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ABSTRACT

Superconducting Mo-based MXenes have been intensively investigated due to their superior $T_c$ values compared with other MXenes. This work reports the unexpectedly strong electron-phonon coupling (EPC) and the highest $T_c$ record ($\approx 38$ K) among the MXenes revealed in the 2H-Mo$_2$N under biaxial stress. At first, its excellent mechanical properties are demonstrated with an ideal strength of 37 GPa and elastic modulus of 438 GPa. We found that the nature of covalent bonding between the N atoms contributes to the extraordinary stiffness and elasticity of 2H-Mo$_2$N compared with the 1T counterpart. Subsequently, EPC and corresponding $T_c$ are elucidated upon the dynamically stable strain range. For strain-free 2H-Mo$_2$N, the EPC constant ($\lambda$) and $T_c$ are 1.3 and 22.7 K, respectively. This $T_c$ is significantly higher than those of 2H-Mo$_2$C (4.3 K), 1T-Mo$_2$N (16.8 K), and other pristine MXenes. The material exhibits substantial improvement in $\lambda$ and $T_c$ when subjected to compressive and tensile stresses. The obvious strong EPC with $\lambda$ over 2.0 occurs at strains of -4%, -2.5%, and 5%, yielding $T_c$’s of 37.8, 35.4, and 28.9 K, respectively. Our findings suggest that the strain-dependent feature and energy levels of electronic bands play an essential role in enhancing EPC. Moreover, the stronger EPC in Mo$_2$N compared with Mo$_2$C is clarified based on lattice vibrations. Therefore, this work paves a practical approach for designing 2D superconducting materials using tuning atomic recipes and strain-dependent engineering.

Introduction

Superconductivity is a physical phenomenon in which the electric current can flow through a superconducting material with zero resistance below a specific superconducting critical temperature ($T_c$). The Bardeen-Cooper-Schrieffer (BCS)-type superconductors have been successfully described by the electron-phonon coupling (EPC), which creates the Cooper pairs. After MgB$_2$ was discovered by processing the $T_c$ of 39 K$^{1,2}$, one of the feasible routes of hunting the high-$T_c$ conventional superconductors is to consider the two-dimensional (2D) superconducting materials. Significant discoveries such as NbSe$_2$ few layers (3 - 7 K)$^{3,4}$, MgB$_2$ monolayer (20 K)$^5$, Mg$_2$B$_6$C$_2$ monolayer (47 K)$^6$, and hydrogenated MgB$_2$ monolayer (67 K)$^7$ have been reported. The advantage of this path is more practical than that of the rare-earth polyhydrides, which must be operated at
extremely high pressure to attain the high-\(T_c\).\(^{8-12}\)

\(\text{Mo}_2\text{X}\)-based MXenes \((\text{X} = \text{C and N})\) have been attractive because they process many promising properties, such as visible-light photocatalysis for \(\text{H}_2\) production\(^\text{13}\), thermoelectricity\(^\text{14,15}\), electrochemical catalysis\(^\text{16-19}\), and energy storage\(^\text{20,21}\). Moreover, \(\text{Mo}_2\text{C}\) and \(\text{Mo}_2\text{N}\) exhibit superconducting materials with significantly high \(T_c\) among the MXene members. Experimentally, 2D ultrathin \(\alpha\)-\(\text{Mo}_2\text{C}\) was successfully synthesized with \(T_c\) around 3-7 K\(^\text{22}\). Its \(T_c\) proportionally depends on sample thickness. As suggested by \textit{ab initio} calculations, two monolayers are possible, namely tetragonal (1T) and hexagonal (2H) structures. The 2H has been proposed to be more energetically favorable in both \(\text{Mo}_2\text{C}\) and \(\text{Mo}_2\text{N}\)\(^\text{23-25}\). These two phases differ by the position of a Mo atom as described in Fig. 1. The \(T_c\) values of 1T and 2H of \(\text{Mo}_2\text{C}\) were calculated to be 7.1 K\(^\text{26}\) and 3.2 K\(^\text{27}\), respectively. For instance, the \(T_c\) of 1T-\(\text{Mo}_2\text{N}\) was theoretically reported as 16 K\(^\text{28}\). Interestingly, replacing C with N can enhance the \(T_c\) of the 1T-\(\text{Mo}_2\text{X}\) more than two times. Moreover, other forms of metal nitride; for example, \(\text{W}_2\text{N}\) also had been reported to be strong EPC with the \(T_c\) about 22-38 K\(^\text{28,29}\). These findings induce more investigations of metal nitrides, particularly the 2H-\(\text{Mo}_2\text{N}\), which is more stable than another and has not yet been investigated in superconductivity.

Incorporating strain engineering into MXenes and other 2D materials enables tuning the electronic band structures, which intrinsically change physical properties. Based on density functional calculations, the spin-gapless semiconductor of \(\text{T}\text{I}\text{I}\text{C}\) could be induced by biaxial strain \((\varepsilon)\) over 2%\(^\text{30}\). The application of compressive strain caused \(\text{Hf}_2\text{CO}_3\) and \(\text{Zr}_2\text{CO}_3\) to transition from semiconductors to metals\(^\text{31}\). The utilization of biaxial stress can induce indirect-to-direct bandgap transitions in \(\text{M}_2\text{CO}_3\) \((\text{M}=\text{Sc}, \text{Ti}, \text{and} \text{Cr})\)\(^\text{32}\). The calculated \(T_c\) value of \(\text{Nb}_2\text{CO}_3\) was increased by 18 K under applying a biaxial tensile strain of 4%\(^\text{33}\). Moreover, a novel method based on machine learning interatomic potentials (MLIPs)\(^\text{34}\) has been achieved to study the mechanical and failure behavior of nanostructures at a continuum scale\(^\text{35}\) and succeed in examining the flexoelectric and piezoelectric properties of \(\text{MSi}_2\text{N}_4\) \((\text{M} = \text{W, Cr, and} \text{Mo})\)\(^\text{36}\). Therefore, the aforementioned examples demonstrate that applying strain has profound consequences on the tuning in various physical properties of 2D materials.

In this work, we systematically investigate the strain-dependent \(T_c\) of 2H-\(\text{Mo}_2\text{N}\) by using density functional theory. Additionally, we examined how the presence of N affects the electron-phonon coupling (EPC) as compared to C in \(\text{Mo}_2\text{X}\), by studying the vibrational modes of X atoms. The structural, mechanical, and electronic properties are also calculated. Based on our findings, there is a promising path towards the development of superconductors based on MXene.

**Methods**

The vacuum-slab model, stress-strain response, and mechanical properties were performed in detail following Supplementary Information (SI). We used the CASTEP code\(^\text{37}\) with ultrasoft pseudopotential\(^\text{38}\) as the electronic configurations of Mo: \(4s^2 \; 4p^6 \; 4d^5 \; 5s^1\) and N: \(2s^2 \; 2p^3\) under GGA-PBE scheme\(^\text{39}\). A dense Brillouin-zone (BZ) sampling grid with a spacing of \(0.04 \times 2\pi\) Å\(^{-1}\) and an energy cutoff \((E_{\text{cut}})\) of 500 eV were utilized for the sufficiently accurate structural optimizations. The magnetic property was accounted for by considering the effect of spin-polarization across the calculated strains. Grimme’s scheme\(^\text{40}\) was used to calculate the van der Waals (vdW) correction as part of the analysis. To ensure dynamic stability, phonon dispersion was evaluated through the use of supercell and finite displacement methods, with a higher degree of accuracy achieved through the use of parameters such as \(5 \times 10^{-8}\) eV/atom for energetic convergence, and 1 meV/Å for force convergence. The isotropic Eliashberg theory was used to investigate phonon-mediated superconductivity by utilizing the Quantum Espresso (QE) code\(^\text{41}\). The plane-wave basis set had an \(E_{\text{cut}}\) of 80 Ry. The EPC matrix elements were computed using an \(8 \times 8 \times 8\) q-mesh in the first Brillouin zone (BZ), while the individual EPC matrices were sampled with a \(64 \times 64 \times 4\) k-points mesh. We employed a Gaussian broadening parameter of 0.02 Ry to assess the electron-phonon interaction by integrating over the Fermi surface (FS). The FS was visualized using the FermiSurfer code\(^\text{42}\). Then, the \(T_c\) values of 2H-\(\text{Mo}_2\text{N}\) versus biaxial strains are calculated using the Allen-Dynes formula\(^\text{43}\). This formula needs the input parameters, including the integration of the lambda \((\lambda)\) and the logarithmic average of the spectral function \((\omega_{\text{log}})\), which are solved by the isotropic Eliashberg theory, as obeyed by equations 3S-7S in SI. Moreover, the \(T_c\) of strong EPC \((\lambda>1.5)\) was obtained by a modified theory \((T_c=\eta\frac{f_1 f_2}{T_c})\)\(^\text{44}\), as expressed in equation 8S. The Coulomb pseudopotential parameter, denoted as \(\mu^*\), has been assigned a value of 0.10.

**Results and Discussion**

We began by evaluating the electronic properties of 1T- and 2H-\(\text{Mo}_2\text{N}\) by analyzing the partial density of states (PDOS) while accounting for the influence of spin polarization. As shown in Figure 1S, both configurations exhibit non-magnetic metals with symmetrical spin up and spin down, with the PDOS intersecting at the Fermi level. Then, the energetic stability of both \(\text{Mo}_2\text{N}\) structures is investigated. By calculating the formation energies \((E_{\text{form}})\) of both phases regarding the total energies of \(\text{N}_2\) and bcc-Mo, the \(E_{\text{form}}\) values of 1T and 2H phase are \(-2.25\) eV/f.u. and \(-1.98\) eV/f.u., respectively. Our findings suggest that the 2H phase is more stable than the 1T phase due to its lower \(E_{\text{form}}\). It was also observed that the 2H phase is energetically preferable when subjected to biaxial strains, as evidenced by the relative total energy and enthalpy in Figure 2S of SI. Furthermore, it was found that the free-strain energy of the 2H phase is lower than that of the 1T phase by 90 meV/atom for both with and without...
Figure 1. Top and side views of atomic arrangements of 2H (a, b) and 1T (c, d) phases in which the small brown balls represent C atoms, and the bigger pink and blue balls refer to Mo atoms at the top and bottom layers, respectively.

Figure 2. Stress-strain responses of the 2H-Mo₂N and 1T-Mo₂N (a), and the inset shows the linear fitting for evaluating elastic modulus. Phonon dispersion at unstressed condition (b) with identifying the zones of atomic contributions.
Figure 3. Electron localization function (ELF) of 2H-Mo\textsubscript{2}N (a-b) and 1T-Mo\textsubscript{2}N (c-d). The cross sections consist of the (001) plane intersecting at the N layer (a, c) and the midpoint between the Mo and N layers (b, d).

vdW correction. This result agrees with a previous report\textsuperscript{45} indicating that the 2H-Mo\textsubscript{2}N should be easier to synthesize than another.

The 2H-Mo\textsubscript{2}N has a lattice constant ($a$) of 2.818 Å and a thickness ($d$) of 5.442 Å at 0% strain ($a$=2.786 Å and $d$ = 5.587 Å for the 1T-Mo\textsubscript{2}N). Subsequently, the stress-strain response shown in Fig. 2a provides the ideal stress, i.e., $\sigma_{\text{max}}$ of 37 GPa at 12% strain and elastic modulus (E) of 438 GPa, which are significantly high regarding those of the 1T-Mo\textsubscript{2}N ($\sigma_{\text{max}}$=19 GPa at 7% and E = 292 GPa). These comparative enhancements of mechanical properties of 2H-Mo\textsubscript{2}N are attributed to the centrosymmetric configuration of 2H atomic layers, similar to the cases of Mo\textsubscript{2}C\textsuperscript{24} and W\textsubscript{2}C\textsuperscript{46}. In addition, the electron localization function (ELF)\textsuperscript{47} was processed in certain planes to examine the chemical bonds of these two phases. The ELFs of the 1T and 2H structures of Mo\textsubscript{2}N MXene are illustrated in Fig. 3(a-d), indicating a significant covalent N-N bond in the 2H phase (Fig. 3a) but not in the 1T phase (Fig. 3c). However, the interconnections between the N and Mo layers remain consistent in both phases, as shown in Figs. 3b and 3d. Hence, it can be addressed that the nature of covalent bonding between the N atoms contributes to the extraordinary stiffness and elasticity of 2H-Mo\textsubscript{2}N.

The dynamical stability of the 2H phase is verified in the unstressed structure as displayed in Fig. 2b. It is found that the vibrations of heavier Mo atoms dominate at low frequencies up to 8 THz, whereas that of a lighter N atom contributes at a higher frequency range of 11-17 THz. Furthermore, stable regimes of both compressive and tensile strains are evaluated, as shown in Fig. 3S. It can be seen that the absence of negative phonon frequency is in the strain range of -5% to 5%, indicating that 2H-Mo\textsubscript{2}N should be dynamically stable within this strain range. Additionally, the relative energy and enthalpy as the functions of strain support the more energetically stable 2H-Mo\textsubscript{2}N throughout this strain range, as shown in Fig. 2S.

The electronic band structure (EBS), as shown in Fig. 4a verifies the insignificant effect of spin-orbit coupling (SOC), corresponding with the previous studies in 1T-Mo\textsubscript{2}N\textsuperscript{26}. Therefore, the SOC will not be included in further calculations. The partial density of states (PDOS) reveals that around the Fermi level (FL) is mainly dominated by the 4$d$-Mo states. Moreover, minor distributions by 5$s$-Mo and 4$p$-Mo states are below the FL, and 2$p$-N states are above the FL. The FL of the unstressed 2H-Mo\textsubscript{2}N is located near the local minimum of the total DOS valley. Consequently, the FL is expected to be easily tuned to higher electronic densities. Applying strain strongly affects band structures respecting the referent bands at $\varepsilon = 0\%$, as seen in Fig. 4b-e. At the tensile strain of 5%, the high-energetic valence band is enhanced to higher energies at the H point, and the low-energetic conduction bands are stretched out with having the lowest touching point with the FL at the H point. Meanwhile, the valence bands at the H point decrease to lower energy at compressive strains, but those at the $\Gamma$ point are pushed up to the FL.

To gain insights into the electronic distribution around the FL, the FS of 2H-Mo\textsubscript{2}N are visualized at varying strains, as shown in Fig. 4f-i. At the reference of $\varepsilon = 0\%$, FS consists of five distinctly different pockets: (i) a pancake-type electron pocket, (ii) a larger circle electron pocket, and (iii) a nest electron pocket around $\Gamma$ point, (iv) six-hole type pockets around H point, and (v) six-hole type pockets around M point, as seen in Fig. 4h. At a tensile strain of 5% (Fig. 4i), pocket (i) significantly extends and nearly touches pocket (ii), and pocket (iii) climbs moderately. Moreover, pockets (iv) and (v) dramatically decline,
respecting the case that \( \varepsilon = 0\% \). At the compressive strains of -2.5\% (Fig. 4g) and -4\% (Fig. 4f), pocket (i) is gradually decreased, and pocket (ii) is transformed to be a nest. Interestingly, an additional nest electron pocket emerges around \( \Gamma \) point, corresponding with a sinking band at this zone. Furthermore, pocket (iii) is moderately reshaped to be a like-hexagon shape at -4\%. It is worth noting that the FS has one more electron pocket around \( \Gamma \) at compressive strains. Hence, it should be noted that the magnitude of both the electron and hole pockets can be attributed to the evolution of superconductive parameters through a strain-induced electronic topological transition. One clear influence is the number of electron densities at the Fermi level (\( N_{E_f} \)).

In Fig. 7a, one can see that the electron and hole pockets on FS with their corresponding band features at calculated strains reflect the value of \( N_{E_f} \). Interestingly, the \( N_{E_f} \) can be rapidly enhanced by compressive strain and gradually increased by tensile strain. The rise in \( N_{E_f} \) at FL increases electron-phonon coupling (EPC) for this material. We will delve into this further.

The patterns of Eliashberg spectral function (\( \alpha^2 F(\omega) \)) of 2H-Mo\(_2\)N at calculated strains have a gap between the spectra contributed by vibrations of Mo and N atoms. The frequency distribution of \( \alpha^2 F(\omega) \) depends on the interaction between atoms, stretching out to higher frequency from tensioned to compressed structures. At stain-free condition, it has the widest gap and has a \( \lambda \) of 1.32, as displayed in Fig. 5c. We demonstrate the enhancement of EPC of 2H-Mo\(_2\)N regarding 2H-Mo\(_2\)C (\( \lambda = 0.58 \)) through the distribution of the phonon linewidth (\( \gamma_q \)), which proportionally contributes to \( \lambda \) and \( \alpha^2 F(\omega) \) as expressed by equations 4S, 6S, and 7S of SI. In Fig. 6a-b, We found that higher \( T_c \) of 2H-Mo\(_2\)N is interplayed by its stronger \( \gamma_q \) at \( \Lambda_1 \) mode (symmetrical bend) of Mo atoms, \( E' \) mode (asymmetrical stretch) of coupling of Mo and N atoms, and \( \Lambda''_2 \) mode (asymmetrical bend) of N atom. Moreover, according to equation 8S, because the lower frequency range of N respects the C atom, it results in stronger \( \lambda_{qv} \) in 2H-Mo\(_2\)N. Intriguingly, Fig. 5a, 5b, and 5d demonstrate that the \( \lambda \) values of 2H-Mo\(_2\)N at -4\%, -2.5\%, and 5\% strains are 2.00, 2.23, and 2.24, respectively. When observing the tendencies of \( \lambda \), it becomes apparent that more than 70% of its magnitude is primarily influenced by the vibrations of Mo atoms. On the other hand, the remaining contribution is attributed to the N atom, which exhibits a notable increase in the \( E' \) mode at the high-frequency region (indicated by the yellow shade). Based on their values, it is clear that these \( \lambda \) values display strong EPC behavior (\( \lambda_\lambda > 1.5 \)). This is a significant finding as it is the first theoretical study to uncover the presence of strong EPC in the bare MXene family. Full details of the relative parameters of EPC are listed in Table 1S.

Here, we plot the related superconductive parameters as a function of strain in Fig. 7a-b to clarify their strain dependencies. At 0\% strain, the \( \omega_{0eg} \) and \( T_c \) of 2H-Mo\(_2\)N are 227 cm\(^{-1}\) and 22.7 K, respectively. This \( T_c \) value is higher than the \( T_c \) of 1T-Mo\(_2\)N (\( T_c = 16.8 \) K with \( \omega_{0eg} = 248 \) cm\(^{-1}\) and \( \lambda = 0.98 \)) that is calculated in this work to validate the result of previous work (\( T_c = 16.0 \) K)\(^{26}\). Furthermore, it is discovered that the \( T_c \) of the 2H-Mo\(_2\)N is extremely higher than that of 2H-Mo\(_2\)C (\( T_c = 4.3 \) K),

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**Figure 4.** EBS and PDOS at (a) unstressed condition with SOC (solid-red line) and without SOC (dot-blue line), and strain-dependent EBS and FS at -4\% (b, f), -2.5\% (c, g), 0\% (d, h), and 5\% (e, i).
Figure 5. The $\alpha^2 F(\omega)$ (blue and yellow shades), $\lambda$ (solid orange line), and phonon density of states (PhDOS) (red and green dash lines) at -4% (a), -2.5% (b), 0% (c), and 5% (d) of 2H-Mo$_2$N. The blue and yellow shades represent the coupling modes with vibrations of Mo and N atoms, respectively.
Figure 6. Phonon dispersions of 2H phase of (a) Mo$_2$N and (b) Mo$_2$C with the decorative phonon linewidth ($\gamma_q$) represented by green balls, and (c) corresponding normal modes of atomic vibrations.

Figure 7. (a) The $\omega_{\log}$ and $N_{Ef}$, and (b) the $T_c$, $T_{cs}$, and $\lambda$ of 2H-Mo$_2$N as a function of strain.
as discussed before. Therefore, it is essential to mention that the $\lambda$ and $T_c$ of bare 2H-Mo$_2$N are significantly higher than other MXenes without surface functionalization and applying external stresses. At -2.5% and 5% strains, the $\omega_{\log}$ increases with increasing $\lambda$, which can be described by the connection of equations 5S and 7S. Moreover, it is found that the $\omega_{\log}$ increases with increasing $\lambda$, which is explicitly explained by equation 5S. By solving equation 3S, the $T_c$ values of 2H-Mo$_2$N are 34.5, 30.1, and 24.4 K for strains of -4%, -2.5%, and 5%, respectively. According to the strong EPC at these strain values, it is important to include the correction factors ($f_1$ and $f_2$) for obtaining a more plausible superconducting temperature ($T_{cs}$) as obeyed in SI. We find that the $T_{cs}$ significantly increases by 9% at $\epsilon$=-4% and 18% at -2.5% and 5% strains, as shown in Fig. 7b. The $T_{cs}$ values are 37.8, 35.4, and 28.9 K for strains of -4%, -2.5%, and 5%, respectively. This finding indicates that strain-induced electronic structures can increase the $T_{cs}$ of 2H-Mo$_2$N. The quantities of the correction and other related factors are also listed in Table 2S. It is important to note that compressive strain can cause 2D materials to ripple and buckle$^{48,49}$. To enable the use of this material and other 2D materials in practical applications, synthesizing planar 2D materials under internal compression presents a challenge.

**Conclusion**

The study has uncovered that 2H-Mo$_2$N possesses a strong electron-phonon coupling (EPC) when subjected to biaxial stress. The 2H-Mo$_2$N is considered because it is more energetically stable than another structure, 1T-Mo$_2$N. In addition, the exceptional strength of 2H-Mo$_2$N is demonstrated by its outstanding mechanical properties, with an ideal strength of 37 GPa and an elastic modulus of 438 GPa. The significant covalent bonding between the N atoms sets it apart from its 1T counterpart, giving it remarkable stiffness and elasticity. The 2H-Mo$_2$N processes to be a dynamically stable structure in the wide strain range of -5% to 5%. The application of stress plays an essential role in tuning the feature and energy level of electronic band structure (EBS), consequently enhancing EPC. A high record $T_{cs}$ of free-strain 2H-Mo$_2$N of 22.7 K is reported. The EBS, FS, and $N_{Ef}$ are carefully elucidated to advocate a strong EPC. The corrected critical temperature for strong EPC, $T_{cs}$, is evaluated, increasing superconducting temperatures by 9 - 18%. Our finding provides a new record for the highest $T_c$ among the MXene family. This result challenges further experiments to prove it and paves the guidance for developing the MXene-based superconductor for modern material applications.

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**Author contributions statement**

K.K.: Conceptualization, Investigation, Data curation, Writing – original draft, preparation, Revision, Methodology, Supervision. P.T.: Data curation, Investigation, Writing – original draft, Revision. T.B., R.A., and W.L.: Visualization, Revision, Software. T.K., R.S., and A.S.: Visualization, Revision.

**Additional information**

The authors declare no competing financial interests.

**Data availability**

The datasets used and/or analyzed during the current study are available from the corresponding author upon reasonable request.

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