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Editorial

The electrical properties and charge transport mechanism of MXenes

Two-dimensional (2D) transition metal carbides and/or nitrides (MXenes) have exhibited many outstanding merits, including good conductivity, tunable bandgap, high electric capacity and optical transparency [1,2]. In the past several years, MXenes have shown promising advantages in the fields of energy storage, electrocatalysis, electromagnetic shielding, and (opto-)electronic devices. These excellent properties can be tuned by controlling the chemical composition, shape and size of the nanosheets, defects, boundaries, and surface functional groups, *etc*.

2D MXene nanosheets can be obtained by selectively etching away the A elements from their parent ternary phase precursors and always terminate with surface functional groups such as -OH, -F and -O. Generally, non-terminated MXenes are normally metallic with a high density of states near the Fermi surface, and the presence of surface functional groups makes MXenes the narrow-band semiconductors. Friedman *et al.* [3] revealed that Nb_2CT_x had an intrinsic conductivity of ~60 Ω^{-1} cm^{-1}, and an intrinsic carrier density of 10^{20} cm^{-3} with the carriers strongly localized due to the disorder and nanoflake boundaries. Short-range, intra-flake free carrier mobility was found to be 30±4 cm^2 V^{-1} s^{-1}, while the flake-boundaries and the disorder suppressed the long-range (inter-flake) mobility to 2.4 ± 0.4 cm^2 V^{-1} s^{-1}. Furthermore, theoretical studies have predicted the efficient band-like transport in MXenes, while device measurements revealed that the conductivity increased at elevated temperature, which was attributed to the thermally activated hopping-type transport in MXenes [4]. This debate between the theoretical and experimental results has sparked issues regarding the nature of the charge carriers and charge transport mechanism of MXenes. Understanding the charge transfer mechanism of MXenes can help to optimize the electrical properties of materials. Clarifying the charge transfer mechanism of MXenes at different temperatures can guide their application in fields such as electronic, optoelectronic devices, energy storage, and electromagnetic shielding, ensuring the stability and performance of the devices. Therefore, the fundamental understanding of electronic properties and charge transport mechanism in MXenes is essential for the fundamental studies and a variety of applications.

Recently, a unified understanding of conductivity and charge transport mechanism in MXenes by employing ultrafast terahertz and static electrical transport measurements has been proposed [5]. This work revealed that the short-range, intra-flake charge conduction in MXenes was band-like transport, while the long-range, inter-flake transport occurred *via* the thermally activated hopping process (Fig. 1a) which limited the charge percolation across the MXene flakes. Due to the presence of charge carriers, it can induce lattice distortion through coulomb interaction, known as polarons. The carrier-phonon coupling constant α characterizes the strength of the coupling between the charge carriers and longitudinal optical (LO) phonons. For the weak coupling ($\alpha < 6$), large polarons are formed. Considering the Fröhlich polaron theory for MXene materials, different types of MXenes have the similar dielectric constants, which leads to the weak coupling between the charge carriers and phonons in MXenes, thereby leading to the formation of large polarons (Fig. 1b). The formation of large polarons in the MXene fundamentally affects the intrinsic charge transport. Despite high density of defects existing in MXenes, the charge carriers may be protected by large polarons, which effectively screens the defect potential and reduces the charge scattering, thus improving charge transfer efficiency. For the semiconducting $Nb_4C_3T_x$, the selected-area electron diffraction pattern demonstrates the high crystallinity and hexagonal symmetry ($P6_3/mmc$), in line with typical MXene structures (Fig. 1c). The photoexcited electrons of $Nb_4C_3T_x$ result in a positive photoconductivity. While for the metallic $Ti_3C_2T_x$, the transient photoconductivity decreases and gives rise to a negative conductivity (Fig. 1d). The photoconductivity of $Nb_4C_3T_x$ (Fig. 1e) decays swiftly within several picoseconds and then slowly decays, which is attributed to the trapped free carriers at defects. The transient photoconductivity decrease in $Ti_3C_2T_x$ confirms the metallic nature of $Ti_3C_2T_x$ (Fig. 1f). The LO-phonon scattering dominates the charge transport over the entire temperature range, while the impurity scattering becomes notable only at the lower temperatures ($T < 150$ K). The transient, picosecond-duration terahertz field drives the charge carrier over approximately tens of nanometers. This provides the short-range, intra-flake charge transport information. Furthermore, the intra-flake charge transport is dominated by the band-like transport, which is mainly influenced by the LO phonons scattering for both semiconducting and metallic MXenes. Moreover, static electrical transport studies provide information on the long-range charge carrier conductance over macroscopic distances. It was investigated that the long-range, inter-flake charge transport was relevant with thermally activated hopping, which was the rate-limiting step for charge percolation through devices consisting of many MXene flakes.

In summary, MXenes exhibit the amazing prospects in various fields due to their excellent merits. The electronic properties, particularly the conductivity and the presence of large polarons in MXenes have been elucidated, and the intra-flake and inter-flake charge transport mechanism of MXene network was also clearly revealed. This is of great significance for the further fundamental

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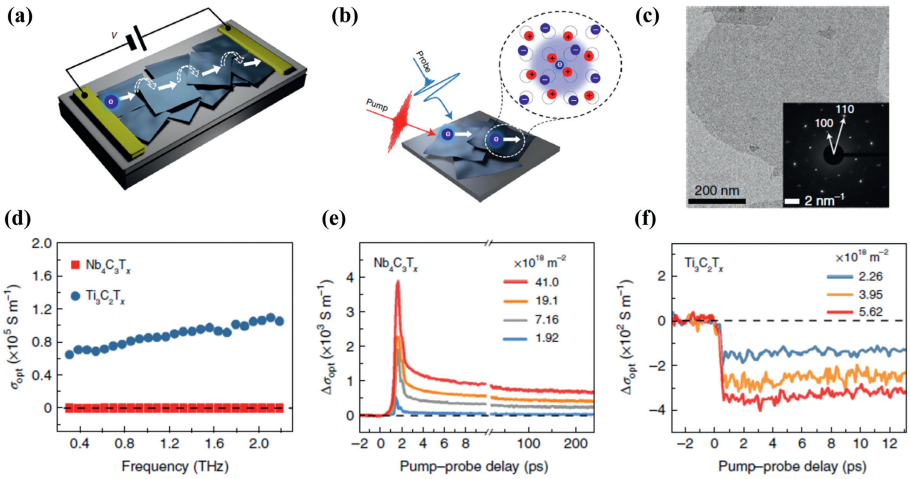

Fig. 1. (a) Schematic of charge transport within the network of MXene flakes. The inter-crystallite charge carrier hopping was indicated by the dashed arrows. (b) Scheme for ultrafast OPTP experiments to characterize the intra-MXene flake transport of charge carriers. Inset: the formation of a large polaron. (c) TEM image of $Nb_4C_3T_x$ MXene. Inset: corresponding SAED pattern. (d) Static terahertz conductivity of $Nb_4C_3T_x$ and $Ti_3C_2T_x$ MXene thin films. The fluence-dependent, time-resolved photoconductivity of (e) semiconducting $Nb_4C_3T_x$ and (f) metallic $Ti_3C_2T_x$ thin films, following 1.55 eV photoexcitation at room temperature. Reprinted with permission [5]. Copyright 2022, Nature.

research on 2D MXenes and various applications in electronic, optoelectronic, and energy devices.

Declaration of competing interest

The authors declare no conflict of interest exists and state that the article is original, unpublished, and not being considered for publication elsewhere.

All authors have participated sufficiently in this work to take public responsibility for it. All authors have reviewed the final version of the manuscript and approved it for publication.

CRediT authorship contribution statement

Bowen Song: Resources. **Chenxu Shi:** Data curation. **Yinghao Qu:** Formal analysis. **Hongjun Liu:** Conceptualization. **Hui Yang:** Conceptualization. **Xiaoming Wu:** Supervision. **Xijun Liu:** Supervision.

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