

Mixed-phase TiO₂ as an intrinsic polarization engine to amplify multi-level interfacial synergy for high-performance electromagnetic wave absorption

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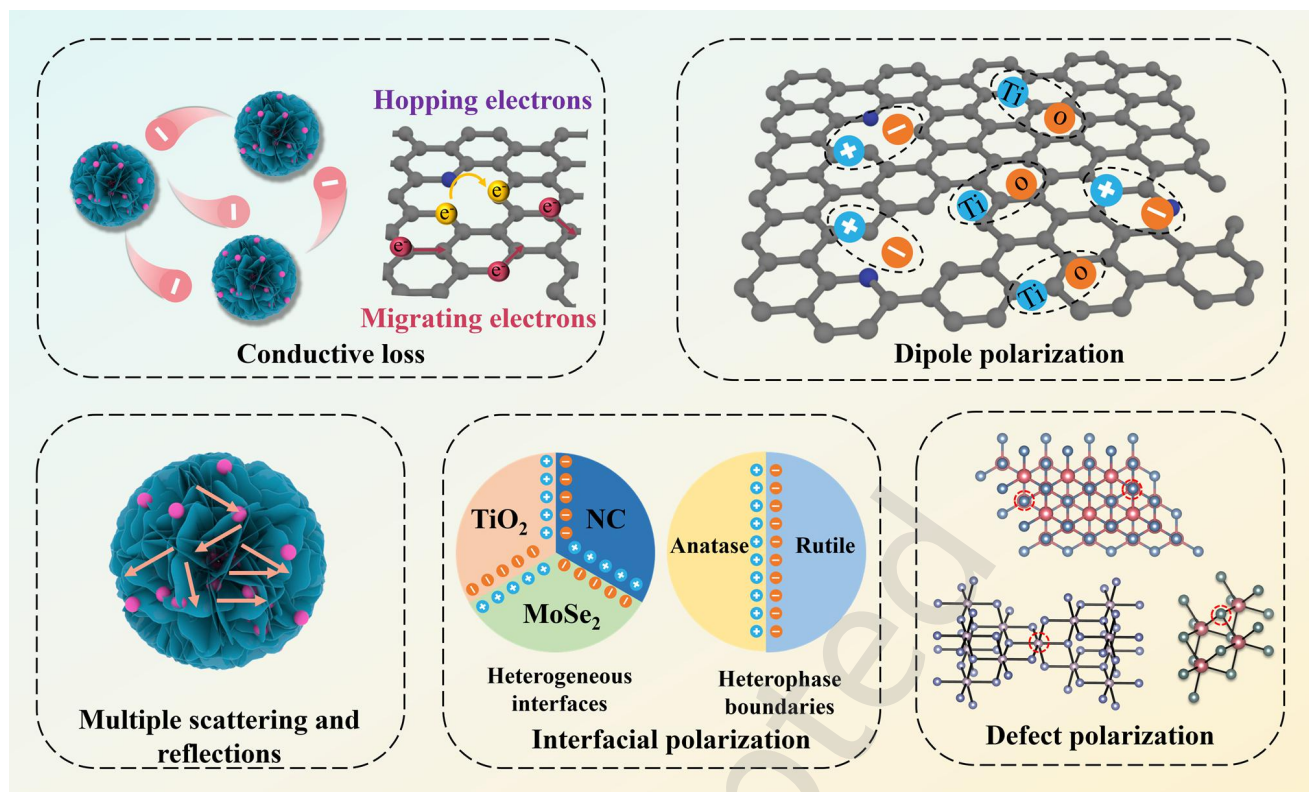
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The superior EMWA capability can be attributed to the cooperative effects of conductive loss and polarization loss. Additionally, the practical usability of the material in the field of EMWA was demonstrated through radar cross-section simulation.

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ABSTRACT: Electromagnetic pollution has become a serious issue, but conventional absorbers often suffer from a trade-off between absorption strength and bandwidth, while traditional interfacial engineering ignores intrinsic polarization within materials. To address this challenge, we propose a strategy to tune electronic structures by integrating anatase/rutile (A/R) mixed-phase TiO₂ into a MoSe₂/nitrogen-doped carbon (NC) matrix. The A/R-TiO₂ acts as an intrinsic polarization engine, inducing spontaneous charge separation and constructing built-in electric fields at phase boundaries, thereby enhancing polarization loss capability. Abundant phase boundaries and structural defects in mixed-phase TiO₂ also serve as charge traps, extending charge relaxation pathways and synergistically enhancing both polarization loss and conductive loss. Combined with density functional theory calculations, electron paramagnetic resonance, and systematic characterizations, this intrinsic polarization amplifies heterogeneous interfacial polarization, defect polarization and dipole polarization, forming an efficient multi-polarization coupling system. The optimized composite achieves a minimum reflection loss of -54.04 dB at 2.18 mm and a broad effective absorption bandwidth of 5.84 GHz. Radar cross-section simulations further confirm its potential for practical radar stealth. This work clarifies the polarization amplification mechanism of TiO₂ phase junctions and provides a new route for designing high-performance electromagnetic wave absorbers.

KEYWORDS: molybdenum selenide, anatase/rutile-TiO₂, intrinsic polarization engine, built-in electric field, electromagnetic wave

1 Introduction

The proliferation of high-frequency electronic devices and communication technologies has inadvertently led to a pervasive issue of electromagnetic radiation pollution, posing significant threats to information security in precision electronics and raising concerns for human health [1-4]. Consequently, the development of advanced electromagnetic wave (EMW) absorption (EMWA) materials featuring "thinness, lightness, broadness, and strength" is of paramount importance [5-7]. Traditional absorbers, however, are often encumbered by inherent trade-offs between absorption intensity and effective bandwidth, fundamentally limiting their utility.

Molybdenum selenide (MoSe₂) has attracted considerable attention because of its distinctive electronic structure, large interlayer spacing, and abundant defect sites [8, 9]. Its layered, graphite-like morphology enables the reflection and scattering of EMWs, while abundant defects enhance polarization losses. However, the limited attenuation mechanisms and relatively low electrical conductivity of pure MoSe₂ reduce EMWA performance. The deliberate construction of heterointerfaces has emerged as a foundational methodology for modulating the electromagnetic response of materials. This

engineering strategy **modulates** key physical parameters, including energy band alignment, electron transport characteristics, and lattice defects, collectively determining the material's interaction with EMW [10,11]. Specifically, the accumulation of charge carriers at junctions between components with varying dielectric properties and conductivities induces interfacial polarization [12,13]. This polarization is subject to relaxation phenomena under the influence of an alternating electromagnetic field, representing a critical pathway for electromagnetic energy attenuation. Although interface engineering has emerged as a cornerstone for manipulating electromagnetic response, a critical research gap persists. Current strategies predominantly focus on macroscopic conductor-semiconductor or Mott-Schottky junctions, often overlooking the untapped potential residing within the materials' intrinsic electronic structure. A particularly promising, yet underexplored, frontier lies in the deliberate engineering of intrinsic phase junctions to act as an internal engine for polarization amplification. Such an approach could orchestrate multiple polarization mechanisms from the inside out, creating a highly integrated and efficient loss network.

Titanium dioxide (TiO_2) exists mainly in three morphologies: rutile (R-TiO_2), anatase (A-TiO_2), and brookite [14]. Brookite TiO_2 is unstable and readily converts to anatase or rutile under thermal treatment. Anatase commonly transforms to rutile between 400 °C and 1200 °C, and the rutile fraction increases with higher calcination temperatures [15]. Composites containing mixed TiO_2 phases often outperform single-phase samples due to synergistic effects between phases [16,17]. Both phases are composed of TiO_6 octahedra, but their distinct bonding arrangements result in different electronic band structures, specifically, a narrower band gap for R-TiO_2 [18]. This fundamental disparity creates a Type-II band alignment at the A/R interface, driving spontaneous charge carrier separation. This internal charge separation not only generates a powerful built-in electric field (BIEF) that enhances carrier transport but also establishes a potent internal polarization source [18]. Despite this well-known phenomenon, previous studies have rarely harnessed this intrinsic polarization source as an active engine for electromagnetic energy dissipation. Instead, the A/R heterojunction has been treated primarily as a structural feature rather than a functional polarization amplifier.

Thus, a critical research gap persists. Current interface engineering strategies predominantly focus on constructing macroscopic conductor–semiconductor or Mott–Schottky junctions, often overlooking the untapped potential residing within the materials' intrinsic electronic structure. A particularly promising, yet underexplored, frontier lies in the deliberate engineering of intrinsic phase junctions to act as an internal engine for polarization amplification. Such an approach could orchestrate multiple polarization mechanisms from the inside out, creating a highly integrated and efficient loss network.

Herein, we bridge this critical gap by presenting a novel and facile heterointerface engineering strategy to fabricate flower-like $\text{MoSe}_2/\text{NC}/\text{A}/\text{R-TiO}_2$ composites. The core of our design is to leverage the A/R- TiO_2 heterojunction as an intrinsic polarization engine. This engine serves a dual purpose: it initiates internal dipole polarization and amplifies the external interfacial polarization occurring at the junctions between the MoSe_2/NC matrix and the TiO_2 nanoparticles. Furthermore, the phase boundaries provide an ideal platform for defect engineering, further enhancing polarization and conductive losses. These multi-level heterostructures are synthesized through a one-step selenization of a Mo-PDA-amorphous TiO_2 precursor, and their complex permittivity can be finely tuned by modulating the TiO_2 content. Benefiting from this synergistic architecture, the optimized composite achieves a minimum reflection loss of -54.04 dB at 2.18 mm and a wide effective absorption bandwidth of 5.84 GHz. This work provides a profound blueprint for leveraging mixed-phase heterojunctions to orchestrate electronic structure, paving a new avenue for the development of next-generation high-performance electromagnetic functional materials.

2 Experimental

Firstly, the Mo-PDA/amorphous- TiO_2 precursors were prepared via a solution stirring route. Subsequently, the precursors were thoroughly blended with selenium

powder and selenized at 800 °C under N_2 protection to obtain target composites. These samples were labeled MNCT-12, MNCT-16, MNCT-20 and MNCT-24 based on different TiO_2 contents of 12, 16, 20 and 24 wt%, respectively. The Electronic Supplementary Material (ESM) contains detailed synthetic procedures and characterizations of all samples.

3 Results and discussion

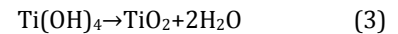
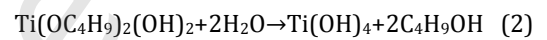
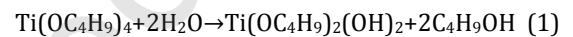
3.1 Composition, Morphology, and Microstructure of $\text{MoSe}_2/\text{NC}/\text{A}/\text{R-TiO}_2$

In the design of advanced EMWA materials, the creation and optimization of interfaces are paramount. The fundamental principle is to introduce multiple interfaces, such as heterointerfaces and phase boundaries to adjust the electromagnetic response, thereby enhancing polarization losses capability [11, 12, 19]. Based on the above theory, our design philosophy is to leverage mixed-phase TiO_2 heterostructures as a tunable platform to orchestrate multi-level electronic structure. This is achieved by integrating phase boundaries and defects within TiO_2 to generate intrinsic dipole polarization, which in turn amplifies interfacial polarization at the $\text{MoSe}_2/\text{TiO}_2$ heterointerfaces. This hierarchical polarization, synergized by the conductive NC network, establishes a comprehensive and controllable loss mechanism for high-performance broadband EMWA. To fundamentally reveal the intrinsic physical mechanism by which mixed-phase TiO_2 acts as an intrinsic polarization engine and enhances multi-level interfacial synergy, we systematically deconstructed the electronic structure of the materials using first-principles calculations. The models were established and subjected to density functional theory (DFT) calculations (Fig. S1-S5). Density of States (DOS) analysis (Fig.1 a-d) clearly delineates the electronic state distribution of each component and the composite system. Pristine A- TiO_2 (Fig.1 a) manifests as a typical wide-bandgap semiconductor where strong electronic localization restricts charge mobility. In the A/R- TiO_2 heterophase (Fig.1 b), significant hybridization of Ti and O states between the anatase and rutile phases disrupts the localization constraints of the pure phase, thereby establishing abundant channels for dielectric polarization and charge transport. Pristine MoSe_2 (Fig.1 c) exhibits superior electronic conductivity, enabling rapid response to EMW induced charge fluctuations. In the $\text{MoSe}_2/\text{NC}/\text{A}/\text{R-TiO}_2$ composite system (Fig.1 d), the DOS of multiple elements exhibits substantial overlap near the Fermi level, constructing a continuous electronic transport network. This network drastically enhances interfacial charge transfer and separation efficiency while accumulating sufficient carriers for EMW dissipation. Work function and Fermi level calculations (Fig.1 e-g) further clarify the driving forces behind interfacial charge transfer. The gradient in work functions between MoSe_2 (4.03 eV), A/R- TiO_2 (4.22 eV), and NC (4.39 eV) establishes a directional built-in electric field extending from MoSe_2 through A/R- TiO_2 to NC. This field effectively promotes interfacial charge redistribution and prolongs charge-relaxation pathways. The Fermi level comparison (Fig.1 h) confirms that upon recombination, the Fermi level of $\text{MoSe}_2/\text{A}/\text{R-TiO}_2$ resides between the individual components, prompting spontaneous charge transfer from MoSe_2 to A/R- TiO_2 . Furthermore, the potential difference

between A/R-TiO₂ and NC drives continued charge migration toward NC. This multistage charge transfer pathway persistently intensifies interfacial polarization and charge relaxation dynamics, significantly enhancing EMW attenuation capability. Band structure analysis (Fig.1 i-k) reveals the modulation of electronic states by heterojunctions. As shown in the Fig.1 (i, j), the bandgap of A-TiO₂ is 3.1 eV, and the bandgap of A/R-TiO₂ is 1.24 eV. Compared to the A-TiO₂, A/R-TiO₂ composite exhibits a lower bandgap. A narrower band gap facilitates the generation of more free charge carriers, elevating the electrical conductivity of the material and strengthening conductive loss. Meanwhile, the A/R two-phase heterostructure possesses abundant interfacial polarization sites, which realize electromagnetic wave attenuation via multiple polarization loss. The MoSe₂/NC/A/R-TiO₂ composite system (Fig.1 k) presents continuous semi-metal-semiconductor features. The introduction of abundant electronic states contributed by MoSe₂, NC and A/R-TiO₂ near the Fermi level significantly enhances carrier absorption and dissipation of EMW energy. Charge density difference and interfacial polarization mechanisms (Fig.1 l-m) intuitively elucidate the core function of the intrinsic polarization engine. In the A/R-TiO₂ heterojunction, electrons transfer directionally from R-TiO₂ to A-TiO₂ (0.278 e), forming distinct electron enrichment (yellow) and depletion (blue) regions (Fig. S6). Within the MoSe₂/NC/A/R-TiO₂ heterostructure, significant charge transfers of 0.733 e and 0.656 e occur at the MoSe₂/A/R-TiO₂ and A/R-TiO₂/NC interfaces, respectively, generating strong interfacial dipole moments (Fig.1 m). This cross-interface directional charge transfer induces built-in electric fields within each layer, synergistically enhancing polarization and conductive loss.

Integrating the space charge region model (Fig.1 n), it is evident that the intrinsic polarization of the A/R-TiO₂ heterophase acts as an engine to drive directional charge migration and relaxation across dual interfaces. Through the synergistic action of dipole polarization, interfacial polarization, and multiple other mechanisms, the system achieves highly efficient EMWA and attenuation.

The synthetic route for the heterogeneous MoSe₂/NC/A/R-TiO₂ composites is schematically depicted in Fig. 2. The initial step involves the complexation of catechol-rich dopamine with MoO₄²⁻ ions to form a Mo-dopamine complex. Subsequent ammonia addition triggers the oxidative self-polymerization and self-assembly of dopamine, yielding globular Mo-polydopamine (PDA) precursor spheres (the step I in Fig. 2) [20]. In the second stage, an amorphous TiO₂ shell is conformally deposited onto the Mo-PDA nanospheres via the controlled hydrolysis of tetrabutyl titanate (the step II in Fig. 2). The governing reactions for TiO₂ genesis can be expressed as:



During this hydrolysis, nascent Ti(OC₄H₉)₂(OH)₂ species polymerizes and migrates into the interior of Mo-PDA microspheres through inherent cavities, preferentially reacting with the more active, highly exposed nanoparticles inside the spheres [21]. After selenization treatment, the Mo-PDA microspheres convert into MoSe₂/NC hybrid while simultaneously inducing the crystallization of the amorphous TiO₂ into the desired mixed anatase/rutile (A/R) phase, thus culminating in the formation of the target MoSe₂/NC/A/R-TiO₂ composite.

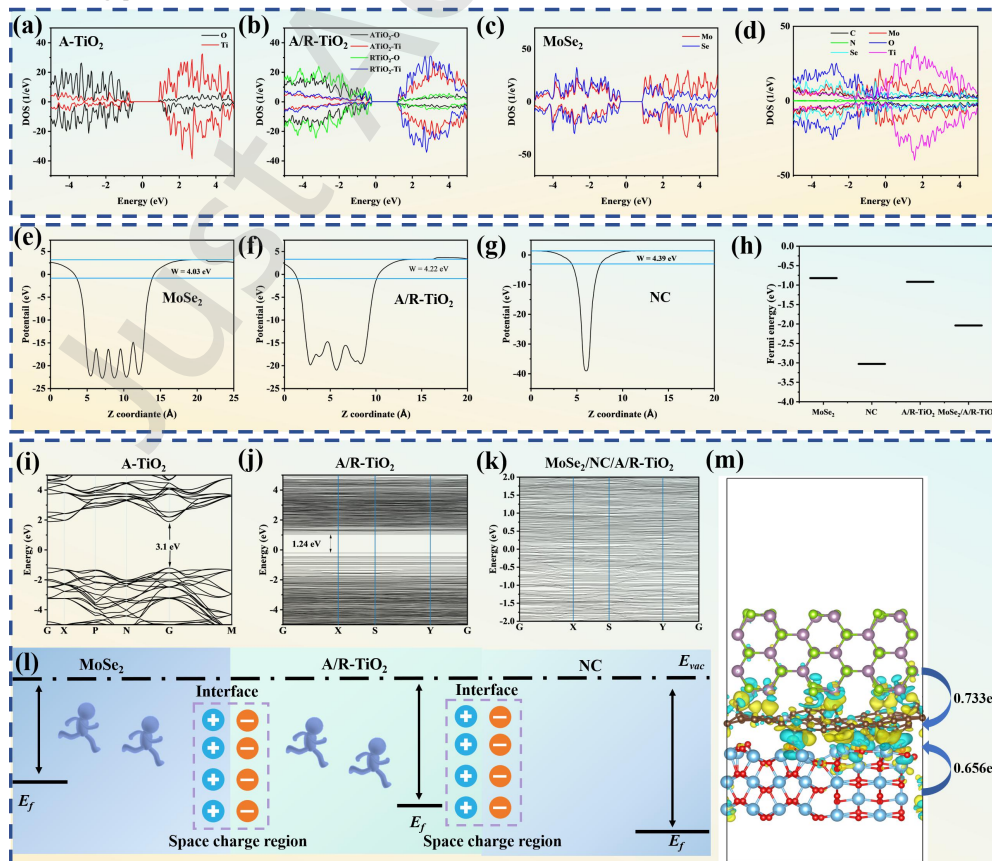


Figure 1 DFT calculations of the MoSe₂/NC/A/R-TiO₂ composites: DOS of the a) A-TiO₂, b) A/R-TiO₂, c) MoSe₂, and d) MoSe₂/NC/A/R-TiO₂. e-g) The work function obtained by calculating the typical crystal planes between the sample interface. h) Fermi level comparison. Projected band

structure of the i) A-TiO₂, j) A/R-TiO₂, and k) MoSe₂/NC/A/R-TiO₂. l) Electron aggregation diagram of heterogeneous interface. m) Charge density difference analysis at MoSe₂/NC/A/R-TiO₂ heterointerface.

The crystal structure of all synthesized samples was analyzed by XRD (Fig. 3a and Fig. S7). As shown in Fig. S7, the Mo-PDA/TiO₂ precursor pattern matches standard cards for ammonium hexamolybdate (NH₄(Mo₆O₁₈), JCPDS No.89-7650), ammonium dimolybdate (NH₄(Mo₂O₇), JCPDS No.70-1706) and molybdenum oxide hydrate (MoO₃·H₂O, JCPDS No.70-1676), [22] respectively, while no TiO₂ diffraction peaks are observed, consistent with TiO₂ being amorphous at this stage. After selenization treatment, as shown in Fig. 3a, main diffraction peaks at 13.64°, 31.43°, 37.83°, 46.97° and 55.81° correspond to the (002), (100), (103), (105) and (110) planes of hexagonal MoSe₂ (JCPDS No. 29-0914), [23] respectively, indicating high-purity MoSe₂. The diffraction peaks are located at 25.25°, 47.98°, 55.06° and 62.63°, belonging to the (101), (200), (211) and (204) crystal planes of A-TiO₂ (JCPDS No. 21-1272) [15], respectively. The diffraction peaks are located at 27.39° and 36.13°, belonging to the (110) and (101) crystal planes of R-TiO₂ (JCPDS No. 21-1276), [15] respectively. These results confirm coexistence of A and R phases of the TiO₂. Furthermore, the TiO₂ content can be easily regulated by controlling the amount of tetrabutyl titanate added to the

precursor, which can be demonstrated by an increase in the peak strength of TiO₂ in the XRD results. To further determine the relative content (W_A and W_R) of A-TiO₂ and R-TiO₂ in mixed-phase TiO₂, the following equation can be used for calculation: [15]

$$W_A = K_A I_A / (K_A I_A + I_R) \quad (4)$$

$$W_R = 1 - W_A \quad (5)$$

where the K_A value is 0.886, I_A is the area of anatase (101) peak, I_R is the area of rutile (110) peak, and the relative TiO₂ content of A and R phases is shown in Table S1. Such a mixed-phase TiO₂ structure favors improved impedance matching, enhanced interfacial polarization, and more effective attenuation of EMW [16]. To delve into the distinctive functional group present, the MNCT-20 sample underwent FT-IR spectroscopic analysis. As illustrated in Fig. S8, the peaks located at 1631 cm⁻¹ and 3438 cm⁻¹ are attributed to COO- and Mo-OH bond vibrations within MoSe₂ [24]. In addition, the peak at 581 cm⁻¹ corresponds to the Ti-O-Ti tensile vibration [25]. The collective outcomes from XRD and FT-IR analyses confirm the successful synthesis of MoSe₂/NC/A/R-TiO₂ composites.

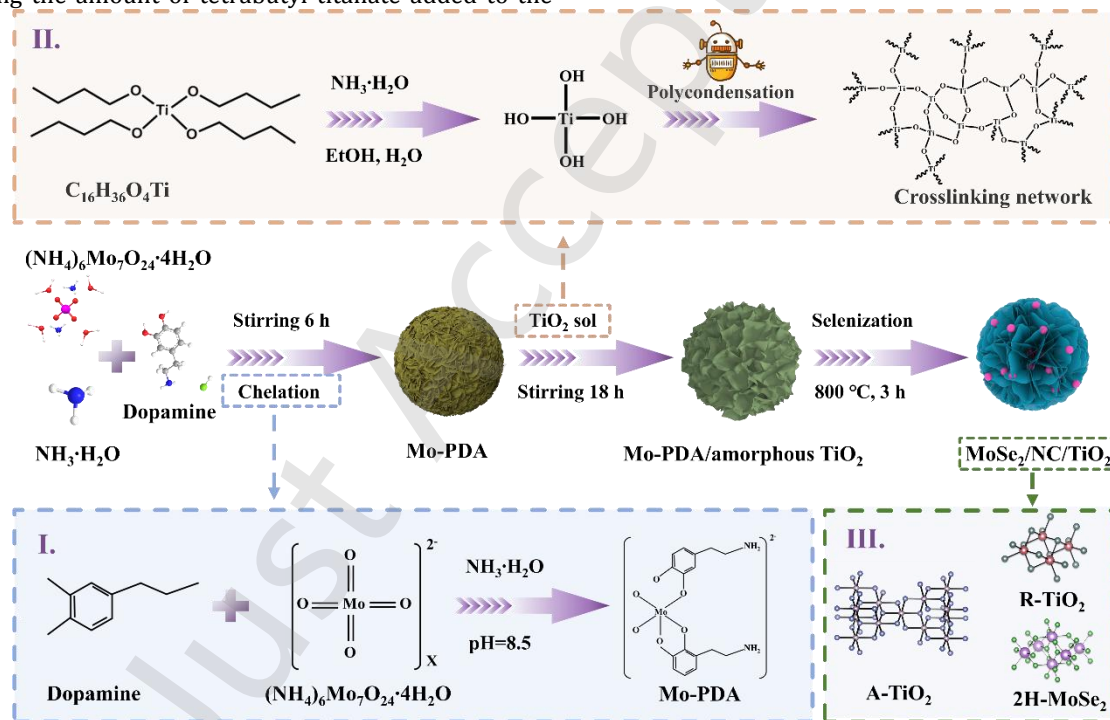


Figure 2 Schematic illustration of the preparation process of the MoSe₂/NC/A/R-TiO₂ composites.

The morphological and structural evolution of the precursor to the final heterostructure was systematically investigated. Initially, SEM analysis of the Mo-PDA/amorphous TiO₂ precursor (Fig. S9) confirms that amorphous TiO₂ nanoparticles are uniformly anchored onto the surface of Mo-PDA nanospheres following a hydrolysis-condensation reaction. Furthermore, the introduction of the TiO₂ precursor fundamentally alters the self-assembly process of the Mo-PDA. Compared to the well-defined, discrete nanospheres of the pristine Mo-PDA precursor we previously reported, [20] the Mo-PDA/amorphous TiO₂ composite is characterized by partial sphere fragmentation and noticeable agglomeration. This morphological evolution provides compelling evidence that the hydrolysis and condensation of tetrabutyl titanate are

integral to the structural formation, exerting a governing influence on the precursor's ultimate morphology rather than being a passive deposition step. After the pivotal selenization process, the resultant MNCT-20 composite undergoes a dramatic structural transformation into a robust, three-dimensional porous network (Fig. 3b). The three-dimensional porous network highly favorable for inducing multiple reflections and scattering of incident EMW, thereby prolonging their propagation path and enhancing dissipation. To resolve the fine details of this architecture, TEM was employed. As depicted in Fig. 3c, it is observed that the TiO₂ nanoparticles with an average size of ~100 nm dispersed on the surfaces of MoSe₂ nanosheets. This intimate contact generates a high density of heterogeneous interfaces, which are critical for attenuating

EMW via interfacial polarization. The HRTEM images of MNCT-20 provide definitive evidence for the formation of the multi-component heterostructure. The clearly resolved lattice spacings of 0.237 and 0.35 nm in Fig. 3d are indexed to the (103) crystal plane of 2H-MoSe₂ and the (101) crystal plane of A-TiO₂, respectively. The colored interfacial regions in Fig. 3e vividly illustrate the seamless integration among MoSe₂, A/R-TiO₂ nanoparticles, and the conformal C layer, confirming the successful construction of MoSe₂/TiO₂ and MoSe₂/C heterojunctions. These junctions are anticipated to significantly facilitate charge carrier migration across the interfaces, a key factor for enhancing

EMWA performance. Further evidence of the mixed-phase TiO₂ is presented in Fig. 3f, where lattice spacings of 0.166, 0.189, 0.237, and 0.248 nm correspond to the (211) crystal plane of A-TiO₂, the (200) crystal plane of A-TiO₂, the (103) crystal plane of MoSe₂, and the (101) crystal plane of R-TiO₂, respectively. In this architecture, A/R-TiO₂ nanoparticles are intricately dispersed throughout the matrix, a configuration highly favorable for inducing the spontaneous redistribution of charge carriers. The resulting charge separation gives rise to a built-in electric field, which not only facilitates rapid carrier transport but also drives the generation of interfacial defects [18].

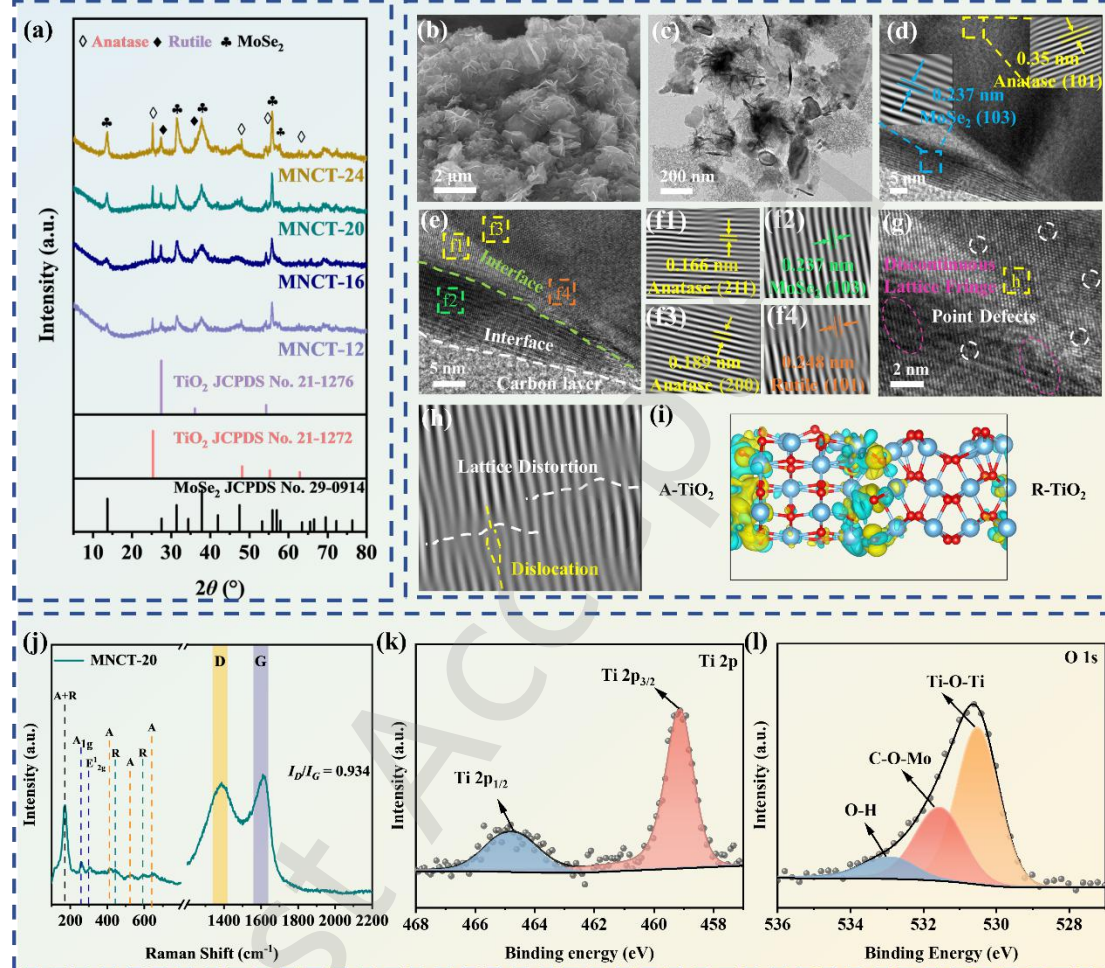


Figure 3 a) XRD patterns of the MoSe₂/NC/A/R-TiO₂. SEM images of b) MNCT-20. c) TEM, d-h) HRTEM of MNCT-20. i) Schematic diagram of TiO₂ phase transition. j) Raman spectrum of MNCT-20. XPS spectra of k) Ti 2p and l) O 1s of MNCT-20.

Critically, the enlarged HRTEM images (Fig. 3g, h) reveal a high concentration of structural defects, including point defects, discontinuous lattice fringes, and significant lattice distortions. These imperfections act as efficient traps for charge carriers, creating localized states that modulate the electron density and transport pathways [10]. Under an alternating EMW field, they also function as abundant defect-induced dipoles, significantly bolstering dipole polarization loss. Overall, the mixed-phase TiO₂ heterostructure serves as an adjustable platform for coordinating multi-level electronic structure, which not only induces the formation of built-in electric fields, further enhancing carrier transport, but also promotes the generation of interface defects (Fig. 3i). The electron paramagnetic resonance (EPR) spectra provide direct evidence for the core role of mixed-phase TiO₂ as an intrinsic polarization engine (Fig. S10). Upon the introduction of A/R-TiO₂, the signal intensity of the Se_v-

MoSe₂/NC/TiO₂ system is significantly higher than that of the Se_v-MoSe₂/NC system without TiO₂. Furthermore, it exhibits a stronger characteristic peak at g=2.03, which corresponds to an increase in oxygen vacancies and defect sites within the system. In fact, the A/R-TiO₂ heterostructure simultaneously introduces three types of defects that synergistically promote EMW attenuation, namely oxygen vacancies, lattice defects, and interfacial structural defects. Oxygen vacancies are typical paramagnetic defects detected by EPR, which act as efficient dipole polarization centers and trigger rapid charge relaxation under EMW excitation. Lattice defects originate from the lattice mismatch and structural distortion between anatase and rutile phases, contributing to intrinsic structural polarization. Interfacial structural defects are generated at the MoSe₂/TiO₂ and TiO₂/NC heterojunction interfaces, inducing intense interfacial charge accumulation and reinforcing interfacial

polarization. Benefiting from the synergistic effect of multi-scale defect polarization, the composite achieves significantly enhanced dielectric loss and EMWA performance. The polycrystalline nature of the composite is further corroborated by the Selected Area Electron Diffraction (SAED) pattern (Fig. S11a), which clearly exhibits diffraction rings corresponding to the (211) A-TiO₂ and (101) of R-TiO₂, respectively, and the (103) and (100) of MoSe₂, respectively. Finally, Energy-Dispersive X-ray Spectroscopy (EDS) elemental mapping (Fig. S11b) confirms the homogeneous distribution of C, N, Mo, Se, Ti, and O elements throughout the entire heterostructure. To further confirm the presence of a mixed phase TiO₂ within the composite the Raman spectra was applied (Fig. 3j). The characteristic peaks at 247 and 291 cm⁻¹ are related to the out-of-plane (A_{1g}) and in-plane (E_{1g}) vibration modes of MoSe₂, respectively [26]. The Raman peaks at 401 cm⁻¹ (B_{1g}) and 516 cm⁻¹ (A_{1g}+B_{1g}) are indicative of A-TiO₂. Peaks centered on 235 cm⁻¹ (second-order Raman scattering), 443 cm⁻¹ (E_g), and 615 cm⁻¹ (A_{1g}) are characteristic of R-TiO₂. The vibration modes at 170 cm⁻¹ are attributed to both A-TiO₂ (E_g) and R-TiO₂ (B_{1g}) [27]. These findings illustrate the TiO₂ occur transitioning from an anatase to a rutile structure, resulting in the formation the mixed phase TiO₂. In addition, two prominent peaks near 1328 and 1589 cm⁻¹ correspond to the D and G bands of the carbon phase, respectively. The D band is associated with defects and lattice distortions, whereas the G band arises from the in-layer stretching vibrations of sp² C atoms [28]. The I_D/I_G ratio is a standard metric for evaluating the graphitization degree of carbon materials. As depicted in Fig. 3j, the I_D/I_G value of MNCT-20 was determined to be 0.934, which serves as evidence that the synthesized MNCT-20 sample is rich in disordered carbon or defects. The presence of these defects can function as polarization centers, thereby promoting polarization behavior, which is advantageous for enhancing polarization loss. Collectively, XRD, FT-IR and Raman results confirm successful synthesis of MoSe₂/NC/A/R-TiO₂ composites.

To further confirm the valence states and chemical composition, the MNCT-20 was investigated by XPS, and the consequential data were performed in Fig. 3k, l and Fig. S12 and S13. As presented in Fig. S12, the MNCT-20 sample contained C, N, Se, Mo, Ti, and O elements. High-resolution C 1s spectrum (Fig. S13a), peaks at 283.2, 284.8, 285.8, and 288.1 eV, indexed to C-Mo, C=C/C-C, C-N, and C=O bonds, respectively [20]. The N 1s spectrum (Fig. S13b) can be deconvoluted into four peaks at 394.8, 398.2, 399.4, and 401.1 eV, correspond to Mo-N bonds, pyridine N, pyrrole N, and graphite N, respectively, indicating that N atoms were successfully doped into the carbon matrix during the selenization of PDA [29]. Under the action of alternating electromagnetic field, pyridine N and pyrrole N can be used as dipole centers to improve the polarization loss. Graphite N can accelerate electron migration and enhance conductive loss. The Se 3d high-resolution spectrum is shown in Fig. S13c, Se 3d_{5/2}, Se 3d_{3/2} and Se-O appear at 54.5, 55.3 and 59.3 eV, respectively, which proves that Se element exists in the form of Se²⁻ [30]. For the Mo 3d high-resolution spectrum (Fig. S13d), two characteristic peaks are observed at 229.0 and 232.1 eV, which are consistent with the double peaks of the oxidation states Mo⁴⁺ Mo 3d_{5/2}

and Mo 3d_{3/2}, while the peak at 230.1 eV belongs to the Mo-C bond. The Ti 2p spectrum (Fig. 3k) describes two characteristic peaks with binding energies of about 459.1 and 464.7 eV, belonging to Ti 2p_{3/2} and Ti 2p_{1/2} of Ti⁴⁺ in TiO₂, respectively [21]. In the O 1s high-resolution spectrum (Fig. 3l), there are three peaks, 530.5, 531.5, and 532.8 eV, which are derived from Ti-O-Ti, C-O-Mo bond, and OH⁻ radical, respectively [31]. Overall, XPS confirms the coexistence of MoSe₂, N-doped carbon and TiO₂ and the presence of interfacial bonds.

3.2 EMWA Performance of MoSe₂/NC/A/R-TiO₂

To assess the EMWA capability of the as-prepared MoSe₂/NC/A/R-TiO₂ absorbers, the reflection loss (RL) values and EAB values were investigated at 2.00–18.00 GHz. Notably, the RL value below -10 dB that represented 90% of EMW was absorbed, and the corresponding frequency range signified the EAB [32]. The RL can be calculated by Equations S1 and S2 according to the transmission line theory. For an intuitive assessment of the impact of TiO₂ loading, 2D and 3D RL plots of the MoSe₂/NC/A/R-TiO₂ across the 2.00–18.00 GHz range were comparatively analyzed. The influence of TiO₂ content on EMWA performance is profound. As depicted in Fig. 4a and Fig. S14 a-c, the initial composite, MNCT-12, achieves an RL_{min} value of -24.62 dB at 2.50 mm, with a corresponding EAB value of 4.32 GHz (9.04-13.36 GHz). The maximum EAB value for MNCT-12 is 5.28 GHz (12.16-17.44 GHz). A significant enhancement is observed for MNCT-16, where the RL_{min} dramatically surges to -49.64 dB at a thickness of 1.88 mm, accompanied by a respectable EAB value of 5.04 GHz (12.96-18.00 GHz). Similarly, MNCT-16 maintains an RL_{min} of -30.12 dB at a thickness of 2.00 mm, with an identical EAB value of 5.04 GHz (12.96-18.00 GHz), as depicted in Fig. 4b and Fig. S14 d-f. This underscores the positive influence of increasing TiO₂ content. The performance culminates in the MNCT-20 composite (Fig. 4c and Fig. S14 g-i), which exhibits a RL_{min} value of -54.04 dB at 2.18 mm, coupled with a broad EAB of 5.84 GHz (12.08–17.92 GHz). This represents the peak absorption capacity achieved within this compositional series. However, this trend is not indefinitely sustainable, as excessive TiO₂ content proves detrimental. For MNCT-24, a marked performance degradation is evident, with the RL_{min} value dropping to -22.58 dB at a thickness of 2.00 mm and its maximum EAB shrinking to 4.96 GHz (Fig. 4d and Fig. S14 j-l). From the analysis of the above results, it can be found that both MNCT-16 and MNCT-20 have achieved good absorption performance. However, compared to other matched thicknesses, the overall absorption performance of MNCT-20 is better than that of MNCT-16 (Fig. 4e, f). These results demonstrate that the TiO₂ content is a critical parameter for precisely attenuation capability, thereby dictating the ultimate EMWA performance of these heterostructures. In addition, it can be observed from the RL curve that the RL_{min} values progressively shift towards lower frequency regions as the matching thickness increases. This phenomenon can be explained via the quarter-wavelength model by the Equation S3. Specifically, when the phase difference between the incident EMW and the reflected EMW at the metal substrate layer at the interface of the air medium is 180°, the electromagnetic energy will be dissipated significantly due to interference

cancellation [33]. Fig. S15 illustrates the correlation between t_m and f_m for MNCT-12, MNCT-16, MNCT-20, and MNCT-24. The red pentagrams represent calculated $RL_{\min}$ values at specific d values, while the gray curve represents t_m values derived from the quarter-wavelength model. Remarkably, there is a close alignment between the red pentagrams and gray curve, providing compelling evidence that EMW attenuation follows the quarter-wavelength model.

To discuss and illustrate the probable dielectric loss mechanism in the $\text{MoSe}_2/\text{NC}/\text{A}/\text{R-TiO}_2$ composites, the corresponding electromagnetic parameters were analyzed. The ϵ_r ($\epsilon_r = \epsilon' - j\epsilon''$) was employed to assess the dielectric characteristics, wherein the real part (ϵ') represented the storing capacity for electromagnetic energy, and the imaginary part (ϵ'') signified the dissipating potential for electromagnetic energy [34]. As illustrated in Fig. 4g, both ϵ' and ϵ'' of the complex permittivity exhibit a clear downward trend as the TiO_2 content increases from MNCT-12 to MNCT-24. This observation demonstrates that the

complex dielectric constant, and thus the intrinsic impedance, can be effectively modulated by varying the proportion of the TiO_2 heterostructure. Frequency-dependent analysis further reveals a characteristic decrease in ϵ' for all samples with increasing frequency, which the behavior attributed to the dispersion effect arising from directional polarization lagging behind the alternating EMW field [35]. The ϵ' values for MNCT-12, MNCT-16, MNCT-20, and MNCT-24 exhibit a decreasing trend with rising frequency, decreasing from 11.03, 9.96, 9.76, and 8.86 to 6.73, 5.33, 5.64, and 5.84, respectively. Simultaneously, the ϵ'' values similarly vary from 5.15, 3.47, 4.98, and 2.35 to 5.25, 3.79, 4.16, and 2.26, respectively. Defect states provide localized polarization centers and may facilitate field-assisted hopping at an appropriate defect density, excessive trapping, however, can suppress long-range carrier transport. When an electromagnetic field is applied, charge accumulates at these grain boundaries due to the external electric field, leading to the formation of local dipoles.

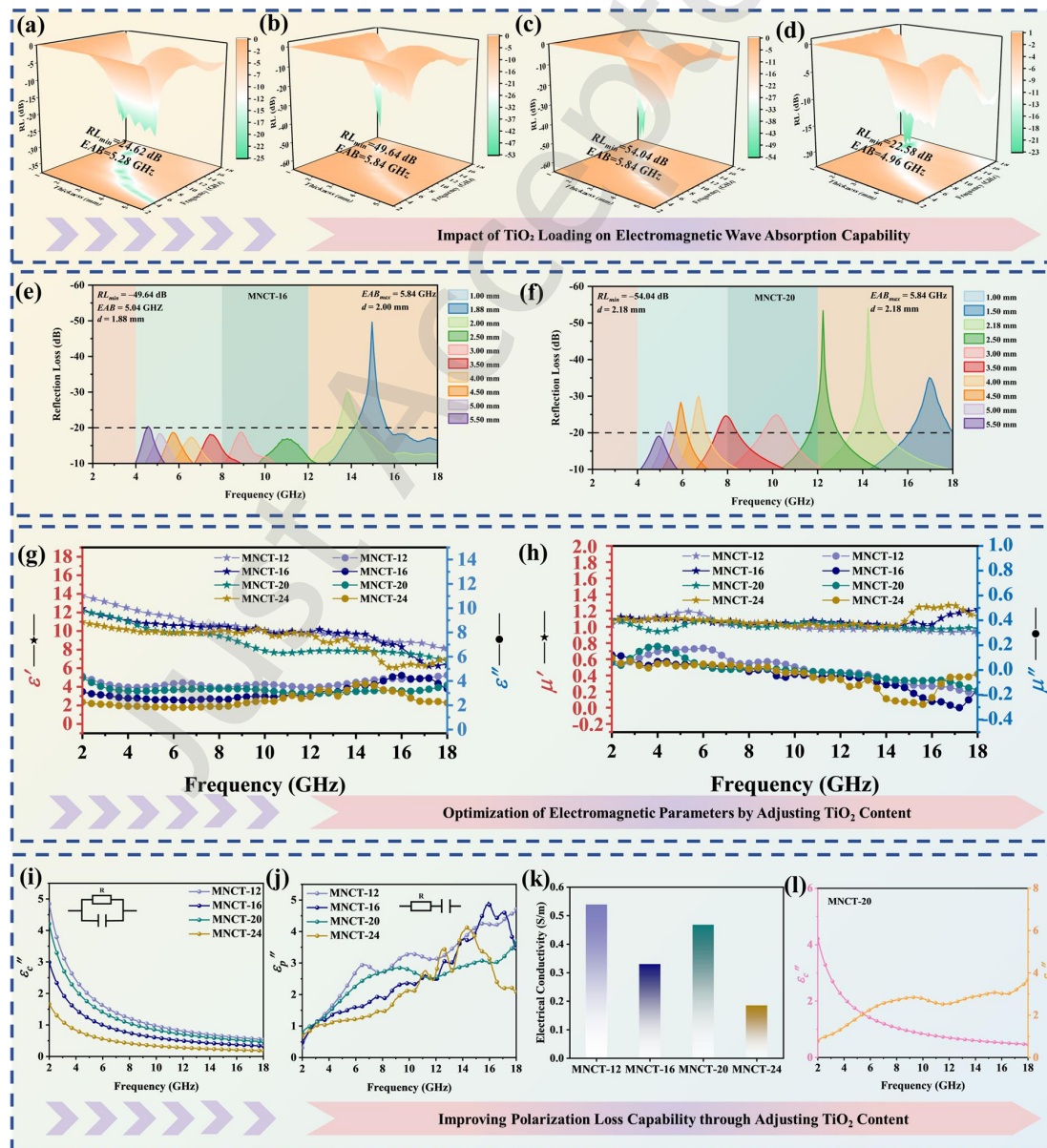


Figure 4 The 3D RL plots of a) MNCT-12, b) MNCT-16, c) MNCT-20, and d) MNCT-24. The RL and EAB curves of e) MNCT-16 and f) MNCT-20. g) ϵ' and ϵ'' of value for MNCT-12, MNCT-16, MNCT-20, and MNCT-24 at 2.00-18.00 GHz. h) μ' and μ'' of value for MNCT-12, MNCT-16, MNCT-20, and MNCT-24 at 2.00-18.00 GHz. i) conductive loss, j) polarization loss, and k) electrical conductivity of all samples. l) comparison chart of

conductive loss and polarization loss of MNCT-20 sample.

These dipoles undergo polarization relaxation under the influence of the applied electromagnetic field, resulting in fluctuations in the dielectric constant. Notably, the ε'' curve exhibits significant fluctuations in the mid-high frequency region due to the multi-polarization relaxation process. This multi-relaxation behavior is a hallmark of the successfully orchestrated electronic structure, originating from three primary sources. Specifically, the abundant heterogeneous interfaces between MoSe₂ nanosheets and the dispersed A/R-TiO₂ nanoparticles, as well as the MoSe₂/NC interfaces, lead to significant charge accumulation at the grain boundaries. The resultant local dipoles relax under the applied electromagnetic field, contributing substantially to dielectric loss. Crucially, the engineered A/R-TiO₂ heterojunction introduces an additional level of interfacial polarization, distinct from the MoSe₂/TiO₂ interface, thereby amplifying the overall polarization loss. Finally, the defects generated during synthesis acts as dipole centers, inducing orientation polarization under the electromagnetic field. To quantify the dielectric loss capacity of MoSe₂/NC/A/R-TiO₂ composites, the $\tan \delta_\varepsilon$ value is utilized based on the complex dielectric constant. As shown in Fig. S16a, the MNCT-20 sample demonstrates a higher $\tan \delta_\varepsilon$ value in the range of 2.00-10.00 GHz, indicating superior dielectric loss characteristics. This optimal performance confirms the efficacy of the design principle. The construction of a mixed-phase TiO₂ heterostructure establishes a synergistic network that allows interfacial, phase-boundary, and defect-induced polarizations to operate in concert, yielding exceptionally strong and tunable dielectric loss. Furthermore, an analysis of the μ' , μ'' , and $\tan \delta_\varepsilon$ curves for each sample (Fig. 4h and Fig. S16b). It was observed that the μ' and μ'' values were less than 1.1 and approximately 0.1, respectively, and $\tan \delta_\varepsilon$ values were lower than $\tan \delta_\varepsilon$ values. Therefore, it was inferred that magnetic loss was not the principal factor involved in the EMWA performance. To understand the dielectric loss mechanisms, the contributions from polarization and conduction were quantitatively separated via a relaxation model fitted with the least squares method (Fig. 4i, j). The intensity of conductive loss for the composites followed the order MNCT-12 > MNCT-20 > MNCT-16 > MNCT-24, which is directly related to their electrical conductivity, as depicted in Fig. 4k. This non-monotonic behavior can be rationalized by the interplay between conductivity and impedance. Initially, increasing TiO₂ content enhances the interfacial network, improving charge transport. However, beyond the optimal point (MNCT-20), the excessive insulating TiO₂ phase increases overall resistivity, while its overabundance can disrupt the continuity of the conductive NC and MoSe₂ pathways, leading to a diminished conductive loss. Crucially, the polarization loss curves for all samples, display significant fluctuations across the mid-to-high frequency range (8.00–18.00 GHz), a hallmark of the rich multi-polarization processes. The superior polarization loss is attributed to the ideal balance of heterogeneous interfaces created by the dispersed A/R-TiO₂ nanoparticles. This confirms that the mixed-phase TiO₂ heterostructure imparts strong polarization-based attenuation to all samples. Furthermore, a comparative analysis reveals that

as frequency increases, polarization loss surpasses conductive loss (Fig. 4l). This indicates a frequency-dependent shift in the dominant loss mechanism: conductive loss is more influential at lower frequencies, while the engineered interfacial and defect-induced polarizations become the primary contributors to attenuation in the crucial middle-to-high frequency bands. This synergistic and tunable loss mechanism is the direct outcome of successful orchestration of electronic structure through the mixed-phase TiO₂ design. Furthermore, the attenuation constant (α) was an essential factor to evaluate the attenuation ability of EMWA materials, which could be expressed by Equation S4. As shown in Fig. S16c, the α value varies with the EMW frequency and TiO₂ content. Compared with the other samples, the MNCT-20 sample shows relatively high α value in the frequency range of 2.00-18.00 GHz, indicating that it has better attenuation ability.

To deconvolute the fundamental dielectric loss mechanisms, the permittivity was further analyzed using *Cole-Cole* plots, a graphical representation derived from Debye relaxation theory (Equation S5). Generally, polarization relaxation primarily originates from electron polarization, ion polarization, dipole polarization, and space charge polarization. However, electron and ion polarizations can be negligible in the gigahertz frequency region, with dipole polarization and interfacial polarization dominating [36]. Each semicircle in a *Cole-Cole* plot signifies a distinct Debye relaxation process, with a larger radius correlating to stronger polarization loss, while a pronounced tail indicates the contribution of conductive loss [37]. As illustrated in Fig. 5a-d, all samples exhibit at least one semicircle and a distinct tail, confirming the coexistence of both polarization and conductive loss. Crucially, the MNCT-20 composite displays the largest semicircle radius, demonstrating its superior polarization relaxation strength. This enhanced polarization is a direct consequence of the successfully orchestrated electronic structure within its mixed-phase TiO₂ heterostructure. Specifically, the optimal dispersion of A/R-TiO₂ nanoparticles maximizes the density of heterogeneous interfaces (MoSe₂/TiO₂, A-TiO₂/R-TiO₂ phase boundaries), which under an alternating electromagnetic field, forces charge accumulation and rearrangement, thereby inducing powerful interfacial polarization. Concurrently, the abundance interface defects, inherently linked to the heterostructure construction, act as dipole centers, further bolstering polarization losses. Furthermore, all samples possess a pronounced tail, confirming a significant conductive loss component. This enhanced conductivity facilitates greater charge carrier migration, leading to stronger conductive loss and contributing synergistically to the overall EMW attenuation. This analysis indicates the construction of a mixed-phase TiO₂ heterostructure is the key to simultaneously optimizing both polarization and conduction pathways.

It is well-known that good impedance matching is essential for excellent EMWA, which can be accessed by Equation S6-8. Theoretically, a smaller $|\Delta|$ value represents better impedance matching. Fig. 5e-h depict the $|\Delta|$ value distribution for different TiO₂ contents. The coverage rates

for MNCT-12, MNCT-16, MNCT-20, and MNCT-24 are 42.5%, 44.7%, 44.6%, and 25.2%, respectively. To achieve optimal impedance matching, the majority of input impedance (Z_{in}) points must fall within the effective absorption region, demarcated by the purple circle on the Smith chart (Fig. S17). The Z_{in} locus initially exhibits inductive behavior at low frequencies, transitioning to a capacitive response with increasing frequency [38]. A resonant condition is identified when the Z_{in} trajectory intersects the horizontal axis. Compared to other samples, MNCT-20 displayed the highest concentration of points

within the purple circle, thereby demonstrating the impedance matching. Due to its exceptional impedance matching, MNCT-20 exhibits extraordinary EMWA capabilities at relatively thin matching thicknesses. Additionally, its EAB value nearly covers the entire Ku band. Owing to the synergy of various electromagnetic attenuation mechanisms, the acquired MoSe₂/NC/A/R-TiO₂ composites with wide EAB value compared to other TMS-based materials and TiO₂-based materials (Fig. 5i, j) [10,16,17,34,39-46].

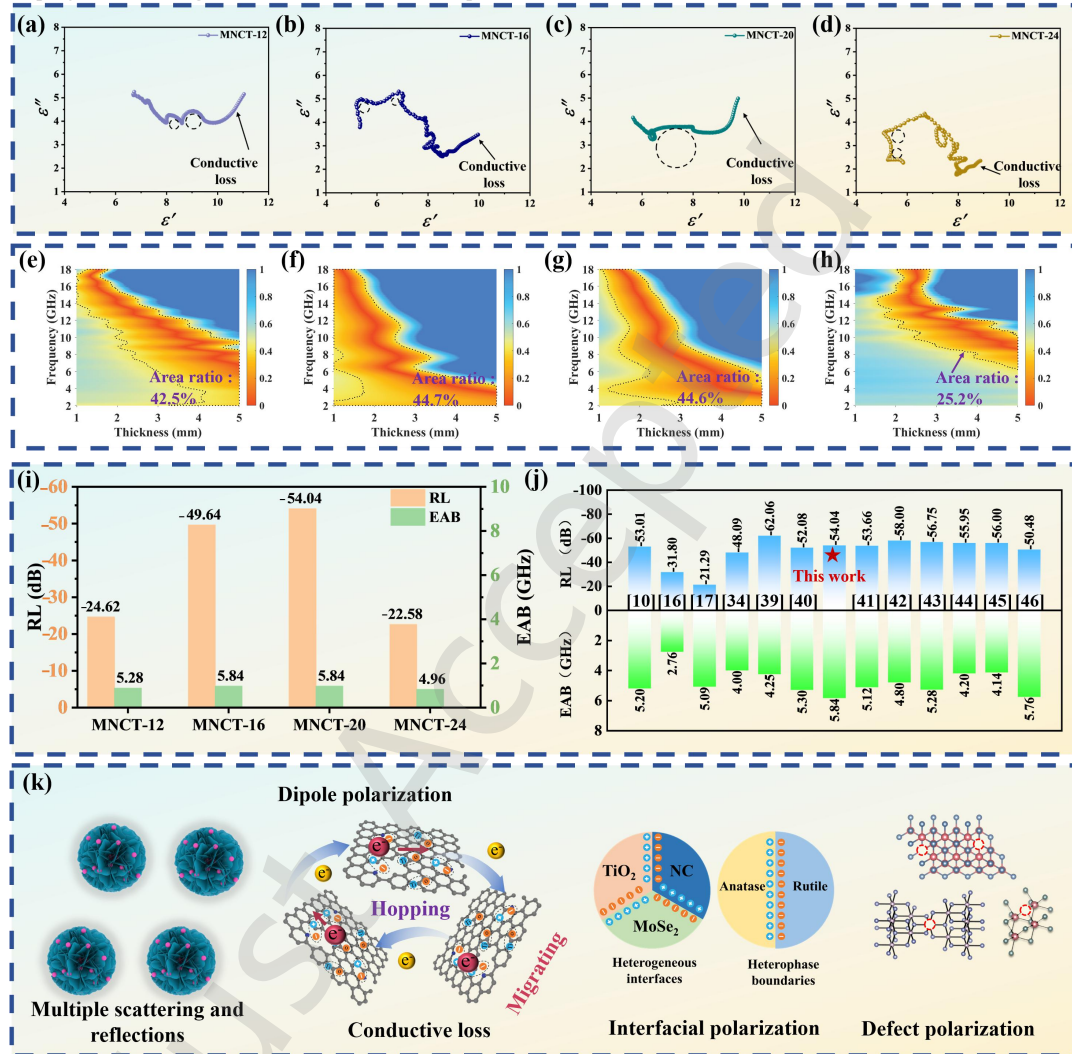


Figure 5 The Cole-Cole plots of a) MNCT-12, b) MNCT-16, c) MNCT-20, and d) MNCT-24. The $|\Delta|$ values of e) MNCT-12, f) MNCT-16, g) MNCT-20, and h) MNCT-24. i) The RL and EAB values of MNCT-12, MNCT-16, MNCT-20, and MNCT-24. j) The EMWA performances for related absorbers compared with this work. k) Schematic illustration of the EMWA mechanisms for MoSe₂/NC/A/R-TiO₂ composites.

Based on the comprehensive analysis, the sophisticated EMWA mechanism of the MoSe₂/NC/A/R-TiO₂ composite is schematically illustrated in Fig. 5k. The superior EMWA performance of the MoSe₂/NC/A/R-TiO₂ composite originates from conductive loss, interface polarization, dipole polarization, and defect polarization. The 3D porous network composed of MoSe₂ nanosheets, TiO₂ nanoparticles, and an NC matrix traps incident EMW via multiple reflections and scattering, while simultaneously providing continuous pathways for electron migration and hopping, thereby yielding strong conductive loss [47]. By adjusting the A/R-TiO₂ content, the overall conductivity can be further tuned, amplifying the conductive loss component. More critically, the mismatch in work functions among the constituents drives charge redistribution at

heterogeneous interfaces (MoSe₂/TiO₂, MoSe₂/NC, TiO₂/NC, A-TiO₂/R-TiO₂), generating powerful interfacial polarization under an alternating electromagnetic field. Notably, the A/R-TiO₂ heterojunction acts as an internal polarization amplifier, lowering the interfacial potential barrier and reducing resistance to carrier transport, thereby enhancing the polarization effect. In parallel, a high density of structural defects (point defects, lattice dislocations, distortions) and selenization process induced vacancies/defects serve as dipoles to induce robust defect polarization [18]. Meanwhile, intrinsic chemical bonds such as Ti-O-Ti and polarized NC groups further boost dipole polarization. Collectively, these multi-level contributions enable broadband, high-efficiency energy attenuation.

To investigate the practical applications in real-world

scenarios, the CST Microwave Studio was utilized to simulate the radar cross-section (RCS) distribution for all samples. The structural schematic of the simulation model as shown in Fig. 6a, b. Generally, the RCS value (σ) of the simulated sample was expressed by the Equation : [47-52]

$$\sigma(\text{dB m}^2) = 10 \lg \left[\frac{4\pi S}{\lambda^2} \left| \frac{E_s}{E_i} \right|^2 \right] \quad (6)$$

where S stood for the simulated plate area, λ designated the wavelength of the incident EMW, E_s was the electric field intensity of the transmitting wave, and E_i represented the electric field intensity of the receiving wave. As depicted in Fig. 6a, the simulation model consists of a perfect electric conductor (PEC) and an absorber in a double-layer configuration. In the simulation, the absorptive coating was set to a thickness of 2.18 mm, while the PEC layer was 2.00 mm thick. Additionally, the model was designed with a side length of 200 mm and positioned within the X-O-Y plane. Linearly polarized EMW were incident from the Z-axis, with the electric field polarization propagating along the X-axis. The direction of the scattered waves was specified by the angles θ and φ . The monitoring frequency was set at 14.24 GHz, and no boundary conditions were defined in all directions. As shown in Fig. 6c-f and Fig. S18, the pure PEC

exhibited the strongest scattering signal, and when the PEC model was coated with different types of MNCT-x absorptive layers, the intensity of the scattering signals was reduced to varying degrees. Notably, the model plate coated with MNCT-20 exhibited a significantly lower scattering signal compared to the other samples, which is consistent with the superior reflection loss performance of MNCT-20 within the MNCT-x series (Fig. S14). Fig. S19 presents the simulated RCS curves for the pure PEC and the four samples on the X-O-Y plane. The RCS values for all samples were substantially lower than that of the PEC, indicating that the MoSe₂/NC/A/R-TiO₂ composites are promising candidates for EMWA materials. To evaluate the intrinsic electromagnetic energy dissipation capabilities of different coatings, the RCS reduction effect relative to the PEC substrate was calculated and analyzed. As illustrated in Fig. 6g, the EMW attenuation characteristics of all samples completely covered the range from -90° to 90°, with peak values exceeding 30 dB m². The RCS simulation results demonstrate that the MoSe₂/NC/A/R-TiO₂ composites can effectively attenuate the scattering and reflection of EMW from the surface of the PEC substrate. While the optimized MNCT-20 absorber demonstrates impressive performance,

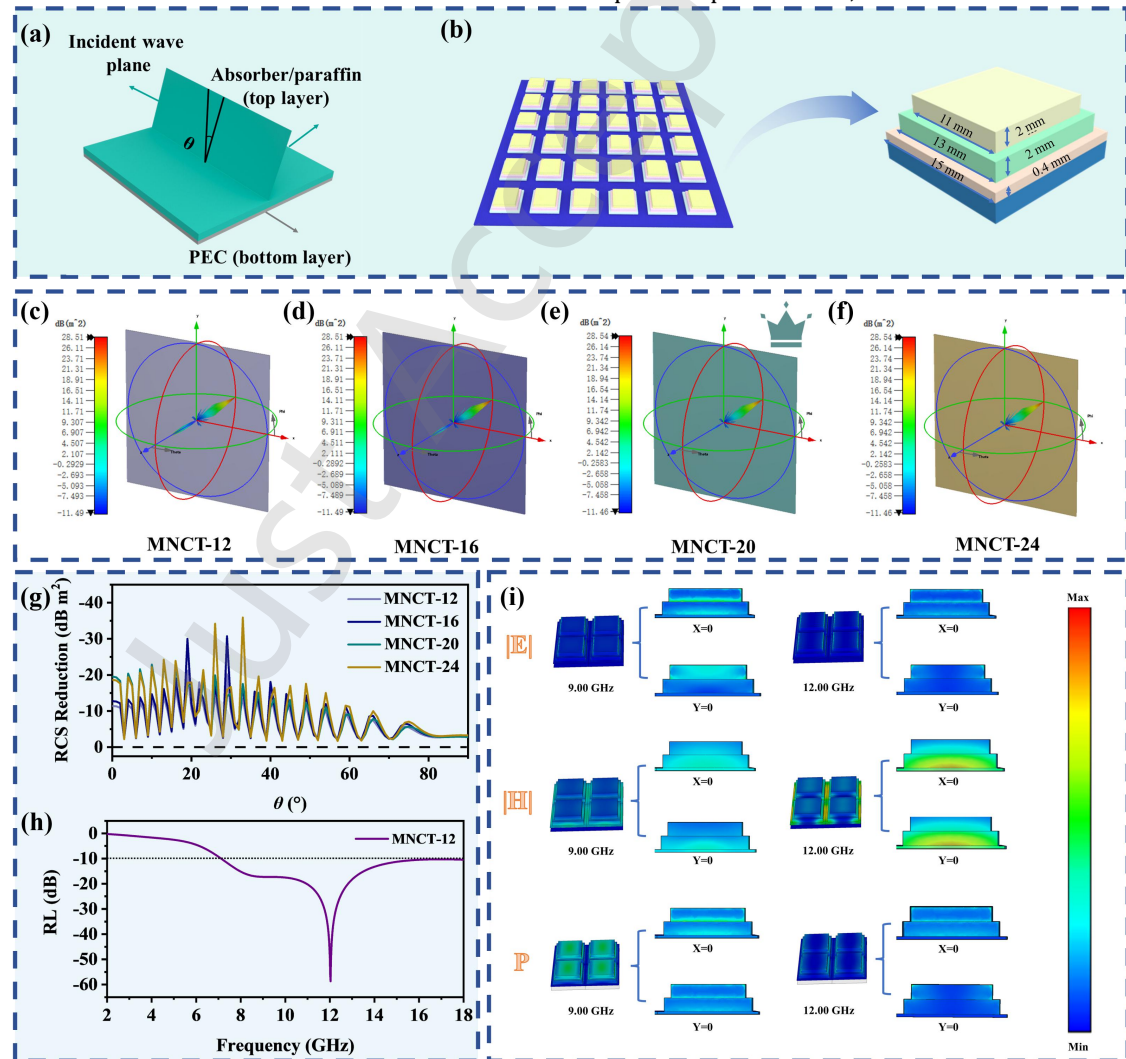


Figure 6 a, b) Structural schematic of the simulation model. CST simulation results. 3D RCS plots for PEC substrate covered with c) MNCT-12, d) MNCT-16, e) MNCT-20, and f) MNCT-24. g) RCS reduction values. h) Gradient structure design of EMWA performance of MNCT-20, i) The distributions of electric field, magnetic field and power loss under normal incidence at 9.00 and 12.00 GHz.

achieving a broadband response across its entire effective bandwidth necessitates varying its thickness, which

presents a limitation for practical integration. To overcome this, a gradient multilayer structure was

designed to further broaden the EAB of MNCT-20 (Fig. 6b). The gradient structure, composed of layers with incrementally increasing side lengths (11, 13, and 15 mm), with a 0.4, 2, and 2 mm per layer, respectively, achieves a remarkable broadening of the EAB from 5.84 GHz to 10.87 GHz (Fig. 6h). To elucidate the mechanism behind this performance enhancement, full-wave electromagnetic simulations were employed to analyze the spatial distribution of the electric field (E), magnetic field (H), and power loss (P) at representative frequencies. At a lower frequency (9.00 GHz), the E and H fields are predominantly localized within the top and bottom, respectively (Fig. 6i), a phenomenon attributed to the formation of standing waves due to a phase difference approaching $\pi/2$ [53]. By correlating the power loss distribution with the RL curve, it becomes evident that the EMWA ability at this frequency is mainly governed by an internal $\lambda/4$ interference phenomenon. The origin of the separate absorption peak at 12.00 GHz, however, is ascribed to resonance within the periodic structure. This assertion is strongly supported by the field maps in Fig. 6i, where the electric field is intensely localized at the cellular cavity edges, the magnetic field is concentrated at the groove's base, and the power loss is primarily confined to the interlayer corners, all characteristic signatures of structural resonance [54]. The EMWA performance is the result of a deliberate synergy between material composition and structural engineering. The high-loss $\text{MoSe}_2/\text{NC}/\text{A}/\text{R}-\text{TiO}_2$ provide the fundamental attenuation capability, while the gradient periodic array serves as an efficient platform. This architecture orchestrates $\lambda/4$ interference and inter-unit electromagnetic resonance, creating complementary loss mechanisms that collectively maximize the absorption bandwidth and intensity. This multi-functional design strategy, empowered by advanced material processing, showcases a viable pathway for creating next-generation absorbers that are not only high-performance but also possess applicable form factors, highlighting their immense practical potential.

4 Conclusions

In summary, the flower-like $\text{MoSe}_2/\text{NC}/\text{anatase-rutile TiO}_2$ composites prepared via a one-step selenization process exhibit tunable electromagnetic parameters and impedance matching through controlled TiO_2 content. The mixed-phase TiO_2 functions as an intrinsic polarization engine, and the formed phase junctions with spontaneous polarization ability, greatly boosting the overall polarization loss. Rich phase boundaries and structural defects also act as charge traps to optimize conductive loss and extend charge relaxation processes. Benefiting from the synergistic effect of multiple polarization and conductive loss, the as-prepared composite exhibits excellent absorption performance with a minimum reflection loss of -54.04 dB and an effective absorption bandwidth of 5.84 GHz. Radar cross-section simulations verify its favorable radar stealth capability. This study systematically reveals the polarization amplification mechanism of TiO_2 phase junctions, and offers a reliable guidance for constructing advanced mixed-phase heterojunction materials toward high-efficiency EMWA.

Electronic Supplementary Material: Supplementary

material (Experimental section, Figs. S1–S23, and Tables S1) is available in the online version of this article at <https://doi.org/10.26599/NR.2026.94909063>.

Data availability

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

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Declaration of competing interest

All the contributing authors reports no conflict of interests in this work.

Author contribution statement

Yuhan Wu and Xiaopeng Li are co-first authors. Yuhan Wu: Data curation, Conceptualization, Investigation, Formal analysis, Writing – original draft. Xiaopeng Li: Data curation, Conceptualization, Investigation, Writing – original draft. Siyu Huzhang: Investigation. Juhua Luo: Conceptualization, Funding acquisition, Project administration, Writing – review & editing. Yu Xie: Formal analysis. Shengci Li: Investigation, Supervision.

Use of AI statement

None.

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Mixed-phase TiO₂ as an intrinsic polarization engine to amplify multi-level interfacial synergy for high-performance electromagnetic wave absorption

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SUPPLEMENTARY EXPERIMENTAL DETAILS

S1. Materials

Dopamine hydrochloride (DA) was purchased from Shanghai Aladdin Reagent Co., Ltd. Ammonium molybdate tetrahydrate ($(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}\cdot 4\text{H}_2\text{O}$) was bought from Tianjin Kemeiou Chemical Reagent Co., Ltd. Ammonium hydroxide ($\text{NH}_3\cdot\text{H}_2\text{O}$, 25%) was provided by Yixing Hengsheng Chemical Co., Ltd. Tetrabutyl titanate ($\text{C}_{16}\text{H}_{36}\text{O}_4\text{Ti}$) was supported by Sinopharm Chemical Reagent Co., Ltd. Selenium powder was supported by Sinopharm Chemical Reagent Co., Ltd. Anhydrous ethanol ($\text{C}_2\text{H}_5\text{OH}$) was supplied by Jiangsu Tongsheng Chemical Reagent Co., Ltd. All chemicals were used directly without further purification.

S2. Synthesis of Mo-PDA/amorphous- TiO_2

In a typical synthesis, 0.12 g of $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}\cdot 4\text{H}_2\text{O}$ and 0.06 g of $\text{C}_8\text{H}_{12}\text{ClNO}_2$ were dissolved in 16 mL of H_2O , stirred for 10 minutes, and then a solution of 32 mL of $\text{C}_2\text{H}_5\text{OH}$ was added to the aforementioned mixed solvent, followed by stirring for 30 minutes. Subsequently, 40 μL of $\text{NH}_3\cdot\text{H}_2\text{O}$ was rapidly added to the reaction solution mentioned above to immediately yield a brownish-red solution. After stirring for 6 hours, varying amounts of $\text{C}_{16}\text{H}_{36}\text{O}_4\text{Ti}$ were added to the mixed solution, and continued stirring for another 18 hours ensued. The precipitate was washed multiple times with distilled water and ethanol before being subjected to vacuum drying at a temperature of 60 $^\circ\text{C}$ for a duration of 12 hours.

S3. Fabrication of $\text{MoSe}_2/\text{NC}/\text{A}/\text{R}-\text{TiO}_2$

Firstly, 0.1 g of precursors and 0.3 g of selenium powder were thoroughly mixed, followed by heating the tube furnace under N_2 atmosphere from room temperature to 800 $^\circ\text{C}$ at a rate of 5 $^\circ\text{C}\cdot\text{min}^{-1}$. The mixture was then kept at this temperature for 3 hours before naturally cooling down to room temperature, resulting in the formation of $\text{MoSe}_2/\text{NC}/\text{A}/\text{R}-\text{TiO}_2$ composite. Based on different TiO_2 content (12, 16, 20 and 24 %), the samples were designated as MNCT-12, MNCT-16, MNCT-20 and MNCT-24 respectively.

S4. Characterizations

The crystal structure of all samples was analyzed using the X-ray diffractometer (XRD, PANALYTICAL, model X'Pert3 Powder) equipped with a Cu K alpha radiation source. The morphology and microstructure were examined using field emission scanning electron microscopy (FESEM, FEI, model Nova Nano SEM 450) and transmission electron microscopy (TEM, JEOL, model JLM-2100F). The elemental valence was determined by X-ray photoelectron spectroscopy (XPS, THERMO SCIENTIFIC, model ESCALAB 250Xi). Fourier-transformed infrared (FT-IR) spectrum was obtained on a FT-IR spectrometer (NICOLET, model NEXUS-670) in the range of 4000-400 cm^{-1} . Raman spectrum was acquired using a Raman spectroscopy system (HORIBA, model Lab RAM HR-800) with 633 nm laser excitation. The electrical conductivity was measured using a four-point-probe tester. Electron Paramagnetic Resonance (EPR, EPR200, Bruker, Germany) was operated at ambient temperature with magnetic field of 0.11–1.5 T and microwave frequency ranging from 2 to 18 GHz. The electromagnetic parameters were evaluated using a vector network analyzer (VNA, Agilent, model N5244A) across the frequency range of 2.00 to 18.00 GHz via the coaxial method. For sample preparation purposes, the samples (30 wt%) were admixed with paraffin wax and compacted into a coaxial ring with an outer diameter of 7.00 mm and an inner diameter of 3.04 mm using a standard mold.

S5. Computational methods

The heterostructure models were constructed by selecting the corresponding low-index surfaces of each component. Specifically, the MoSe_2 (110) surface, anatase TiO_2 (204) surface, and rutile TiO_2 (101) surface were cleaved from their bulk structures to construct the surface slabs. The surface layers were generated with sufficient thickness to preserve the bulk-like characteristics, while a vacuum layer was introduced along the surface normal direction to avoid artificial interactions between periodic images.

We have employed the VASP to perform all the spin-polarized density functional theory calculations within the generalized gradient approximation using the Perdew-Burke-Ernzerhof formulation. We have chosen the projected augmented wave potentials to describe the ionic cores and take valence electrons into account using a plane wave basis set with a kinetic energy cutoff of 400 eV. Partial occupancies of the Kohn-Sham orbitals were allowed using the Gaussian smearing method and a width of 0.05 eV. The electronic energy was considered self-consistent when the energy change was smaller than 10^{-6} eV. A geometry optimization was considered convergent when the force change was smaller than 0.05 eV/ $\text{\AA}$. Grimme's DFT-D3 methodology was used to describe the dispersion interactions among all the atoms. During structural optimizations of the surface models, the $2\times 2\times 1$ gamma-point centered k-point grid for Brillouin zone was used. The charge transfer between different components was evaluated using Bader charge analysis. The optimized heterostructure charge density was partitioned into atomic basins according to the Bader scheme, and the total charge variation of each component was obtained by summing the atomic Bader charges. The charge transfer amount (ΔQ) was calculated by comparing the Bader charges of each component before and after heterostructure formation.

S6. RCS simulation

The assessment of the electromagnetic energy attenuation capability of the prepared samples was conducted by simulating the radar cross-section using CST simulation software under far-field conditions. The simulation model featured a 2.18 mm thick absorbent coating on the top and a 2.00 mm thick perfect conductor layer on the bottom. Moreover, the model was square-shaped with a side length of 200 mm. Positioned in the X-O-Y plane, the plate of the model had a linearly polarized electromagnetic wave

incident from the Z-axis, with electric polarization propagating along the X-axis. The direction of the scattering wave was determined by the theta and phi angles. The field monitoring frequency was set at 14.24 GHz, and boundary conditions were left undefined in all directions.

S7. Electromagnetic Measurements

Calculation of the reflection loss value (RL) of the sample according to the transmission line theory to assess the EMWA capability [1, 2].

$$RL = 20\log|(Z_{in} - Z_0)/(Z_{in} + Z_0)| \quad (S1)$$

where Z_0 and Z_{in} were the impedance of free space and the input impedance of the material, respectively, as described by **Equation S2**.

$$Z_{in} = Z_0 \sqrt{\frac{\mu_r}{\epsilon_r}} \tanh(j \frac{2\pi f d \sqrt{\mu_r \epsilon_r}}{c}) \quad (S2)$$

where μ_r and ϵ_r were the relative complex permeability and the relative complex permittivity, respectively, f , d , and c referred to the EMW frequency, the thickness of the absorber and the light velocity in vacuum, respectively.

The RL_{min} values progressively shift towards lower frequency regions as the matching thickness increases. This phenomenon can be explained via the quarter-wavelength model by the following **Equation S3** [3].

$$t_m = \frac{n\lambda}{4} = \frac{nc}{4f_m \sqrt{|\mu_r| |\epsilon_r|}} (n = 1, 3, 5 \dots) \quad (S3)$$

where t_m denoted the matching thickness of material and f_m represented the peak frequency.

The attenuation constant (α) was an essential factor to evaluate the attenuation ability of EMWA materials (**Equation S4**) [4].

$$\alpha = \frac{\sqrt{2}\pi f}{c} \sqrt{(\mu_r''\epsilon_r'' - \mu_r'\epsilon_r') + \sqrt{(\mu_r''\epsilon_r'' - \mu_r'\epsilon_r')^2 + (\mu_r'\epsilon_r'' + \mu_r''\epsilon_r')^2}} \quad (S4)$$

Debye relaxation model fitting

To further understand the possible dielectric loss mechanisms, the ϵ' and ϵ'' can be expressed by **Equation S5** [5].

Equation S5:

$$\left(\epsilon - \frac{\epsilon_s + \epsilon_\infty}{2}\right)^2 + (\epsilon'')^2 = \left(\frac{\epsilon_s - \epsilon_\infty}{2}\right)^2 \quad (S5)$$

where ϵ_s was the static dielectric constants and ϵ_∞ represented the limiting frequency dielectric constants.

The normalized impedance is the key to determine whether the waves enter the interior of the material (**Equation S6-8**) [6].

$$|\Delta| = |\sinh^2(Kfd) - M| \quad (S6)$$

$$K = (4\pi\sqrt{\epsilon'\mu'} \sin \frac{\delta_e + \delta_m}{2}) / (\cos\delta_e \cos\delta_m) \quad (S7)$$

$$M = \frac{4\mu' \cos\delta_e \cos\delta_m}{(\mu' \cos\delta_e - \epsilon' \cos\delta_m) + \left[\tan\left(\frac{\delta_m - \delta_e}{2}\right)\right]^2 (\mu' \cos\delta_e + \epsilon' \cos\delta_m)^2} \quad (S8)$$

where δ_e ($\delta_e = \epsilon''/\epsilon'$) and δ_m ($\delta_m = \mu''/\mu'$) stand for the loss tangent values of the permittivity and permeability, respectively.

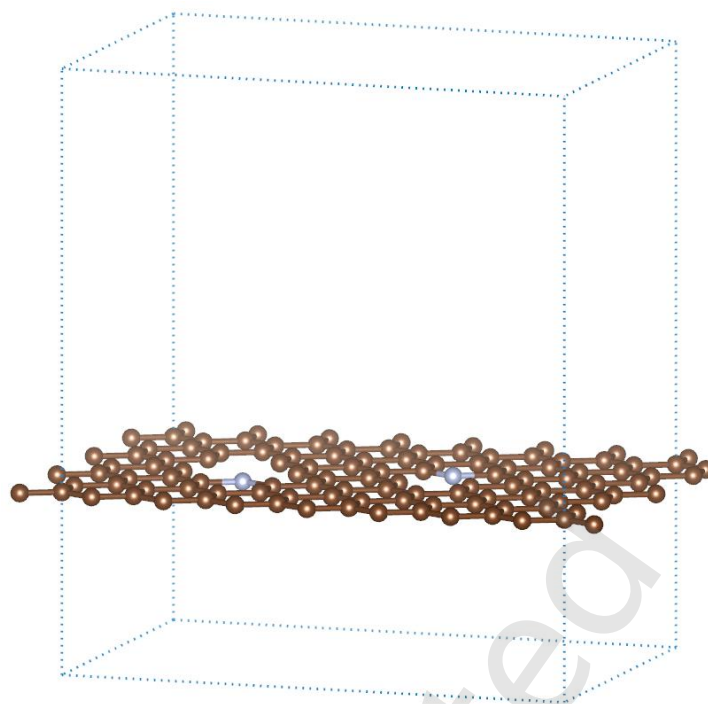


Figure S1 Model of NC.

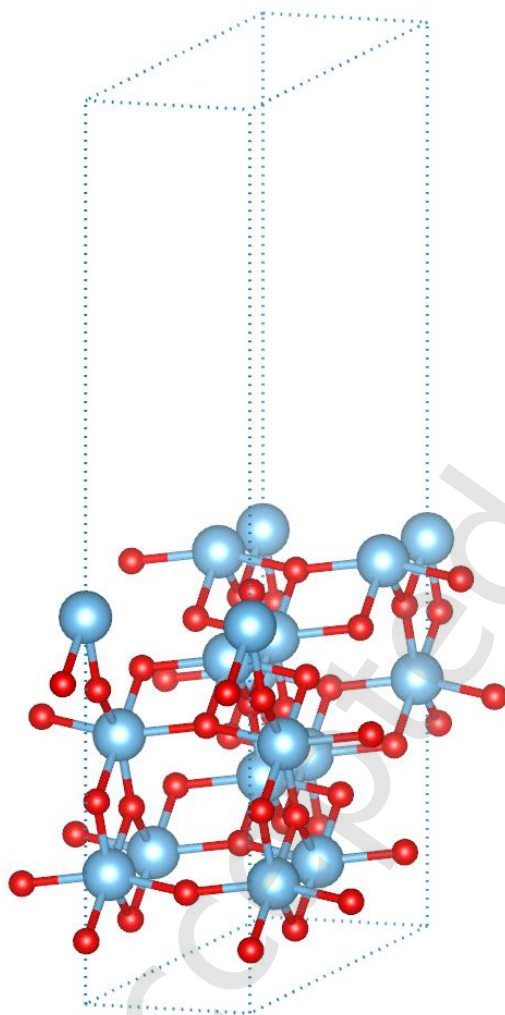


Figure S2 Model of A-TiO₂.

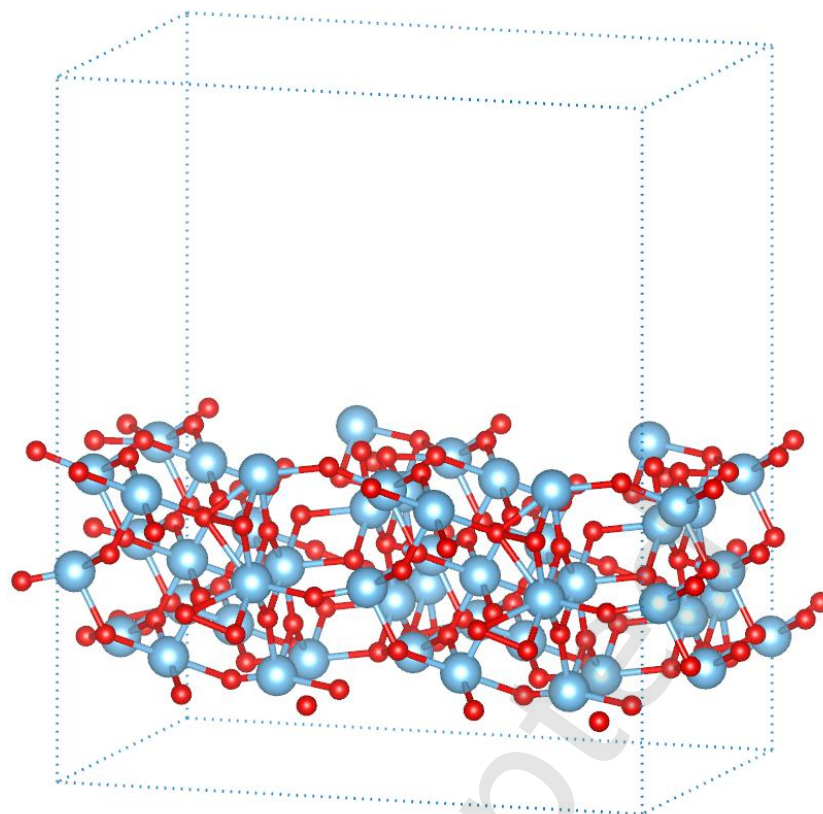


Figure S3 Model of A/R-TiO₂.

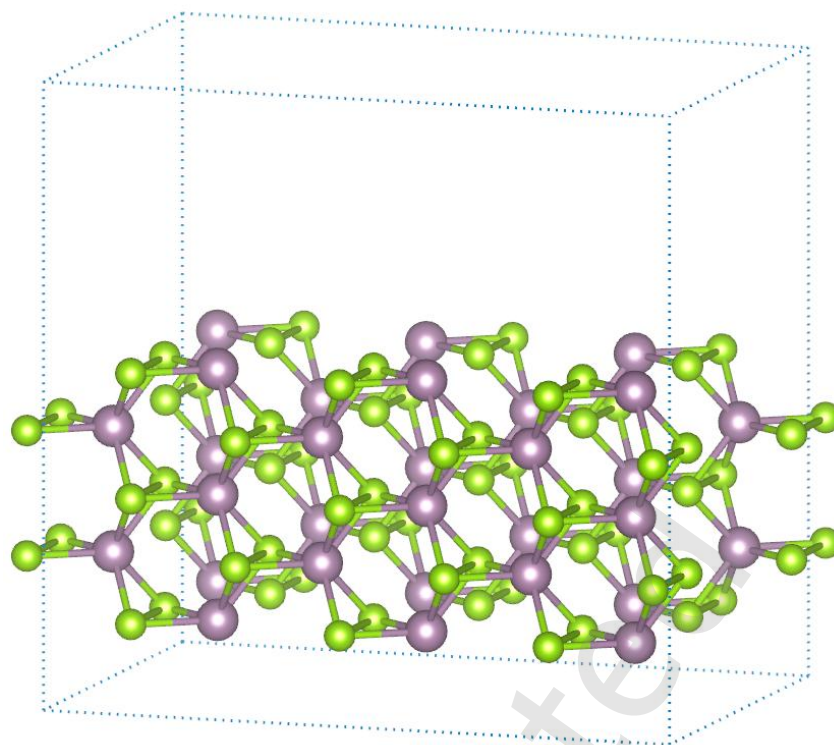


Figure S4 Model of MoSe₂.

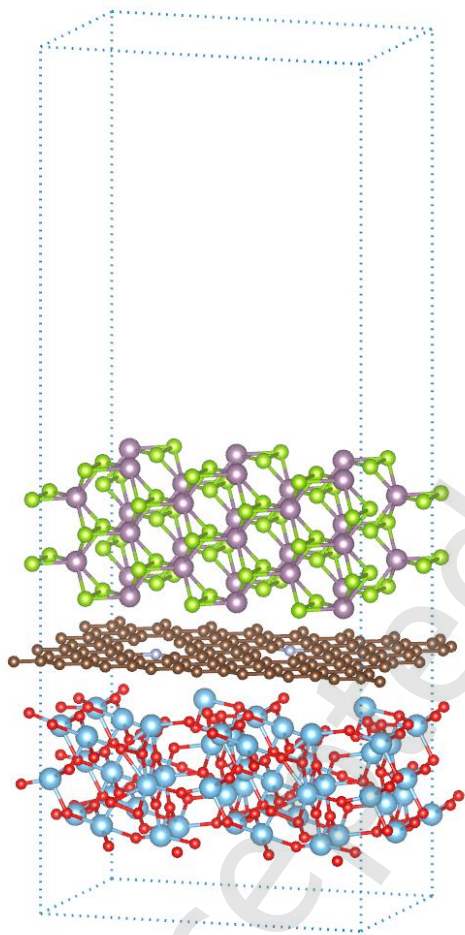
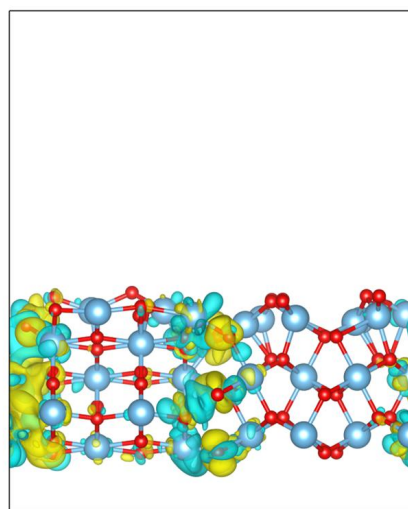


Figure S5 Model of MoSe₂/NC/A/R-TiO₂



0.278e

Figure S6 Charge density difference analysis and at A/R-TiO₂ heterointerface.

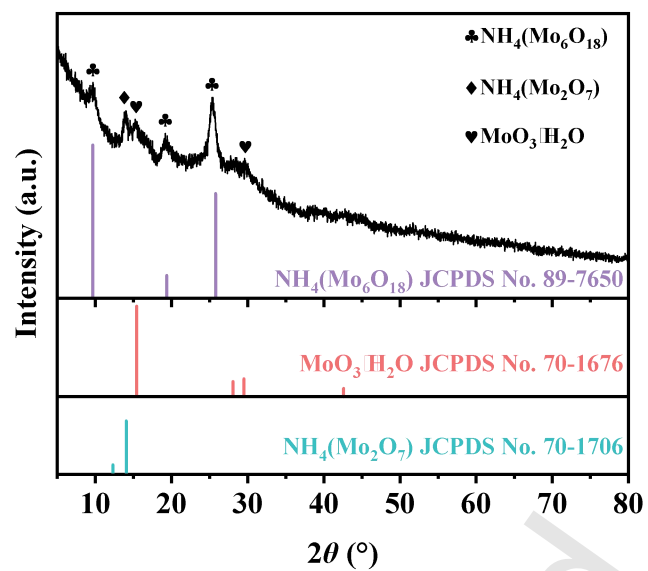


Figure S7 XRD patterns of Mo-PDA/TiO₂ precursor.

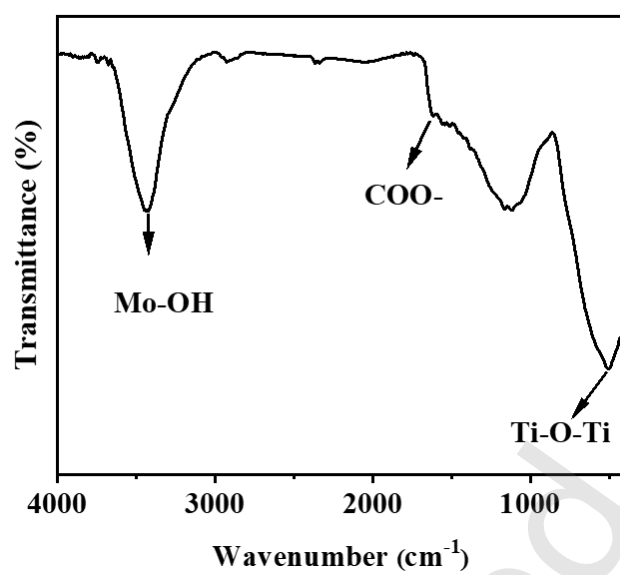


Figure S8 FT-IR spectrum of MNCT-20.

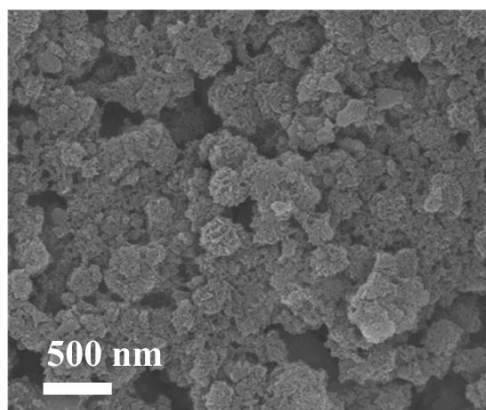


Figure S9 SEM images of (a) Mo-PDA/amorphous TiO₂

Just Accepted

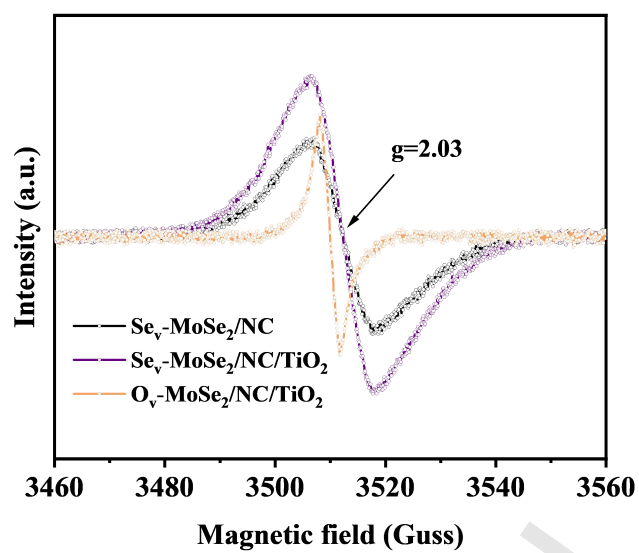


Figure S10 EPR spectra (g value)

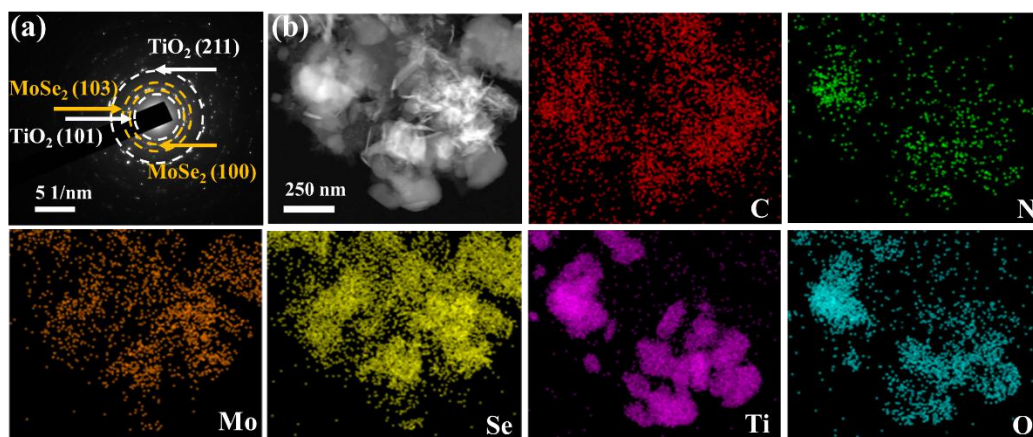


Figure S11 a) SAED and (b) mapping images of MNCT-20.

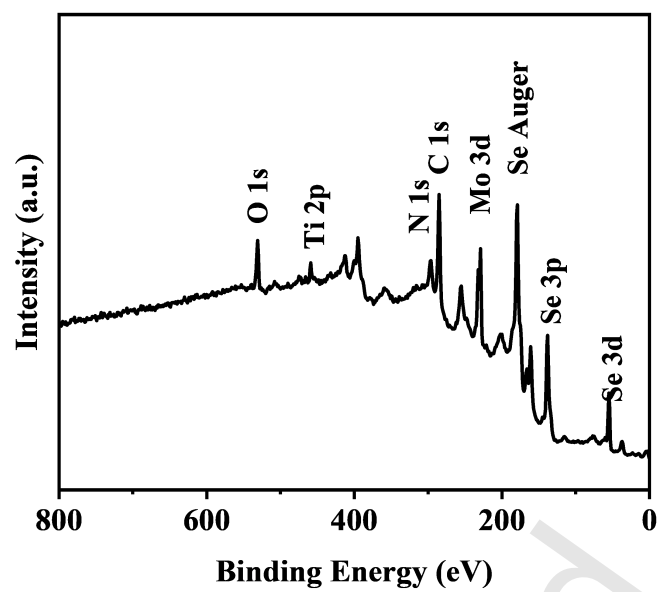


Figure S12 XPS survey spectrum of MNCT-20.

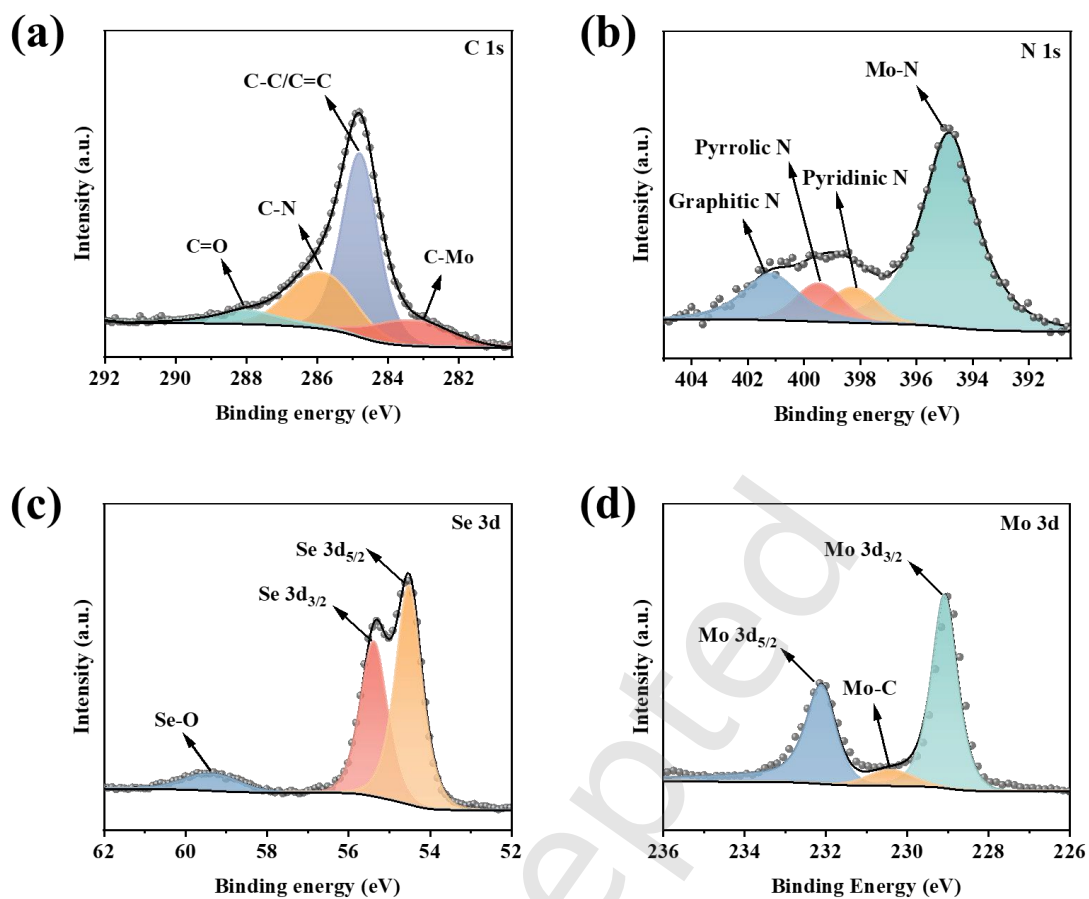


Figure S13 XPS spectra of c) C 1s, b) N 1s, c) Se 3d, and d) Mo 3d in MNCT-20.

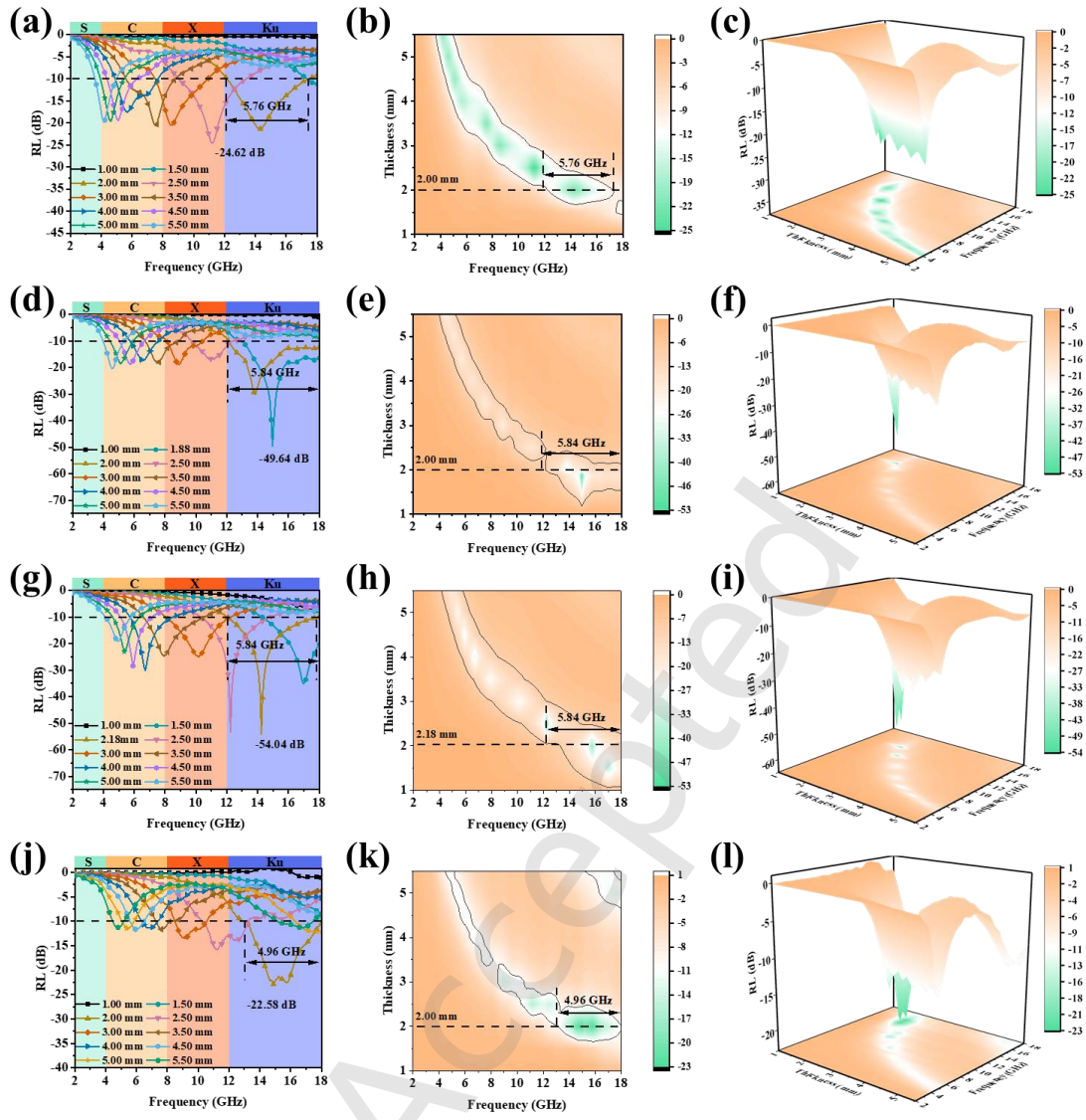


Figure S14 The 2D and 3D RL plots of (a-c) MNCT-12, (d-f) MNCT-16, (g-i) MNCT-20, and (j-l) MNCT-24.

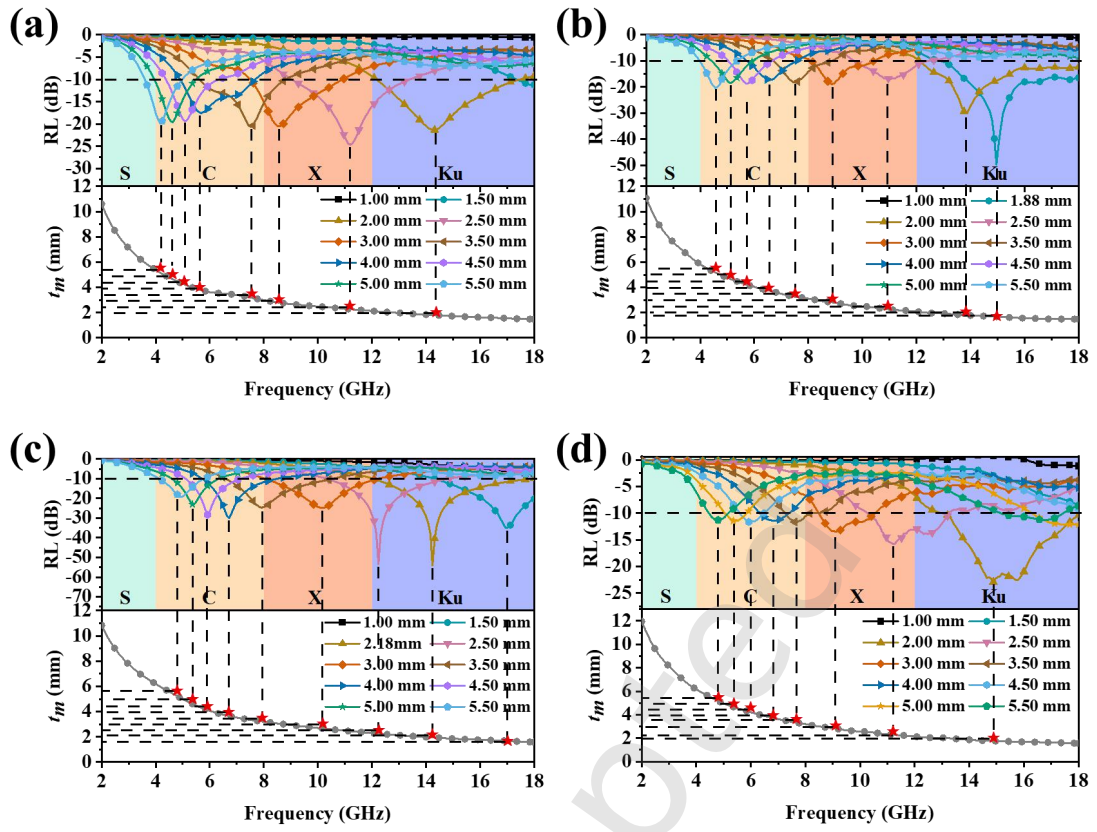


Figure S15 The quarter-wavelength matching plots of (a) MNCT-12, (b) MNCT-16, (c) MNCT-20 and (d) MNCT-24

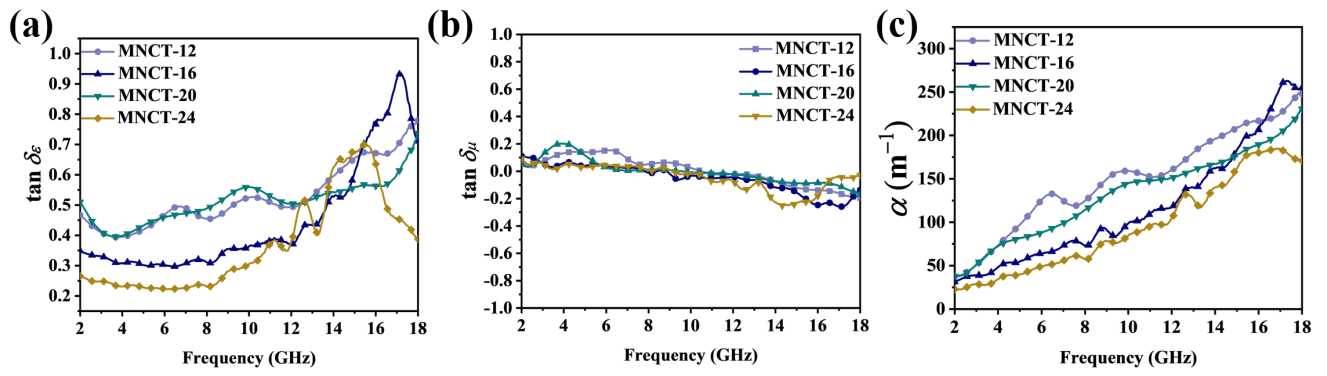


Figure S16 a) $\tan \delta_\epsilon$, b) $\tan \delta_\mu$, and c) α for MNCT-12, MNCT-16, MNCT-20, and MNCT-24 at 2.00-18.00 GHz.

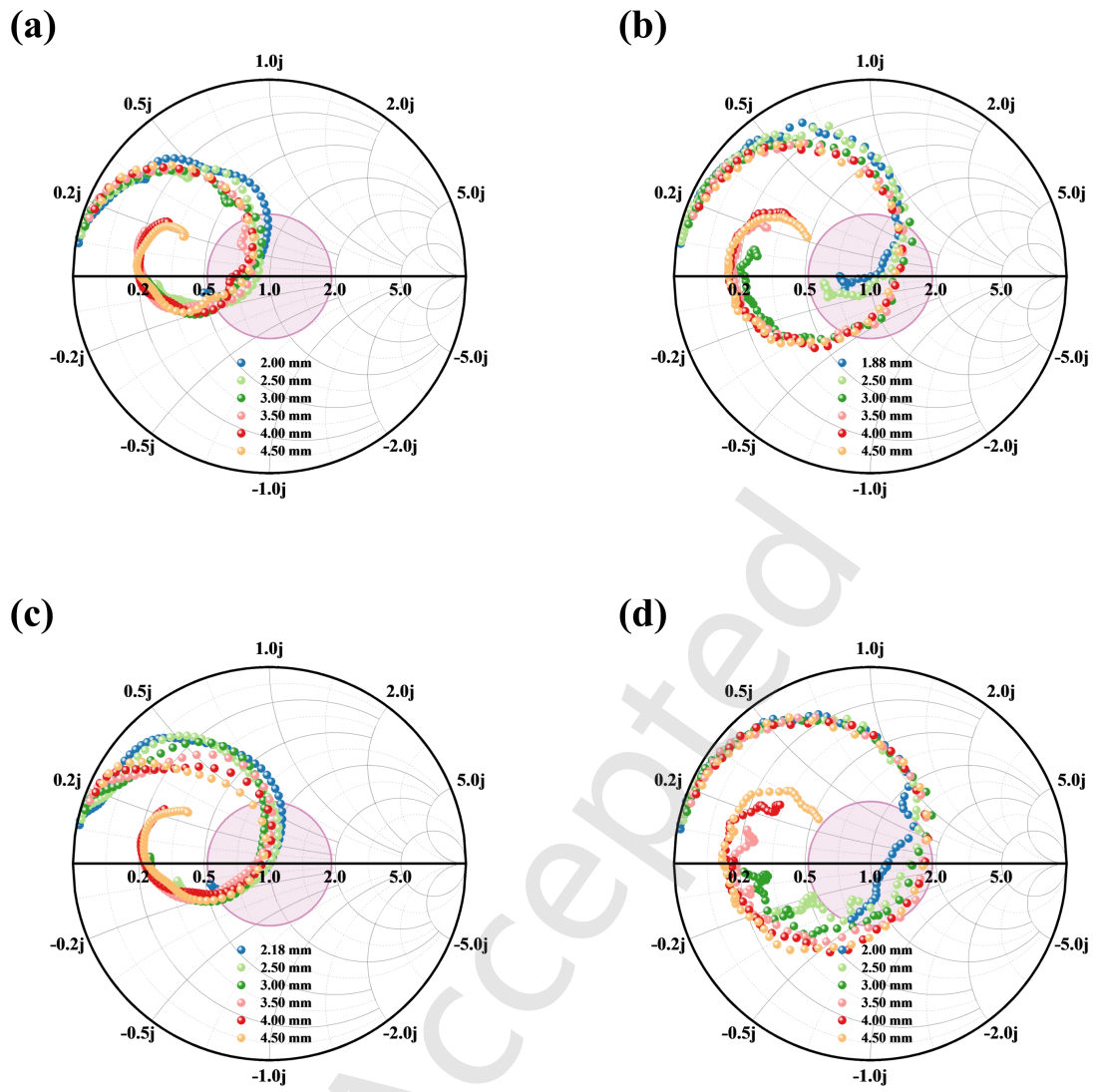


Figure S17 Smith chart of a) MNCT-12, b) MNCT-16, c) MNCT-20, and d) MNCT-24.

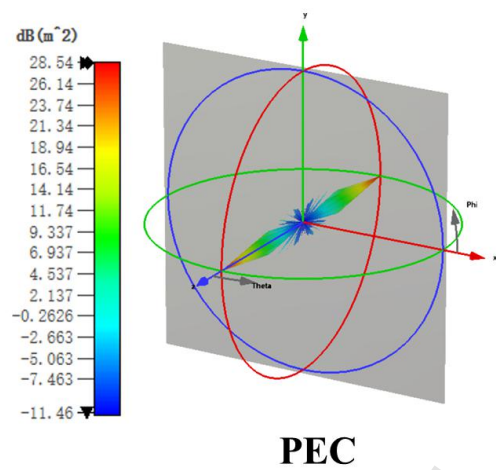


Figure S18 3D RCS plots for b) PEC substrate.

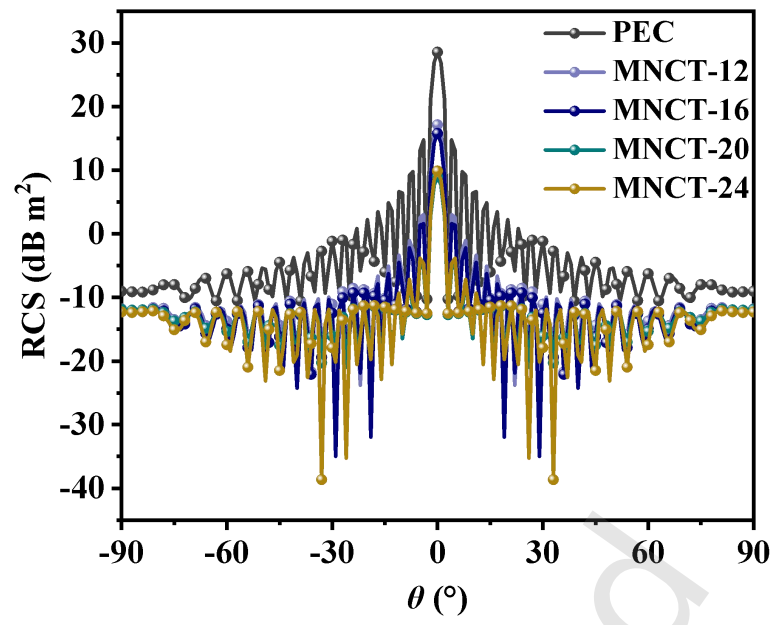


Figure S19 Simulated RCS values of all samples under certain detecting angles.

Table S1. Phase content of TiO₂ in MoSe₂/NC/TiO₂ composites

Samples	I_A	I_R	$W_A\%$	$W_R\%$
CT-12	4273	4253	53.14	46.86
MNCT-16	8973	7568	51.23	48.77
MNCT-20	9045	7142	52.87	47.13
MNCT-24	11283	8407	54.31	45.69

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