Investigation of mixed surface termination groups in Ti₃C₂T_x: XAS and electronic analysis

Mahdieh Zeynali¹, Saeid Asgharizadeh¹



¹Faculty of Physics, University of Tabriz, Tabriz, Iran

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Introduction

Physical and chemical properties of MXenes are highly controlled by their surface terminations; thus, by adjusting the surface functional groups of MXenes, two-dimensional transition-metal carbides, their applicability may be expanded to a wider range of applications¹.

By using electron energy-loss spectroscopy and DFT-based simulation in two-dimensional MXene, the rule of surface termination groups in chemical bonding becomes clearly noticeable.

The influence of terminated atoms on the K-edge shift is measured by focusing on the 1s core electron excitation of C, Ti, and terminated atoms.



All of our calculations have been based on density function theory (DFT) utilizing their project argument with a potential technique by quantum espresso with an energy cut-off of 730 eV. electron energy loss at the C, Ti and terminated atoms' Kedge structure. The experimental data were chosen from damine². To eliminate physical mutual interaction between neighboring excited at atoms, we employed a $2 \times 2 \times 1$ supercell and conducted calculations using a $12 \times 12 \times 2$ K-point sample of the first billion zone on a Monkhorst-Pack grid.

Result

of $T_{i3}C_2T_x$ with the $T_x = 0$, OS



Fig2. Comparison between the simulated O-K edge and Site-projected density of states



Because the phonon band dispersion curve of functionalized MXene does not contain any imaginary frequencies, this makes them dynamically stable according to our calculations. Focusing first on the top part of Fig2, it is obvious that around the Fermi level, the surface Ti d-states dominate the electronic structure of $Ti_3C_2T_x(T_x=0,OS)$. The highest valence band contribution from -6 to around -4 eV comes from the O-p and S-p states. The predominant part of the higher conduction bond for $Ti_3C_2T_X$ between 1 and 5 eV relates to a strong hybridization between C-p states and Ti-d states. However, using various atoms as surface termination has a significant effect on these bands. The peak intensity for Kedge spectrum considerably is correlated with DOS of $Ti_3C_2T_X$. The EELNS at the C-k edge is shown to be sensitive to the composition of the X termination atoms and their placement on the MXene's surface. When comparing the O-K and S-k edges in Fig3, various differences can be seen: the splitting between the structures A and B is bigger for O, and their relative intensities fluctuate. Moreover, it is demonstrated that the hybridization of this atom with the Ti Bands determines the EELNS at the C-k boundary. generally, careful inspections of the EELNS at the C, O-K and S-K edges show that the peaks at the edge onset arise from hybridizations with the d states of either the surface or volume Ti atoms. Further, it is shown that the EELNS for the Ti1-k and Ti2-k edges are changed for the functionalized O and OS atoms due to the alteration in their bond length.

Conclusion

The electronic structure of Ti3C2Tx has been investigated using DFT calculations. It is also demonstrated that the chemical nature of the T-groups has a significant impact on the ELNES at the C-K edge, Considering that the C-K edge is to a good approximation a probe of the unoccupied C-p DOS. These may be utilized to determine the best synthesis finding strategy based on the desired applications because of the significant influence that T-groups play in the characteristics of MXenes as a whole.



Energy loss (ev)

References

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