (f) Na-ion batteries.

Supplementary Files

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