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Chemical bonding in carbide MXene nanosheets

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Highlights

- i) The valence band of a new 2D material called MXene is probed by X-ray photoelectron spectroscopy.
- ii) Al K_α radiation is used to enhance the Ti 3d - C 2s features.
- iii) The results indicate that the Ti-C bond is weaker in Ti₂C-T_x compared to Ti₃C₂-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 TiO₂ 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,

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