INVESTIGATING THE MAX PHASES

Larousse Charlot[1], Vincent Yannello[2], and Micheal Shatruk[2]

1. Manard Evans High School, 4949 Silver Star Rd, Orlando, Florida 32801
2. Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States

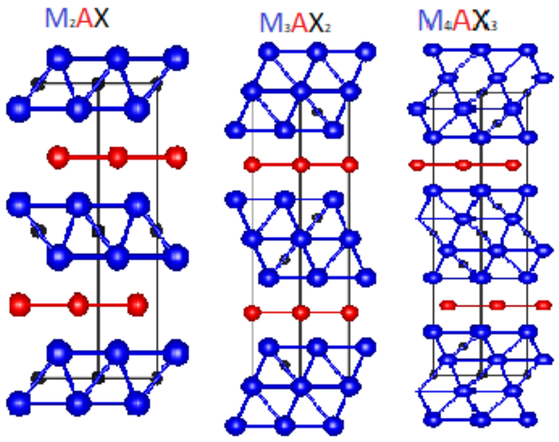
NATIONAL MAGLAB

ABSTRACT

MAX phases are layered hexagonal carbide and nitride compounds with the general form $M_{n+1}AX_n$, where *M is a transition metal*, *A is a main group element, and X is either carbon or nitrogen.* In this investigation, we will be observing the constitutions of the MAX phases, their structures, stabilities, and other properties. Here, we will be investigating the stability of the various MAX phases, and attempting to understand the reasons for the formation of different compounds.

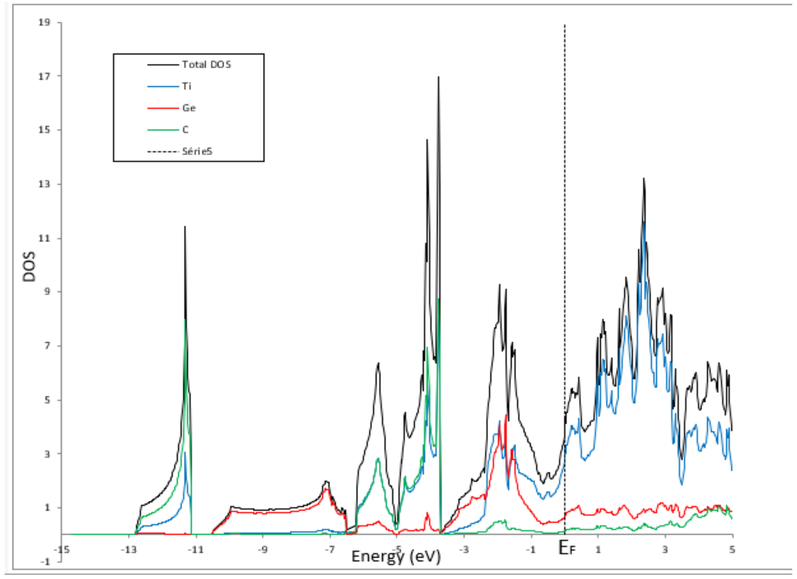
INTRODUCTION

To begin our investigation, we have revisited a few MAX phases to confirm their behavior and properties. Let us take a close look at some depictions of the MAX phases.



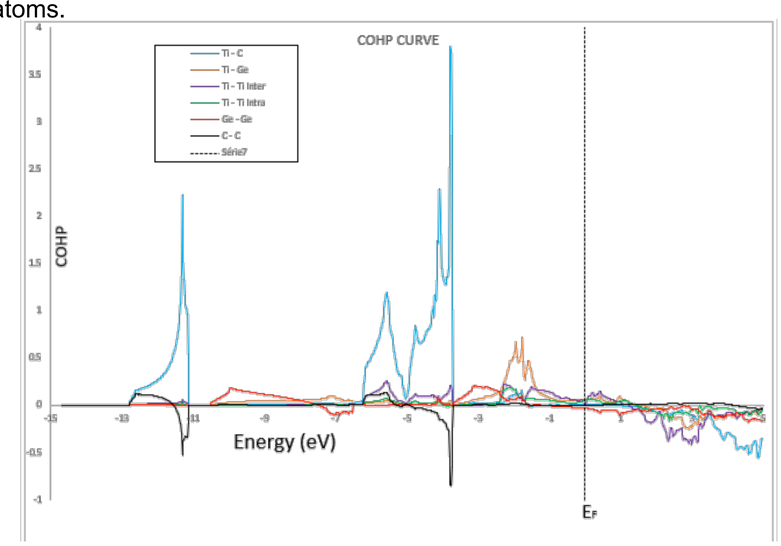
Types of MAX phases composed of X-centered M-Octohedra with the A atom separating the MX layers

Black is carbon, blue is the transition metal and red is the main group atom. To obtain a better sense of the reaction contribution of each element, we calculated the density of states (DOS) of each element



The Density of States (DOS) curves for Ti_2GeC, including projected DOS curves (pDOS) for each of the elements

The density of states informs us of the available states for the system, and the breakdown for each atom's contribution to these. Reading the DOS curve, the higher the density at a particular energy, the more states available to be occupied. Referring to the DOS graph above, take notice how the M and X atoms strongly contribute to the total DOS curve. That indicates the strengths of the bonding between the two atoms. Also, take notice that as we approach the Fermi Energy, the reaction between the M and A atoms strengthens a bit, however, not as strong as that of the M – X atoms. To further confirm our intuition, we look at the Crystal Orbital Hamilton Populations (COHP). The COHP indicates at which energies we have bonding (+) and antibonding (-) interactions between particular atoms.



The COHP of Ti2GeC – displaying the stability around the fermi energy (EF)

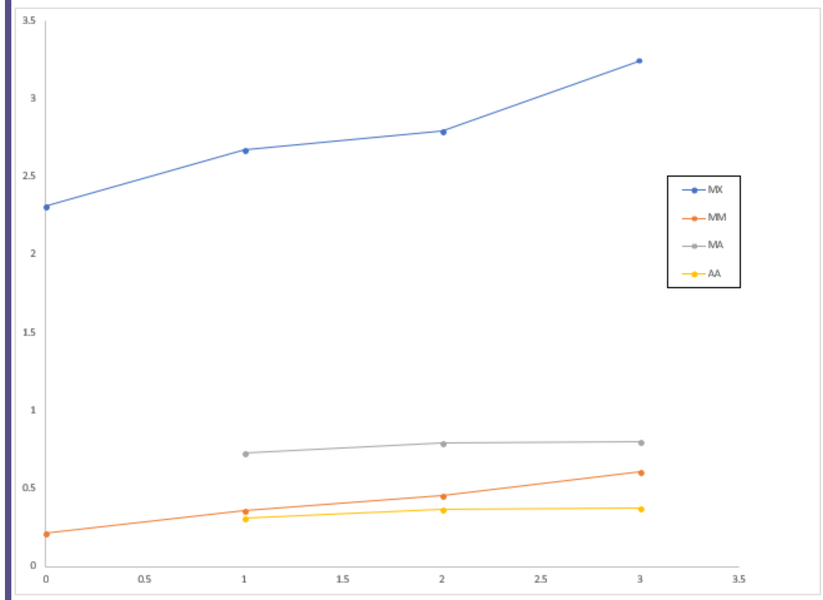
Analyzing the COHP curve above, the bonding between Titanium and Carbon (Ti – C) is very strong, stronger than any other bonding taking place this compound. The result is coherent to what is observed in the DOS curve. As we approach the Fermi energy, the bonds stabalize, indicating more of paramagnetism state.

MA vs. MX BONDING

Investigating the MAX Phases, we decided to compare the bonding strengths of the MA and the MX, for we wish to know how far we can move in either direction of the periodic table with respect to the transition materials. Due to finding that the MX bonding tend to be of higher strength than that of MA, we looked at the bonding as we increase the layers. Our finding is as displays below

	TaC	Ta_4AlC_3	Ta_3AlC_2	Ta_2AlC	TaAl
M-X	2.31	2.67	2.79	3.24	---
M-M	0.26	0.36	0.45	0.61	2.02
M-A	---	0.72	0.79	0.80	1.39
A-A	---	0.31	0.37	0.38	0.72

We also investigated the bonding strengths through other atomic compounds to observe the trend. Thus far, the bonding strengths is of the same pattern, the individual bonding grows weaker with more layers, the overall strength is greater than that of less layers. Below is a depiction of our observation.



The bonding pattern of TaC, Ta_2AlC, Ta_3AlC_2, Ta_4AlC_3, and TaAl

CONCLUSION

In conclusion, we have come to notice the structural layers could be increased indefinitely. However, having additional layers would not be structurally beneficial, due to the weaking of the various bondings as the number of layers increase.

REFERENCES

Magnuson, Martin and Mattesini, Maurizio (2017). Thin Solid Films. *Chemical bonding and electronic-structure in MAX phases as view by X-ray spectrocospy and density function theory. Vol 621* Pages 108 – 130.

Tan, Xiaoyan, Tener, Zachary and Shatruk, Micheal (2018). Account of Chemical Research. *Correlating Itinerant Magnetism in RCo_2Pn_2 Pnictides (R= La, Ce, Pr, Nd, Eu, Ca; Pn = P) to Their Crystal and Electronic Structures. Vol 51* Pages 230 – 239.

Hoffmann, Roald (1987). Angewandte Chemie International Edition. *How Chemistry Physics Meets in the Solid State*. Vol. 26, issue 9. Pages 805 – 938

ACKNOWLEDGEMENT

I want to thank the following individuals and programs which have rendered my profesional development possible. Without each and everyone of you, the experience would not be what it is today. Thank you to: Dr. Micheal Shatruk, Dr. Vincent Yannello, The Department of Chemistry and Biochemistry at FSU. Jose Sanchez, the Director of the RET Program and National High Magnetic Field Laboratory made possible through a generous grant: DMR-1704712