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Electronic Band Structure of MXene Material (V_2C)

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Abstract

MXene materials have received a strong boost of interest due to the prediction of behaving as topological dielectric or non conductor which is used in spintronic devices and for future technology device. In this experiment DFT (Density Functional Theory) based Quantum Expresso code is used to calculate the band structure and DOS of MXene material (i.e. V_2C) by setting non-polarized spin polarization framework. From the geometric optimization, lattice parameter is found to be a = 2.945 Å, b = 8.836 Å, c = 28.19 Å. Since its bulk is insulating in nature, we observed MXene layer as conducting i.e. bands overlapping within fermi surface. Similar kind of scenario is observed in DOS which resembles escorted by the previously predicted results.

Key Words: MXene, V_2C, Density functional Theory, QE code, Fermi surface

Introduction:

MXene is an exotic material which lies under the category of topological insulators of which surface or edge states are conducting whereas the bulk state is insulating. As it has a property of topological insulators it gives interesting topic for scientific studies. Therefore, it is very important for us to understand the core theoretical structure of this broad concept. The theoretical framework of this MXene material has its root in the basic foundation of quantum mechanics.

Before 1980, all states of matter in condensed-matter systems could be classified by the principle of broken symmetry. The quantum Hall (QH) state, discovered in 1980, provided the first example of a quantum state that has no spontaneously broken symmetry. Its behavior depends only on its topology and not on its specific geometry; it was topologically distinct from all previously known states of matter. However, this MXene material is quantum spin hall (QSH) state which differs from other states of matter. Therefore, this theoretical framework covers the basic ingredients of the enhanced topological band theory and quantum spin hall effect. The emphasis will be on the understanding of core concepts with as simple mathematical tools as possible. In physics ab initio study or study from first principle is very popular in qualitative analysis of the physical laws. The Latin word *ab initio* is made of two words 'ab' means 'from' and

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'initium' means 'beginning', hence, the meaning 'from the beginning'. It means to understand the observed phenomenon of real world we have to break things down to the basic fundamental laws of physics and understand them from ground level. In Physics, Hamiltonian mechanics and Schrödinger's equation are considered as the basic fundamental laws because they cannot be further breakdown to have the understanding of electrons in quantum scale.

Methodology

In problem solving criteria of physics, computer has been extensively used in the recent days. The development of quantum mechanics has lead to the complex mathematical formulation of simple natural phenomenon.

It is very difficult to solve the problems by just using different mathematical techniques. Therefore, computer simulation programs are required to solve those issues. The use of computer drastically reduces the time and power required to solve those problems. With the engagement in Computer we can model, analyze and interpret different structures of physical system. In the Solid state physics, it is mainly used in modeling of structure and study of different physical properties embedded in it.

Simulation is the imitation of the operation of a real-world process or system over time. The act of simulating something first requires that a model be developed; this model represents the key characteristics or behaviors of the selected physical or abstract system. Then the model represents the system itself, whereas the simulation represents the operation of the system over time. Simulation can be used to show the eventual real effects of alternative conditions and courses of action in the computer world. Simulation is also used when the real system cannot be engaged, because it may not be accessible, or it may be dangerous or unacceptable to engage, or it is being designed but not yet built, or it may simply not exist. In this study, different simulation soft wares are used for the purpose of modeling and interpretation of structure.

Quantum ESPRESSO is a software suite for ab initio quantum chemistry methods of electronic-structure calculation and materials modeling, distributed for free under the GNU General Public License. It is based on Density Functional Theory, plan wave basis sets, and pseudo-potentials (both norm-conserving and ultra soft). ESPRESSO is an acronym for *Open Source Package for Research in Electronic Structure, Simulation and Optimization.*

The different tasks that can be performed include

— Ground state calculations.
— Structural optimization.
— Transition states and minimum energy paths.
— Response properties (DFPT), such as phonon frequencies, electron- phonon interactions and EPR and NMR chemical shifts.
— Ab initio Molecular Dynamics: Car-Parinello and Born-Oppenheimer MD.
— Spectroscopic properties.
— Quantum transport.

The program, written mainly in fortran-90 with some parts in C or in Fortran-77, was built out of the merging and re-engineering of different independently-developed core packages, plus a set of packages, designed to be inter-operable with the core components, which allow the performance of more advanced tasks.

The basic packages include PWSCF which solves the self-consistent Kohn and Sham equations, obtained for a periodic solid, CP to carry out Car-Parrinello molecular dynamics, and PostProc, which allows data analysis and plotting. Regarding the additional packages, is noteworthy to point out atomic for the pseudo-potential generation, Phonon package which implements density-functional perturbation theory (DFPT) for the calculation of second- and third-order derivatives of the energy with respect to atomic displacements.

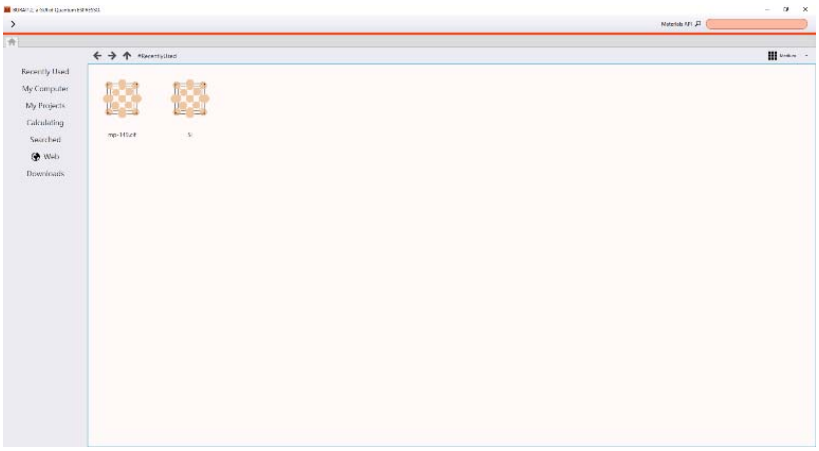
BURAI Program

BURAI is a GUI system of Quantum ESPRESSO. We can download and use it freely. This system is developed as JavaFX application, and requires Java Runtime Environment (JRE).

Initial Window

The initial window of BURAI Program consists of two items:

I. Main menu

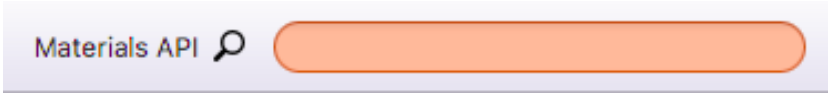


Courtsey: http://burai.readthedocs.io/en/latest/usage/initial_window.html

Figure 1: Initial Window

II. Materials API

We can get crystal structure through Materials API.

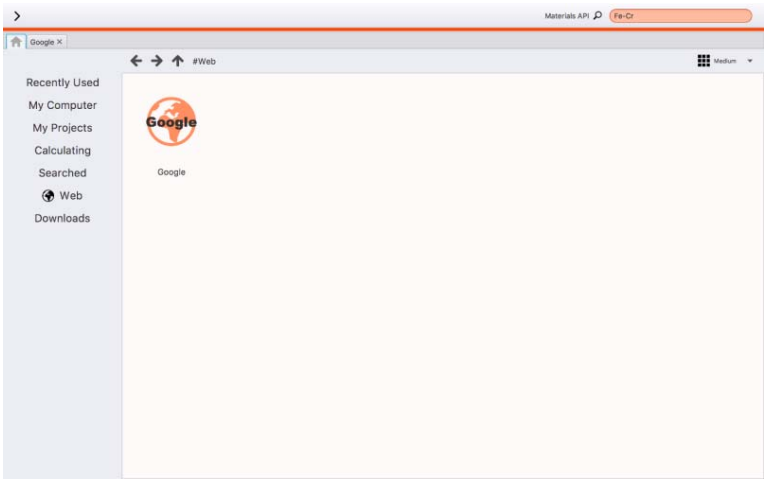


Courtsey: http://burai.readthedocs.io/en/latest/usage/initial_window.html

Figure 2: Materials API

Web browser

BURAI has *build-in* web browser. if you want to search something at the internet, you should select "Web" from menu. Different crystal structures and pseudopotentials are downloaded from various websites through the web browser.



Courtsey: http://burai.readthedocs.io/en/latest/usage/web_browser.html

Figure 3: Web browser embedded in BURAI Program

Calculations

Choices are collectively given in the homepage to perform any kind of calculations that are available.

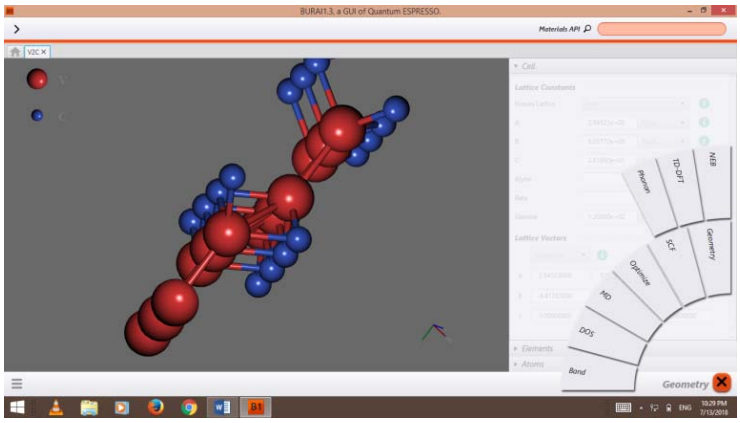


Figure 4: Calculations using BURAI

Self-consistent field calculation

Appropriate inputs should be given to perform SCF calculation.

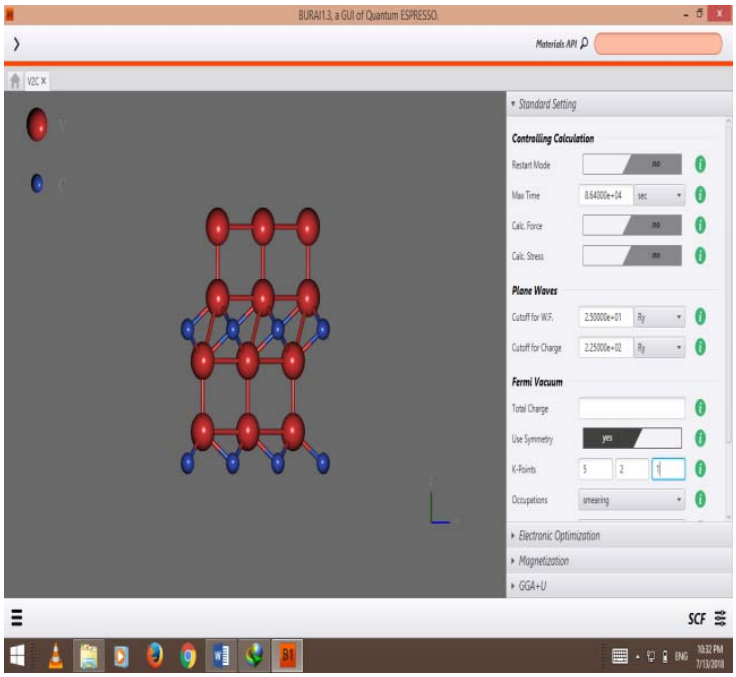


Figure 5: SCF Calculation Inputs

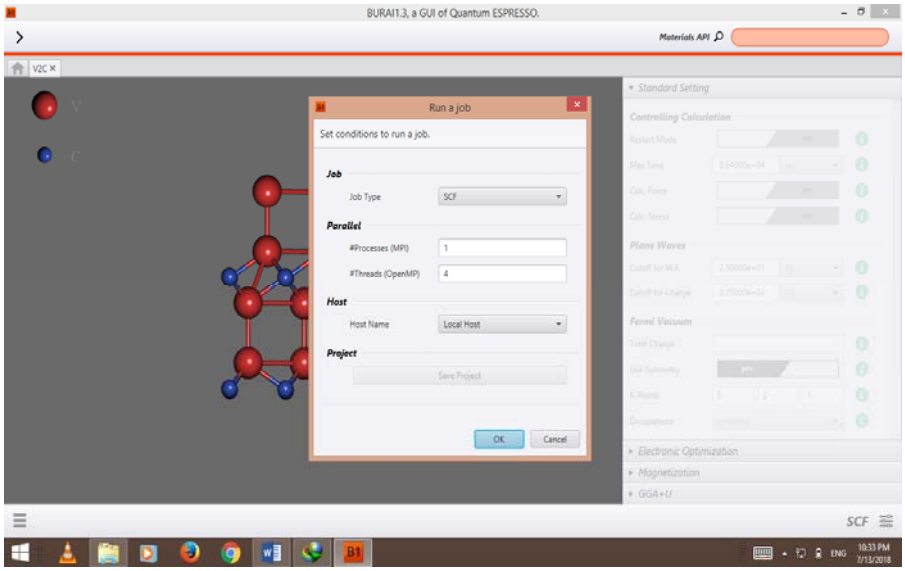


Figure 6: Calculation of SCF

Geometric Optimization Calculation

Appropriate inputs should be given to perform Geometric Optimization calculation.

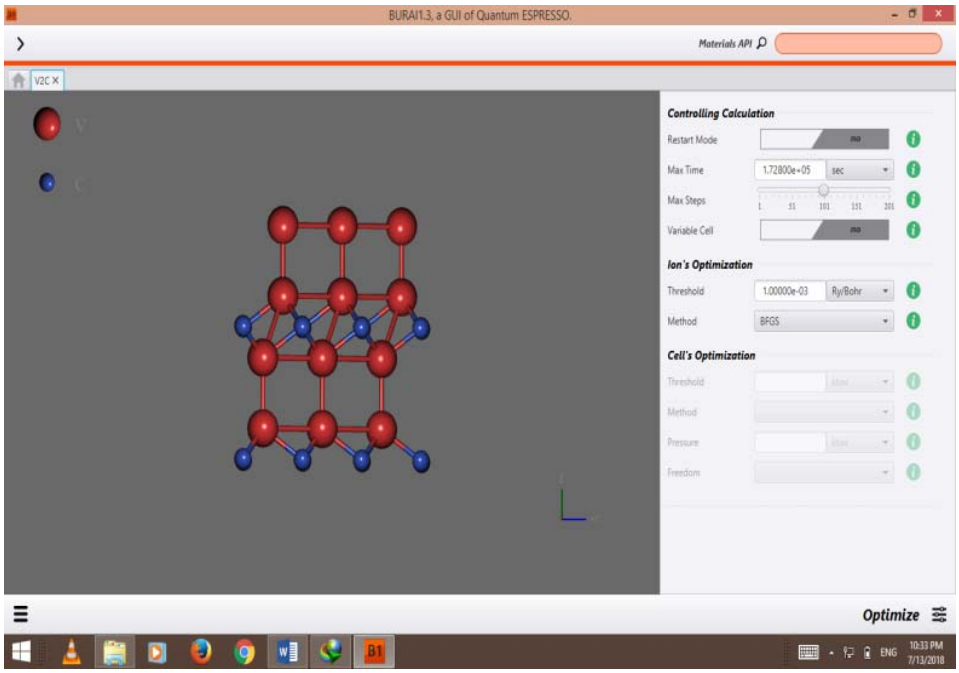


Figure 7: Geometric Optimization Inputs

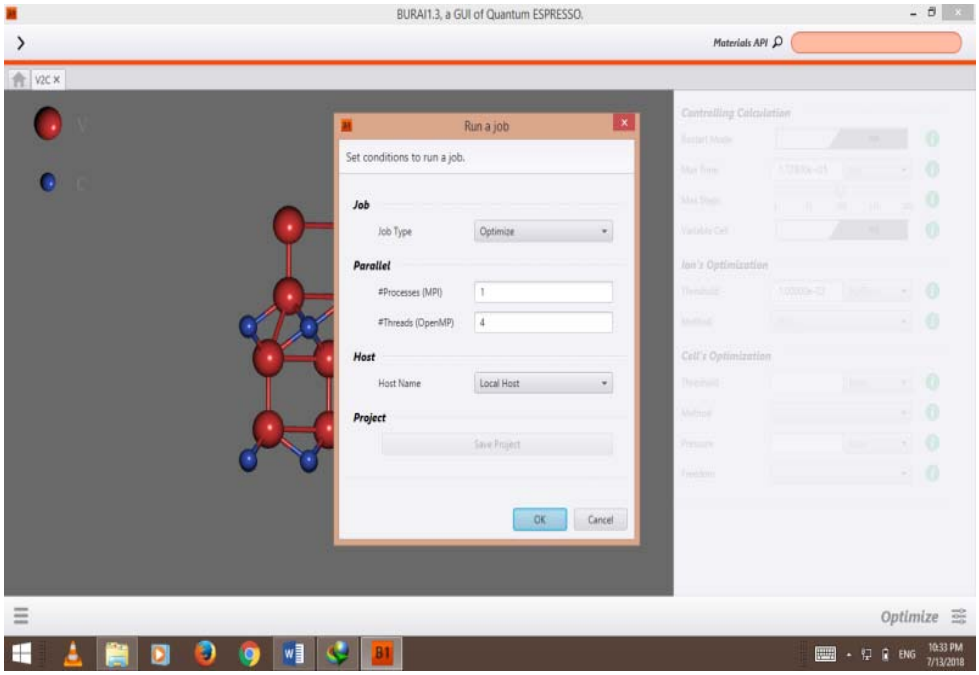


Figure 8: Calculation of Geometric Optimization

Density of States Calculation

Appropriate inputs should be given to perform DOS calculation.

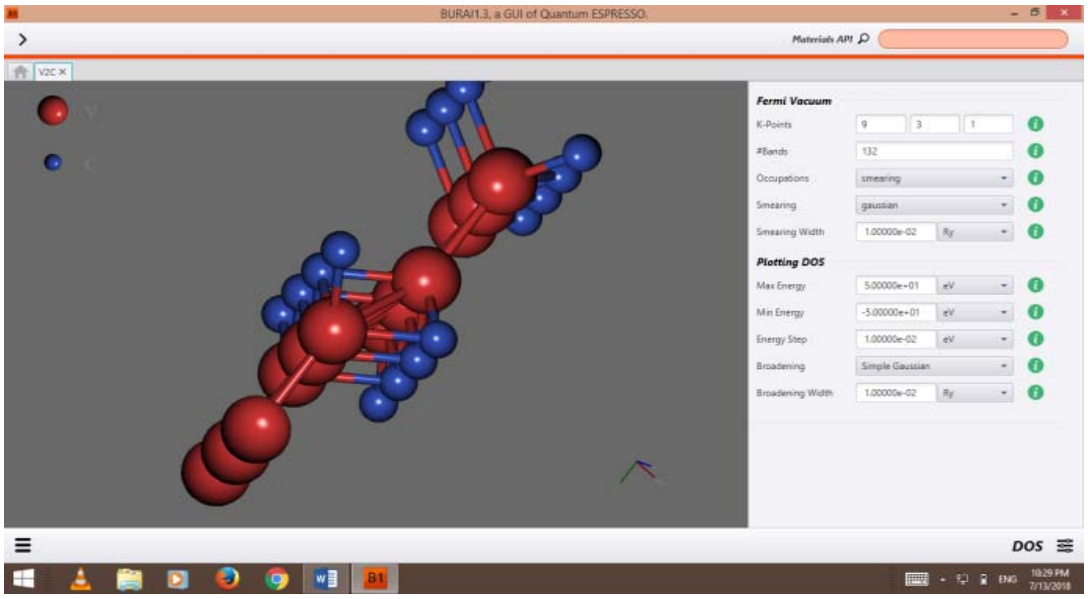


Figure 9: Density of States Inputs

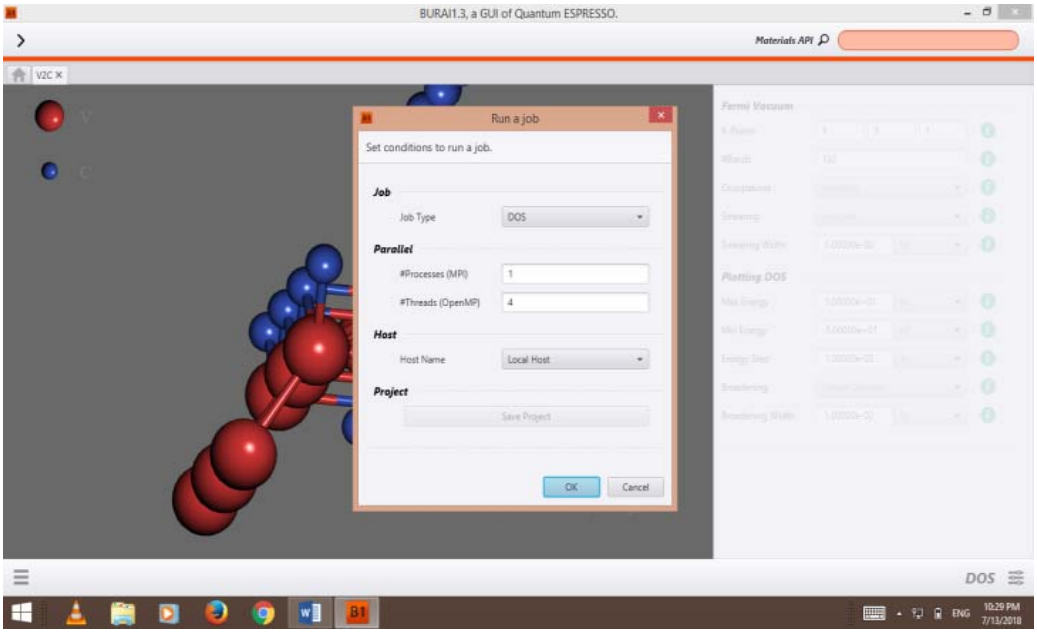


Figure 10: Calculation of Density of States

Electronic Band Structure Calculations

Appropriate inputs should be given to perform Electronic Band Structure Calculation.

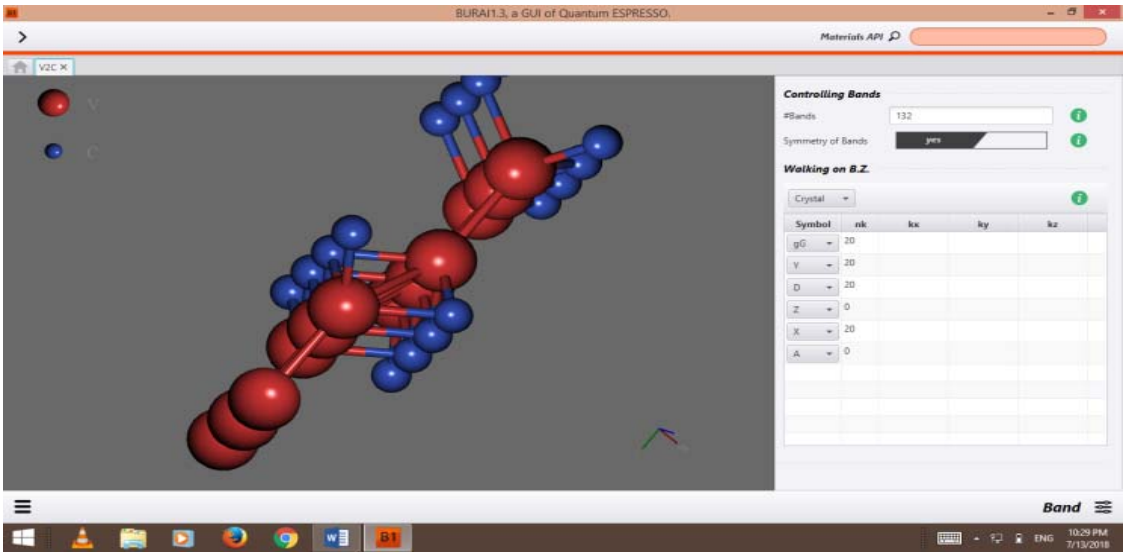


Figure11: Electronic Band Structure Inputs

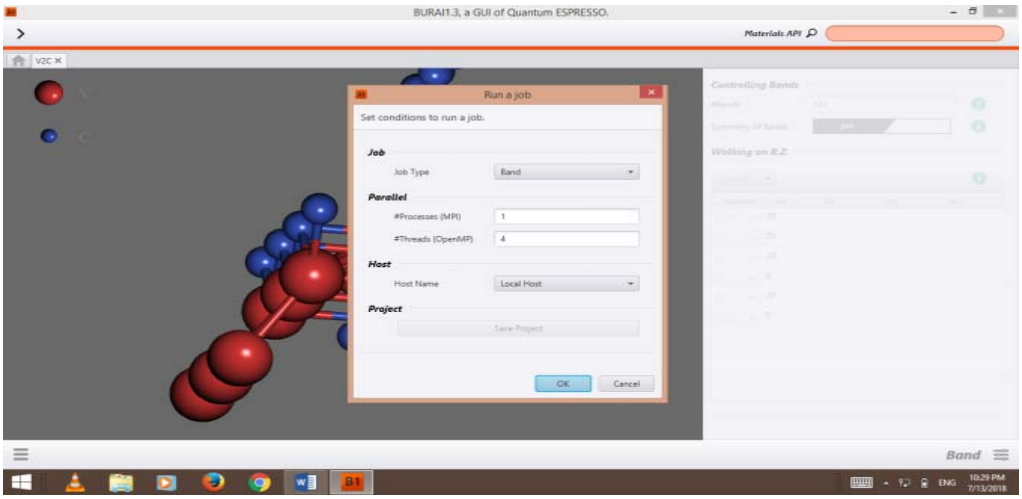


Figure 12: Calculation of Electronic Band Structure

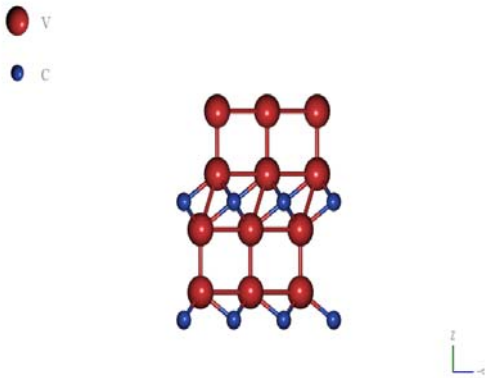
Bravais Lattice	Monoclinic P, Unique axis c
P.P type	Ultra soft Pseudo-potential (USPP)
XC Function	PBE
Cutoff of WF	25.000 Ry
Cutoff of Charge	225.000 Ry
Spin Polarization	Non – polarized
K - points	9, 3, 1
Occupation	Smearing
Number of Bands	132

Table 1: Parameters taken for Electronic Band Structure and DOS Calculation

Result and Discussion

General Consideration

In this chapter, the result obtained from the calculation of SCF, geometric optimization, band structure and density of states are shown and analyzed. Calculations are performed by providing the parameter information of BURAI software which is the GUI of Quantum ESPRESSO is used for the calculation.



SCF Analysis

From the self consistent calculation, it is observed that it will be in stable state at energy of -399.4879 Ry. It is observed that SCF is converged after 27 iterations.

Figure 13 : Surface state of V C model using BURAI
2

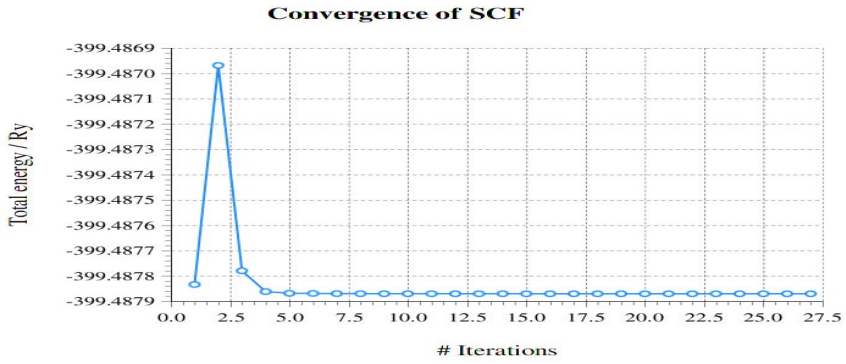


Figure 14: Energy vs. Number of Iterations in SCF

The graph of energy Vs No of iterations in SCF is shown in figure 14 which shows that the first increased rapidly up to pick after that it will decreases rapidly up to 2.5 Iterations and at last it becomes constant.

Geometric Optimization Analysis

From the geometric optimization, optimization is converged after 12 iterations as shown in fig 5.3. The force exerted on each atom is 0.001419 Ry/Bohr.

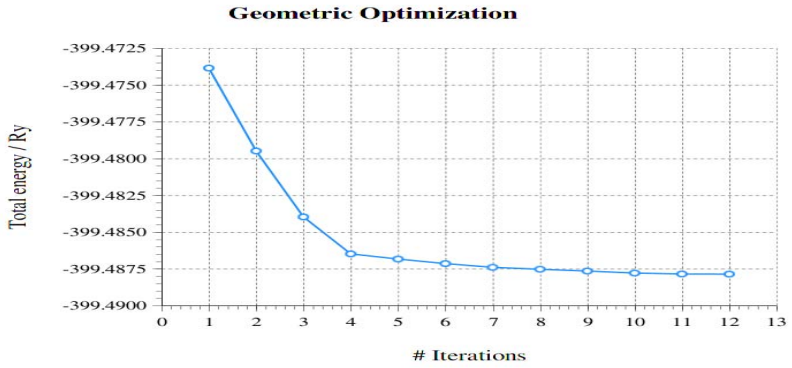


Figure 15: Energy vs. Number of Iterations in Geometric Optimization

Figure 15 is the graph of energy Vs No of Iterations in Geometric Optimization which shows that the total energy of atom decreases rapidly from initial phase to up to 4 Iterations after that it will becomes constant.

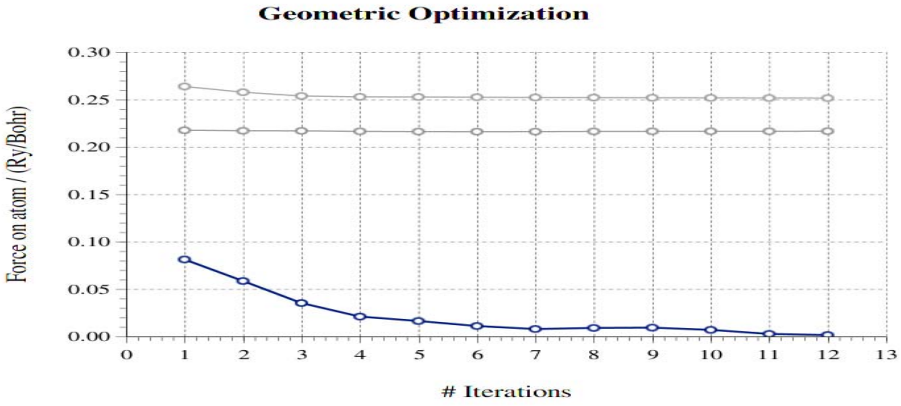


Figure 16: Force on atoms vs. Number of Iterations in Geometric Optimization

Figure 16 shows the graph of force on atom Vs Iterations. It shows that the when the iterations rate increases the force on atom decreases.

Electronic Band Structure Analysis

Electronic band structure plot presents the variation of energy range within the reciprocal high symmetry points (k-points).

The analysis of band structure is shown in figure 17. It is the graph of Energy vs. High Symmetry Points in Band Structure.

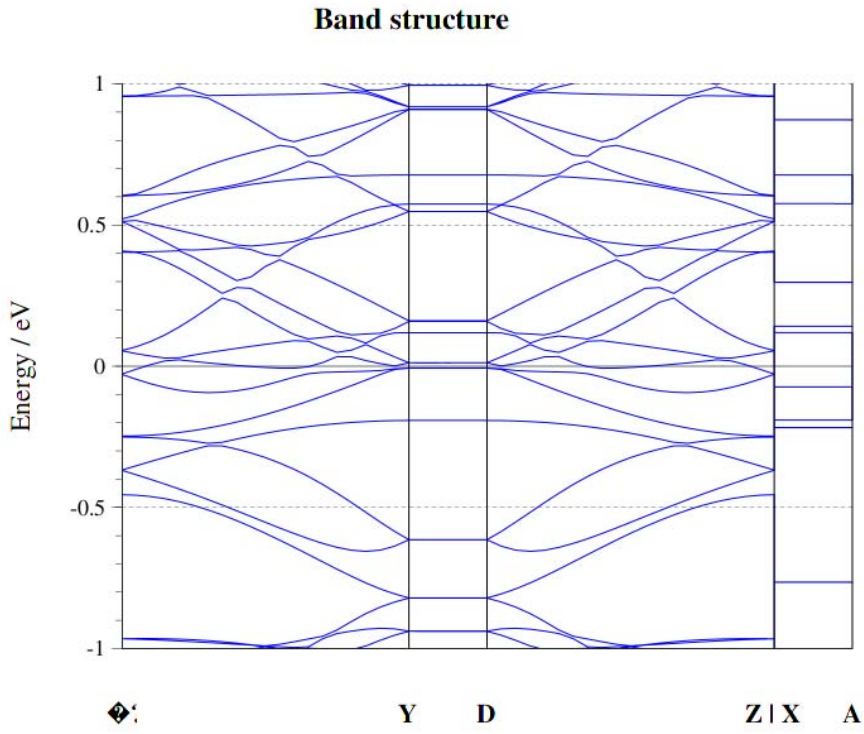


Figure 17: Energy vs. High Symmetry Points in Band Structure

Band Structure of V_2C MXene gives the metallic in nature being conduction band and valence band lines cross the fermi level.

Density of States Analysis

From the DOS plot it is observed that DOS of V and DOS of C are overlapping near the fermi level which is resemblance with the band structure. Due to the effect of which we found highest peak of DOS near the fermi level as shown in figure 18.

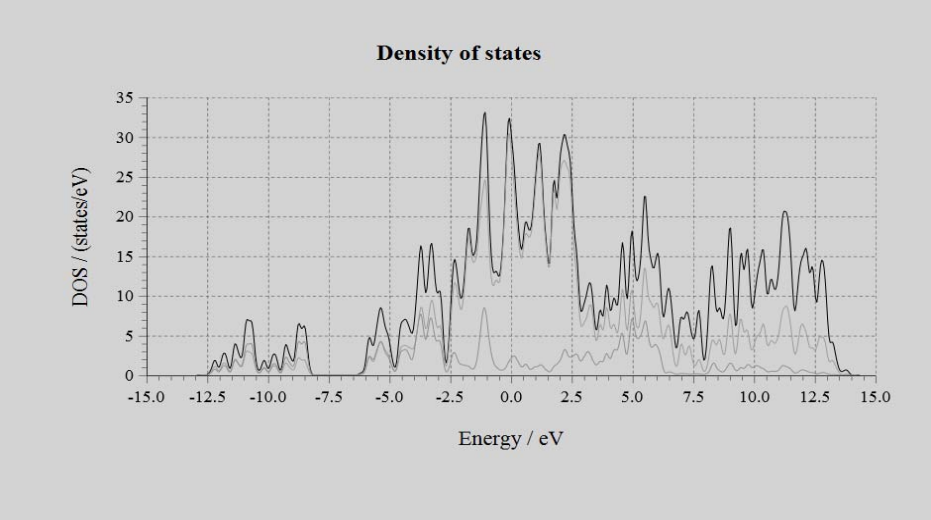


Figure 18: Density of States vs Energy

In short, the monolayer of V_2C MXene shows the conducting behavior at the surface.

The current work presents the calculation and analysis of the Vanadium Carbide (V_2C) which is a MXene material. The calculation was performed on BURAI software which is the GUI of Quantum ESPRESSO. The electronic properties were examined through band structure and density of states, confirms the metallic nature of V_2C at the surface level. As shown in figure 17 and 18 the lines cross the Fermi level, which also confirms the metallic behavior.

Conclusion

In conclusion, the MXene material Vanadium Carbide V_2O is very novel material which behaves as a metallic at the surface level. The fermi level and cross line in the i.e the density of state and the band structure confirms its metallic behavior. We can use such material as a electrode in the electronics components.

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