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Chemical bonding and electronic-structure in MAX phases as viewed by X-ray spectroscopy and density functional theory

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Abstract

This is a critical review of MAX-phase carbides and nitrides from an electronic-structure and chemical bonding perspective. This large group of nanolaminated materials is of great scientific and technological interest and exhibit a combination of metallic and ceramic features. These properties are related to the special crystal structure and bonding characteristics with alternating strong M-C bonds in high-density MC slabs, and relatively weak M-A bonds between the slabs. Here, we review the trend and relationship between the chemical bonding, conductivity, elastic and magnetic properties of the MAX phases in comparison to the parent binary MX compounds with the underlying electronic structure probed by polarized X-ray spectroscopy. Spectroscopic studies constitute important tests of the results of *state-of-the-art* electronic structure density functional theory that is extensively discussed and are generally consistent. By replacing the elements on the M, A, or X-sites in the crystal structure, the corresponding changes in the conductivity, elasticity, magnetism and other materials properties makes it possible to tailor the characteristics of this class of materials by controlling the strengths of their chemical bonds.

Keywords: Nanolaminates, chemical bonding, X-ray emission spectroscopy, electronic structure calculations, elastic and magnetic properties, Seebeck measurements

Contents

1. Introduction
2. Crystal structures and stability of MAX phases
3. X-ray spectroscopy – absorption and emission
4. Electronic structure calculations – theory and modeling
5. Anisotropy and polarization dependence
6. Chemical bonds in MAX phases
7. Balanced crystal orbital overlap population analysis
8. Transport properties - resistivity and thermopower
9. Phonon and optical properties of MAX phases: Raman and infrared spectroscopies
10. Elastic properties of MAX-phases
11. Charge-transfer in MAX phases
12. Magnetic properties in MAX phases
13. Concluding remarks

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