DFT calculatin of High-Entropy MXene

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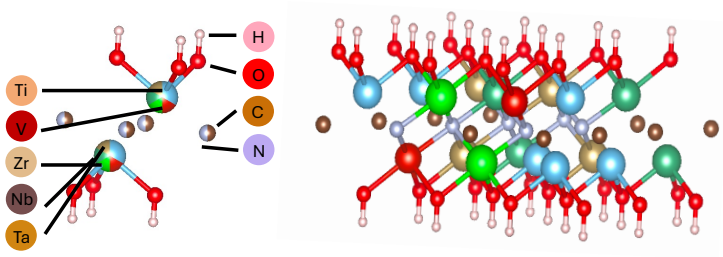
MXene is a two-dimensional material with a thickness of a few nm and is expected to be applied as an electrode material, sensor material, and battery. MXene is represented by the chemical formula $M_{n+1}X_nT_X$, where M is a transition metal such as Sc, Ti, V, or Cr, X is C or N, and T is a functional group such as O or OH. MXene is obtained by selectively etching A atoms from the precursor MAX phase ($M_{n+1}AX_n$).

High-entropy alloys are mixtures of five or more metals, each with a high concentration, and the mixing of multiple metals creates new functions. In 2021, Du *et al.* discovered a high-entropy MAX layer, $(Ti_{1/3}V_{1/6}Zr_{1/6}Nb_{1/6}Ta_{1/6})_2AlC_XN_{1-x}$, and applied it to synthesize high-entropy MXene, $(Ti_{1/3}V_{1/6}Zr_{1/6}Nb_{1/6}Ta_{1/6})_2C_{1/2}N_{1/2}$ T_X[1,2]. In this study, first-principles calculations are performed to deeply understand the properties of this High-Entropy MXene.

Density functional calculations of the high-entropy MXene $(Ti_{1/3}V_{1/6}Zr_{1/6}Nb_{1/6}Ta_{1/6})_2C_{1/2}N_{1/2}OH$, shown in Figure 1 with OH as a functional group, are carried out using the VASP package with PBE-GGA functional. We consider 100 supercell realizations of the random alloy, and investigate their elastic properties up to ductile fracture.



(a) (b)

Figure1. Structure of $(Ti_{1/3}V_{1/6}Zr_{1/6}Nb_{1/6}Ta_{1/6})_2C_{1/2}N_{1/2}(OH)_2$, (a) Unitcell and (b) supercell representations.

References

1. Zhiguo Du et al, High-Entropy Atomic Layers of Transition-Metal Carbides MXenes, 2021

2. Zhiguo Du et al, High-Entropy Carbonitride MAX Phases and Their Derivative MXenes, 2022