

Title: On the C(1s) core level binding energy calculations of MXene carbides.
A theoretical approach.

Student: Néstor Mauricio García-Romeral González

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Supervisor/s: Dr. Ángel Morales García
Departament de Ciència de Materials i Química Física.
Dr. Francesc Illas Riera
Departament de Ciència de Materials i Química Física.

One of the latest families incorporated to the group of bidimensional (2D) materials is the low-dimensional transition metal carbides, nitrides and carbonitrides known as MXenes. These materials have generated a great interest in Material Science due to the potential use as catalysts, (bio-) sensors, neural electrodes, ion batteries, water purification, electrochemical capacitors and photodetectors. Such applications are directly related with the surface properties demanding thus exhaustive analysis by using sensitive techniques such as X-ray Photoelectron Spectroscopy (XPS). Essentially, XPS measures core level electron binding energies, constituting a notorious method for accessing to the information of the materials composition. In the present study, first-principles calculations based on the Density Functional Theory (DFT) are employed to investigate C(1s) binding energy of MXenes along with additional parameters such as the charge of carbon atom. In particular, MXene carbides with M_2C stoichiometry ($M = \text{Ti, Zr, Hf, V, Nb, Ta, Cr, Mo}$ and W) are selected to this purpose. The goal is to stablish tentative correlation between C(1s) binding energy and the carbon charge that allows one to understand MXenes based on their composition, and the XPS based experiments.