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# Full potential theoretical investigations for electronic, optical, mechanical, elastic and anisotropic properties of $X_2Se_2C$ (X = Ta, Nb) compounds

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**Abstract.** To study the structural properties of $X_2Se_2C$ ($X$ = Ta, Nb) MXenes, we have used an FP-LAPW method based on functional density theory GGA-PBE-sol, which is based on the method of plane waves increased by linear waves at full potential. From the most stable state, we determined other properties such as electronic, optical, and mechanical ones. Band structure calculations reveal the metal character of GGA. MXenes exhibit hexagonal crystal structures at zero temperature. Calculated elastic constants show the alloy's mechanical stability and ductility. Due to its high elasticity anisotropy, the alloy possesses excellent tensile strength. The dielectric function, absorption, reflectance, optical conductivity, and other optical properties were also investigated. In the ultraviolet region, $X_2Se_2C$ ($X$ = Ta, Nb) is an effective absorber and has a high refractive index.

## 1 Introduction

Two-dimensional (2D) materials are key materials for today's technology. Amongst them, Mxenes are prevalent examples of 2D materials. Early transition metal (TM) carbides and nitrides form the materials known as MXenes [1]. They are also the most efficient and promising materials for production technology. Mxenes are ideal for energy storage [2–6], electronics and magnetics [7–10]. catalysis [11–14], and so on. Early TMs that are well known include the Sc. Ti, V, Cr, Mn, Zr, Nb, Mo. Hf, Ta, and W elements. Besides, different arrangements of these elements lead to the formation of various Mxenes. Thus, different MXenes emerge with distinguished and tunable magnetic. optical. and electronic aspects. So, it is still important to clarify the physical insights of this variety. Literature involves many works, especially for Ti–C [15–20] Mxenes. However, the intriguing physical aspects of other Mxenes combinations remain unclear. On the other hand, as is well known. like other 2D materials, MXene nanosheets tend to stack together via van der Waals interactions. This stacking leads to a limited number of active sites, sluggish ionic kinetics, and finally the ordinary performance of MXene materials/devices. Constructing 2D MXenes nanosheets into 3D architectures has been proven to be an effective strategy to reduce restacking. So, it is possible to get, a larger specific surface area, higher porosity, and shorter ion and mass transport distances over normal 1D and 2D structures [21]. For this reason, we addressed the several bulk properties of $Nb_2Se_2C$ and $Ta_2Se_2C$ MXenes for the first time in this work. We surveyed the elastic, electronic. and optical properties of $Nb_2Se_2C$ and $Ta_2Se_2C$ MXenes during this study.

The second part of the article outlines the theoretical calculation details used in the research. In the third part of the paper, we provide a detailed evaluation of our present findings through results and discussion. Finally, we underline the main outcomes of the study via conclusions.

## 2 Materials and methods

The calculations were performed using the full-potential linearized augmented plane wave (FPLAPW) method of density functional theory (DFT) using the Vienna package (WIEN2k) [22]. The exchange–correlation potential was calculated using the local density approximation, LDA [23], and the generalized gradient approximation based on Perdew, Burke, and Ernzerhof (PBE-GGA) [24]. According to Perdew, Burke. and Ernzerhof (PBE-GGA) [24], the

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