Ab initio studies of stability, magnetism, and electronic properties of titanium carbonitride MXenes

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Two-dimensional (2D) materials have been investigated extensively in recent years. In the broad class of 2D systems, transition metal carbides, nitrides, and carbonitrides have also received a lot of attention [1]. In addition to common MXene materials, titanium carbonitride MXenes where carbon and nitrogen atoms form alloy structures are intriguing materials with interesting physical properties [2]. However, monolayer $Ti_2C_xN_{1-x}$ alloy MXenes have not been investigated using *ab initio* calculations so far. In this work, we examine the stability, magnetism, and electronic properties of $Ti_2C_xN_{1-x}$ alloy MXenes by employing state-of-the-art density functional theory calculations.

Our calculations reveal that all $Ti_2C_xN_{1-x}$ systems are magnetic. Furthermore, the $Ti_2C_xN_{1-x}$ alloy MXenes are found to be stable in the whole carbon concentration range, which can be seen from Fig. 1, where the alloy formation energies are shown for anti-ferromagnetic (AFM), ferromagnetic (FM), and non-magnetic (NM) phases. Our analysis of the alloy MXenes also shows that their lattice parameters, layer thicknesses, and magnetic moments depend on the carbon concentration and magnetic phase remarkably.

We determine the electronic band structures for representative alloy MXenes in the whole carbon concentration range and find them to be metallic. Only Ti_2C is a semiconducting material with a band gap of around 0.20 eV. Computing the projected density of states for alloy MXenes indicates that the N 2p and C 2p states hybridise with the Ti 3d states. This hybridisation is related to the strong tendency of Ti_2C and Ti_2N towards mixing in $Ti_2C_xN_{1-x}$ systems. The results of our work demonstrate clearly that the physical properties of alloy MXenes can be tuned significantly by changing the carbon concentration. Moreover, our calculations can give new insights into the studies of other alloy MXenes.

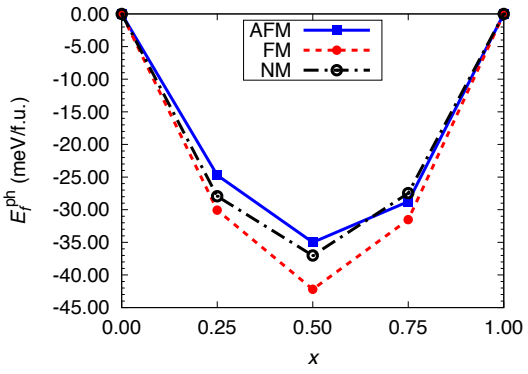

Figure 1. Alloy formation energy E_f^{ph} (in meV per formula unit) for the AFM, FM, and NM phases of $Ti_2C_xN_{1-x}$ MXenes as a function of the carbon concentration x.

References:

[1] X. Jiang, A. V. Kuklin, A. Baev, Y. Ge, H. Ågren, H. Zhang, P. N. Prasad, Phys. Rep. **15**, 1 (2020).

[2] A. N. Enyashin, A. L. Ivanovskii, J. Solid State Chem. **207**, 42 (2013).