Supplementary Material
Superconductivity in functionalized niobium-carbide MXenes

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Bulk Nb$_2$CCl$_2$ structures with $P6_3mmc$ and $P-3m1$ symmetries

![Diagram showing bulk Nb$_2$CCl$_2$ structures](image)

**Figure S1:** (a) Schematic representation of the periodic unit-cell of the Nb$_2$CCl$_2$ crystals with space group symmetries (a) $P6_3mmc$ and (b) $P-3m1$. The calculated phonon dispersion along with phonon density of states, and electronic band structures of Nb$_2$CCl$_2$ crystals with space group symmetries (c) $P6_3mmc$ and (d) $P-3m1$.

**Exfoliation energies ($E_x$)**

\[ E_x = \left( E_{\text{bulk}} - n^*E_{\text{2D}} \right)/N \]

- $E_{\text{bulk}}$ = Total energy of the bulk structure
- $E_{\text{2D}}$ = Total energy of the single layer
- $n$ = Number of layers in the bulk unit cell
- $N$ = Number of atoms in the unit cell of the bulk structure

| Materials     | $E_x$ (meV/Atom) |
|---------------|------------------|
| Nb$_2$CS$_2$  | -1.08            |
| Nb$_2$CCl$_2$ | -1.03            |
| Nb$_3$C$_2$S$_2$ | -0.53         |
| Nb$_3$C$_2$Cl$_2$ | -0.52       |

Note: Total energies were obtained using the PBE functional, without the inclusion of vdW interactions.
**Monolayer Nb\(_2\)CCl\(_2\)**

**Superconducting properties**
\[ ts\text{mear} = 0.0075 \text{ Ha} \; \mu' = 0.13 \; T_C = 9.6 \; K \]

(a) Periodic unit-cell
(b) Phonon dispersion
(c) Band structure
(d) Eliashberg function and e-ph coupling (\(\lambda\))

*Figure S2:* (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with e-ph coupling (size of red circles) and phonon density of states, (c) electronic band structure, and (d) Eliashberg function and integrated e-ph coupling constant (\(\lambda\)). The size of red circles is scaled with 1/100 for a better view. Here the red, grey, and green lines correspond to the Nb, Cl, and S atoms, respectively.

**Monolayer Nb\(_2\)CCl\(_2\)**

**The Fermi level dependent superconducting properties of monolayer Nb\(_2\)CCl\(_2\)**

(a) Eliashberg function and integrated e-ph coupling constant for Fermi level shifted by gating to 0, -70, and -110 meV. (b) The calculated superconducting transition temperature \(T_C\), along with electronic density of states at \(E_F\).

*Figure S3:* (a) Eliashberg function and integrated e-ph coupling constant for Fermi level shifted by gating to 0, -70, and -110 meV. (b) The calculated superconducting transition temperature \(T_C\), along with electronic density of states at \(E_F\).
Bulk-layered Nb$_2$CS$_2$

*The calculated nesting function*

![Graph showing calculated nesting function for Nb$_2$CS$_2$ (bulk).](image)

**Figure S4:** The calculated nesting function for Nb$_2$CS$_2$ (bulk).

Monolayer Nb$_2$CS$_2$

*The change in Eliashberg function and integrated e-ph coupling constant ($\lambda$) with applied strain*

| Strain | $T_c$ (K) |
|--------|-----------|
| (a) 0% | 10.7      |
| (b) 2% | 11.0      |
| (c) 4% | 12.0      |
| (d) -2%| 4.9       |

![Graphs showing Eliashberg function and integrated e-ph coupling constant for different strains.](image)

**Figure S5:** The calculated Eliashberg function and integrated e-ph coupling constant ($\lambda$) for different strain values (tensile (+) and compressive (-)). Here, $\mu^* = 0.13$ and $t_{\text{smear}} = 0.005$ Ha.
**Bulk Nb$_2$CSe$_2$**

**Superconducting properties**

\[ t_{\text{smear}} = 0.0015 \text{ Ha} \quad T_c = 0.0 \text{ K} \]

Figure S6: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with e-ph coupling (size of red circles) and phonon density of states, (c) electronic band structure, and (d) Eliashberg function and integrated e-ph coupling constant ($\lambda$). The size of red circles is scaled with 1/100 for a better view. Here the red, grey and green lines correspond to the Nb, Se, and C atoms, respectively.

**Monolayer Nb$_3$C$_2$**

**Superconducting properties**

\[ t_{\text{smear}} = 0.010 \text{ Ha} \quad T_c = 1.0 \text{ K} \]

Figure S7: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with e-ph coupling (size of red circles) and phonon density of states, and (c) Eliashberg function and integrated e-ph coupling constant ($\lambda$). The size of red circles is scaled with 1/100 for a better view. Here the blue, and red lines correspond to the Nb, and C atoms.
**Bulk Nb$_3$C$_2$Cl$_2$**

Space group $P-3m1$

**Phonon dispersion**

$t_{\text{smear}} = 0.0075$ Ha

(a) Periodic Unit-Cell

![Diagram of periodic unit-cell](image)

(b) Phonon dispersion

![ Phonon dispersion diagram](image)

Figure S8: (a) Schematic representation of the periodic unit-cell of the considered crystal. (b) The calculated phonon dispersion along with $e$-$ph$ coupling (size of red circles) and phonon density of states.

**Superconducting properties**

$t_{\text{smear}} = 0.0050$ Ha $T_c = 28.1$ K

(a) Periodic unit-cell

![Diagram of periodic unit-cell](image)

(b) Phonon dispersion

![ Phonon dispersion diagram](image)

(c) Band structure

![ Band structure diagram](image)

(d) Eliashberg function and $e$-$ph$ coupling ($\lambda$)

![ Eliashberg function diagram](image)

Figure S9: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with $e$-$ph$ coupling (size of red circles) and phonon density of states, (c) electronic band structure, and (d) Eliashberg function and integrated $e$-$ph$ coupling constant ($\lambda$). The size of red circles is scaled with 1/10 for a better view. Here the red, grey and green lines correspond to the Nb, S, and C atoms, respectively.
**Bulk Nb$_2$CCl$_2$**

The calculated electronic density of states and carrier doping level

![Graph](image)

**Figure S10**: The calculated electronic density of states and corresponding electron doping for bulk Nb$_2$CCl$_2$. Here, the Fermi level is set to 0 eV.

**Monolayer Nb$_2$CCl$_2$**

The calculated electronic density of states and carrier doping level

![Graph](image)

**Figure S11**: The calculated electronic density of states and corresponding electron doping for monolayer Nb$_2$CCl$_2$. Here, the Fermi level is set to 0 eV.
Monolayer Nb$_2$CCl$_2$

The change in band structure with tensile strain

| Tensile Strain (%) | Band Structure |
|--------------------|---------------|
| 0.00 %             | ![Band Structure](image1) |
| 0.25 %             | ![Band Structure](image2) |
| 0.50 %             | ![Band Structure](image3) |
| 0.75 %             | ![Band Structure](image4) |
| 1.00 %             | ![Band Structure](image5) |

**Figure S12:** The calculated band structures for different tensile strain values.
Monolayer Nb$_2$CCl$_2$

The change in Eliashberg function and integrated $e$-$ph$ coupling constant ($\lambda$) with tensile strain

| (a) 0.00% $T_c = 10.5$ K | (b) 0.25% $T_c = 11.8$ K |
|---|---|
| ![Graph](image1.png) | ![Graph](image2.png) |

| (c) 0.50% $T_c = 16.4$ K | (d) 0.75% $T_c = 25.6$ K |
|---|---|
| ![Graph](image3.png) | ![Graph](image4.png) |

| (e) 1.00% $T_c = 4.3$ K |
|---|
| ![Graph](image5.png) |

**Figure S13:** The calculated Eliashberg function and integrated $e$-$ph$ coupling constant ($\lambda$) for different tensile strain values. Here, $\mu^* = 0.13$ and $t_{smear} = 0.0075$ Ha.
The change in phonon dispersion with tensile strain

Figure S14: The calculated phonon dispersions for different tensile strain values.
Monolayer Nb$_2$CS$_2$

Superconducting properties
$t_{\text{smear}} = 0.0015$ Ha $T_c = 10.7$ K

Figure S15: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with $e$-$ph$ coupling (size of red circles) and phonon density of states, (c) electronic band structure, (d) Eliashberg function and integrated $e$-$ph$ coupling constant ($\lambda$). The size of red circles is scaled with 1/10 for a better view. Here the red, grey, and green lines correspond to the Nb, S, and C atoms, respectively.

Monolayer Nb$_2$CS$_2$

The change in band structure with applied strain

Figure S16: The calculated band structures for different strain values (tensile (+) and compressive (-)).
**Monolayer Nb$_2$CS$_2$**

*The change in phonon dispersion with applied strain*

| (a) 0.00 % | (c) 4.00 % |
| --- | --- |
| ![Graph](a) | ![Graph](c) |

| (b) 2.00 % | (d) -2.00 % |
| --- | --- |
| ![Graph](b) | ![Graph](d) |

**Figure S17**: The calculated phonon dispersions for different strain values (tensile, + and compressive, -).

**Monolayer Nb$_2$CS$_2$**

*The calculated nesting function*

![Graph](nesting_function)

**Figure S18**: The calculated nesting function for Nb$_2$CS$_2$ (2D).