Turning the structural, electrical, optical, and excitonic properties of two-dimentional M_2XT_2 (M=Y, Sc; X=C and T=O, F, S, Cl, Se, Br, Te ,I , H, OH) MXene monolayers for solar harvesting efficiency.

B. D. Aparicio-Huacarpuma[a,b,*], M. L. Pereira Junior[c], M. J. Piotrowski[d], C. R. C. Rêgo[e], D. Guedes-Sobrinho[f], L. A. Ribeiro Junior[a,b] and Alexandre C. Dias[a]

[a]*Institute of Physics, University of Brasília, 70910-900, Brasília, Brazil*
[b]*Computational Materials Laboratory, LCCMat, Institute of Physics, University of Brasília, 70910-900, Brasília, Brazil*
[c]*University of Brasília, College of Technology, Department of Electrical Engineering, University of Brasília, 70919-970, Brasília, DF, Brazil*
[d]*Department of Physics, Federal University of Pelotas, PO Box 354, 96010-900, Pelotas, RS, Brazil*
[e]*Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Hermann-von-Helmholtz-Platz, 76344, Eggenstein-Leopoldshafen, BW, Germany*
[f]*Chemistry Department, Federal University of Paraná, 81531-980, Curitiba, PR, Brazil*

Abstract

In this work, we study the structural, electrical, optical and excitonic properties of the 2D M_2CT_2 (M=Y, Sc and T= O, F, S, Cl, Se, Br, Te, I, H, OH) MXene monolayers have been investigated using using a computational protocol that combines first-principles and semi-empirical methods. We performed systematic simulation to explore the stability and electronic structure of the MXene systems.From the 22 MXene monolayers, we found from phonon calculations that 10 systems are stable, 5 meta-stable and 7 unstable. It is found for that Y_2CCl_2, Y_2CBr_2, Y_2CH_2, Y_2CI_2, Sc_2CCl_2, Sc_2CBr_2, Sc_2CF_2 and Sc_2CH_2 are semiconductors with indirect band gaps of about 1.68, 1.66, 1.59, 1.25, 1.70, 1.65, 1.90, and 1.85 eV, respectively, employed the hybrid functional Heyd-Scuseria-Ernzerhof (HSE06) approach. Moreover, excitonic correction will be explored in the optical properties, using tight binding based on maximum localized Wannier functions, and the Bethe-Salpeter equation. Excitonic effects induced by quantum confinement contribute to exciton binding energies from 210 meV to 470 meV, consistent with typical 2D materials. Additionally, some monolayers demonstrate potential for solar harvesting applications, with predicted power conversion efficiency (PCE) approaching 30% under full photon absorption. Hence the obtained results are promising to optoelectronic applications.

Keywords: MXenes, Density functional theory (DFT), structural and optical properties, band gap.