Crossian Resonance

A Multidisciplinary Research Journal **ISSN 0976-5417**
(A refereed Biannual Published in June and December)
Vol. 15, No.2, December 2024
https://research.holycrossngl.edu.in/

Electronic Band Structure and Density of States of Alkali metals Rubidium and Cesium

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ABSTRACT

The electronic band structure, density of states and the behaviour of conduction and valence bands in body-centered cubic rubidium and cesium, particularly under varying pressure conditions. The research examines how rubidium's and cesium's lattice constant and pressure change with reduced volume, providing insights into its structural properties. Furthermore, the distribution of electron energy levels is analysed through the density of states across different energy regions. In the Brillouin zone, the conduction and valence band widths are mapped across important symmetry sites and computed in relation to the Fermi level.

Keywords: *Alkali metals, Band Structure, Density of States*

1. Introduction

Rubidium (Rb) and cesium (Cs) are alkali metals with comparable chemical characteristics, including low ionization potentials and strong reactivity. Both elements have unique electronic structures that significantly impact their behaviour under various conditions. Understanding their conductive characteristics and how they react to changes in pressure requires knowledge of their electronic band structures and density of states (DOS).This study focuses on the electronic band structure and DOS of cesium and rubidium, using the Full-Potential Linear Muffin-Tin Orbital (FP-LMTO) method to explore their behaviour under different pressures.

2. Band Structure

An illustration of the energy levels that electrons in a material can inhabit is provided by the electronic band structure. Cesium, being a metal, exhibits overlapping conduction and valence bands, which is characteristic of metallic elements. This overlap allows for the free movement of electrons, contributing to its high conductivity. Rubidium, while similar in behavior to cesium, exhibits slight differences in the overlap of its conduction and valence bands, based on the FP-LMTO computations.

For both cesium and rubidium, the band structures were calculated along key

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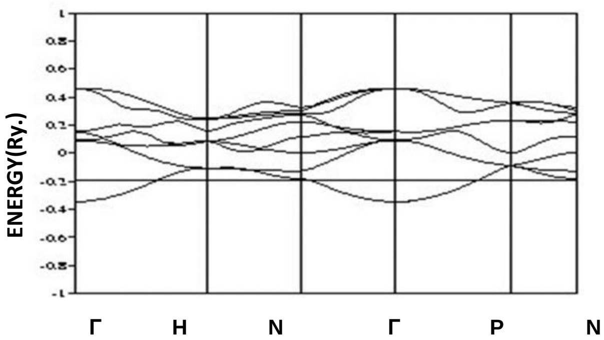
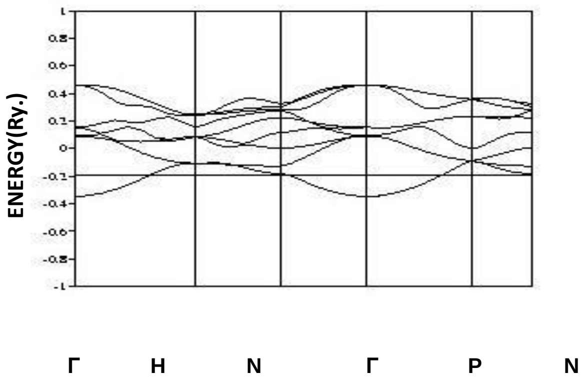
symmetry directions in the Brillouin zone: Γ-H-N-Γ-P-N.The metallic character of the conduction and valence bands was confirmed by the Fermi level, which was situated between them.According to the band structure data for cesium, the 6s orbital is the primary source of the conduction band, where rubidium's conduction band also features contributions from the 5s orbital, but the overlap with the valence band is somewhat less pronounced than in cesium.



CESIUM



RUBIDIUM

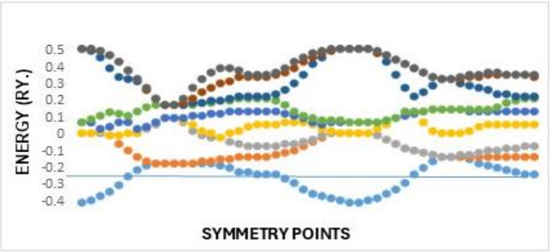


Fig. 2. Band structure of cesium using M.S. Excel

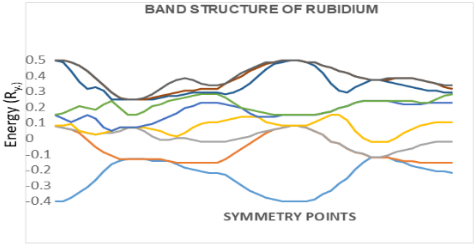


Fig. 3. Band Structure of rubidium using M.S. Excel

Graphs of the band structures for cesium and rubidium show that, as pressure increases and the reduced volume decreases, the bands shift accordingly. This shift in the band structure is a reflection of how the material's lattice constants and reaction to external forces have changed.

3. Density of States

The quantity of electronic states that can be occupied at each energy level is measured by the density of states (DOS). For cesium and rubidium, the DOS was calculated across various energy levels, disclosing important comprehension into their electronic structures. Both metals show significant peaks in the DOS near the Fermi level, providing evidence of a high density of states at the energy levels most likely to be occupied by electrons.

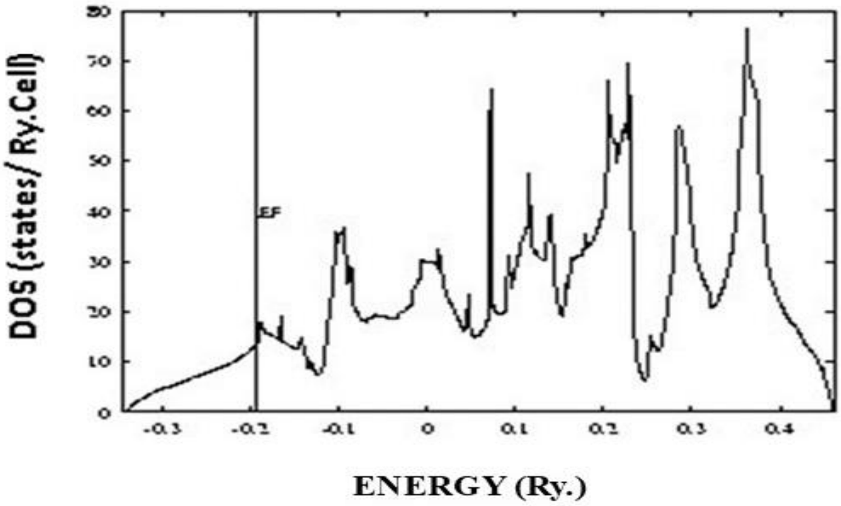


Fig. 4: Density of States of Cesium using FP-LMTO method.

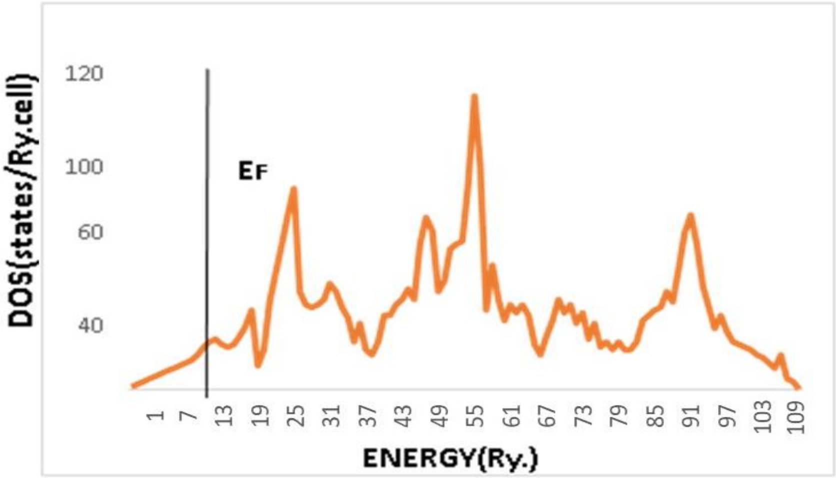


Fig. 5: Density of States of Cesium using M.S. Excel

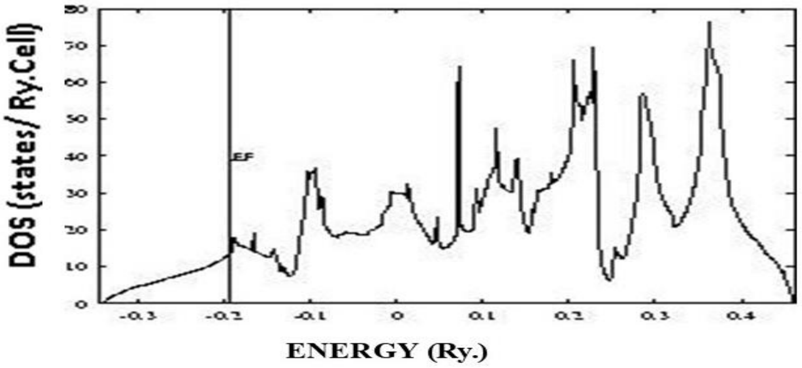


Fig. 6: Density of States of Rubidium using FP-LMTO method.

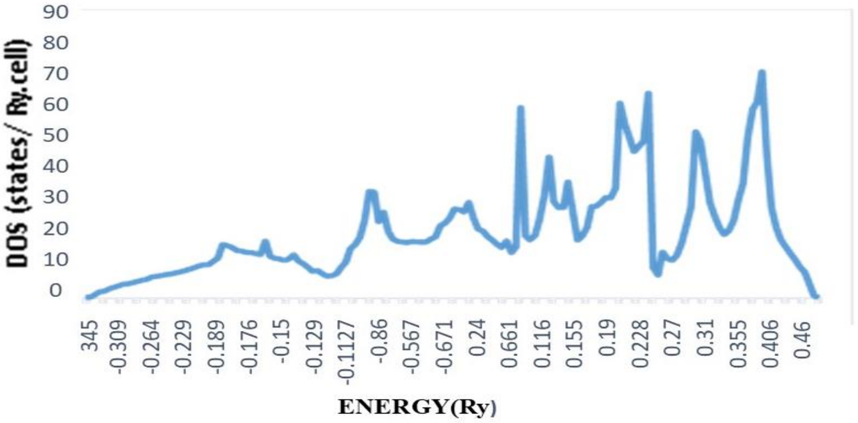


Fig. 7: Density of States of rubidium using M.S. Excel

The DOS for cesium is characterized by a broad distribution, with significant contributions from the 6s orbital, while rubidium’s DOS has a more localized distribution, primarily stemming from its 5s and 4d orbitals. The increased electron density at the Fermi level in cesium suggests stronger metallic behavior compared to rubidium.

For both cesium and rubidium, the DOS shows a pronounced shift in the peak positions as pressure is applied, reflecting the changes in their electronic environments under different volume conditions.

4. Ground State and Its Properties

The total energy as a function of decreased volume (V/V0) was used to study the ground state characteristics of cesium and rubidium, using the Murnaghan equation of state. The results showed that as the reduced volume decreases, the total energy increases for both metals, indicating an increase in internal pressure.

For cesium, the equilibrium lattice constant is 11.427 Å at normal pressure. As the pressure increased, the lattice constant decreased, confirming the typical behavior of alkali metals under pressure. The pressure values at various reduced volumes were also computed, and it was observed that asthe lattice constant increases, the pressure decreases.

Rubidium’s ground state properties showed similar trends, however the particular numbers for lattice constant and pressure were somewhat lower than those for cesium, reflecting differences in their atomic radii and bonding characteristics.

5. Conclusion

This study provides a detailed analysis of the electronic band structure and density of states of cesium and rubidium, with a focus on how these properties evolve under pressure. The findings confirm that both cesium and rubidium exhibit metallic behaviour, with overlapping conduction and valence bands. Cesium has a larger density of states around the Fermi level, indicating stronger metallic properties than rubidium. The ground state study indicated typical alkali metal behavior, with decreasing lattice constant and increasing pressure as volume is lowered. These findings contribute to the understanding of cesium and rubidium’s electronic structures and provide a foundation for future studies on these metals under varying pressure conditions.

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