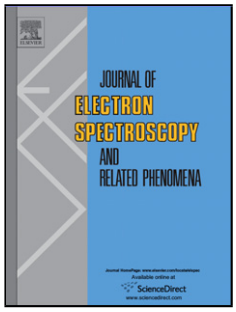

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Chemical bonding in carbide MXene nanosheets

Martin Magnuson[1*], Joseph Halim[1,2] and Lars-Åke Näslund[1]

[1]*Department of Physics, Chemistry and Biology, IFM, Thin Film Physics Division, Linköping University, SE-58183 Linköping, Sweden.*
[2]*Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA*

* Corresponding author: Martin.Magnuson@ifm.liu.se

Highlights

i) The valence band of a new 2D material called MXene is probed by X-ray photoelectron spectroscopy.

ii) Al K_alpha radiation is used to enhance the Ti *3d* - C *2s* features.

iii) The results indicate that the Ti-C bond is weaker in Ti_2C-T_x compared to Ti_3C_2-T_x due to more interfaces that also affect the transport and elastic properties of the materials.

iv) The O *2p* and F *2p* band positions are sensitive to the site and the bond distances of the termination groups in MXene.

Abstract

The chemical bonding in the carbide core and the surface chemistry in a new group of transition-metal carbides $Ti_{n+1}C_n$-T_x (n=1,2) called MXenes have been investigated by surface-sensitive valence band X-ray photoelectron spectroscopy. Changes in band structures of stacked nano sheets of different thicknesses are analyzed in connection to known hybridization regions of TiC and TiO_2 that affect elastic and transport properties. By employing high excitation energy, the photoelectron cross-section for the C *2s* - Ti *3d* hybridization region at the bottom of the valence band is enhanced. As shown in this work, the O *2p* and F *2p* bands are shown to strongly depend both on the bond lengths to the surface groups and the adsorption sites. The effect of surface oxidation and Ar^+ sputtering on the electronic structure is also discussed.

1. Introduction

In the quest for new 2D materials outperforming graphene [1], research on other more advanced 2D materials has greatly intensified. Despite the large interest in graphene,