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Revealing Structural, Electronic and Elastic Properties of $NaPaO_3$ Compound Theoretically

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ABSTRACT

In this study, structural, electronic and elastic properties of $NaPaO_3$ are investigated by Density Functional Theory (DFT). The lattice parameter, ground state energy and energy-volume-pressure relations are revealed by volume optimization. The electronic band diagram and total and partial Density of States (DOS) of $NaPaO_3$ compound are computed and graphs are plotted. It is revealed that $NaPaO_3$ is a semiconductor. Finally, the elastic properties are calculated and interpreted. It is seen that $NaPaO_3$ is an elastic material and it is mechanically stable.

Keywords: *Density Functional Theory, Elastic Properties, Electronic Properties, $NaPaO_3$*

ÖZET

Bu çalışmada, $NaPaO_3$'ün yapısal, elektronik ve elastik özellikleri ABINIT programı kullanılarak Genelleştirilmiş Gradyan Yaklaşımı (GGA) dahilinde Yoğunluk Fonksiyonel Teorisi (DFT) ile incelenmiştir. Örgü parametresi, temel durum enerjisi ve enerji-hacim-basınç ilişkileri hacim optimizasyonu ile ortaya çıkarılmıştır. $NaPaO_3$ bileşiğinin elektronik bant diyagramı ve toplam ve kısmi Durum Yoğunluğu (DOS) hesaplanmış ve grafikleri çizilmiştir. $NaPaO_3$'ün bir yarı iletken olduğu ortaya konmuştur. Son olarak, elastik özellikler hesaplanmış ve yorumlanmıştır. $NaPaO_3$'ün elastik bir malzeme olduğu ve mekanik olarak kararlı olduğu görülmüştür.

Anahtar Kelimeler: *Elastik Özellikler, Elektronik Özellikler, $NaPaO_3$, Yoğunluk Fonksiyonel Teorisi*

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INTRODUCTION

Materials with perovskite crystal structure are materials that are worth examining in theoretical and experimental research due to their widespread industrial use. In these materials, formalized as XYO_3, X and Y represent cation and O represents anion. It has wide application areas due to its properties such as ferroelectricity [1], superconductivity [2] and great light absorption [3].

Nalbanyan et al. experimentally investigated the structural properties of $NaSbO_3$ crystal [4]. Saeed et al. calculated the structural, electronic and optical properties of $NaNbO_3$, $KNbO_3$ and $RbNbO_3$ crystals for their cubic, rhombohedral, tetragonal and orthorhombic structures [5]. Sayed demonstrated the structural, electronic and optical properties of the thin film obtained by mixing nano-sized $NaTiO_3$ structures with polymethylmethacrylate [6]. Wang et al. investigated the photovoltaic performance of $NaNbO_3$ ferroelectric ceramics [7]. Yang et al. experimentally examined and declared the energy storage feature of $NaNbO_3$-based ceramics [8].

With computational materials science, the electronic, dynamic, optical, elastic and thermodynamic properties of many crystal structures, synthesized or unsynthesized in the laboratory, have been calculated [9-15]. These results have guided researchers regarding the suitability of crystals for their application areas. With the motivation derived from this, the properties of $NaPaO_3$ crystal were revealed in this study. It is anticipated that the findings of this study will inform future research endeavors.

COMPUTATIONAL METHOD

In this study, the structural, electronic and elastic properties of $NaPaO_3$ crystal were investigated using the ABINIT [16] software package. While examining the properties of NaPaO3 crystal, the exchange-correlation energy difference was expressed with the Generalized Gardient Approximation [17,18]. Perdew-Burke-Ernzerhof pseudopotentials were used when performing the calculations. The k grid sampling from the Brillouin region was chosen as 12 x 12 x 12 according to the Monkhorst-pack special points [19]. To express Kohn-Sham [20] wave functions, the cut-off energy was taken as 24 Ry. These values were determined by performing convergence tests.

RESULTS AND DISCUSSION

Some properties of $NaPaO_3$ compound was calculated which is a cubic crystal with $Pm\bar{3}m$ space group (No:221) and $m\bar{3}m$ point group.

We first performed volume optimization to calculate the lattice parameters, ground state energy. Volume optimization also gave us the total energy- volume, total energy-pressure and pressure-volume relations. The calculated lattice parameter of $NaPaO_3$ is 8.9409 Bohr and its volume is 714.73 $Bohr^3$. Examination the data of volume optimization have shown that the pressure versus volume behavior is inversely proportional as expected.

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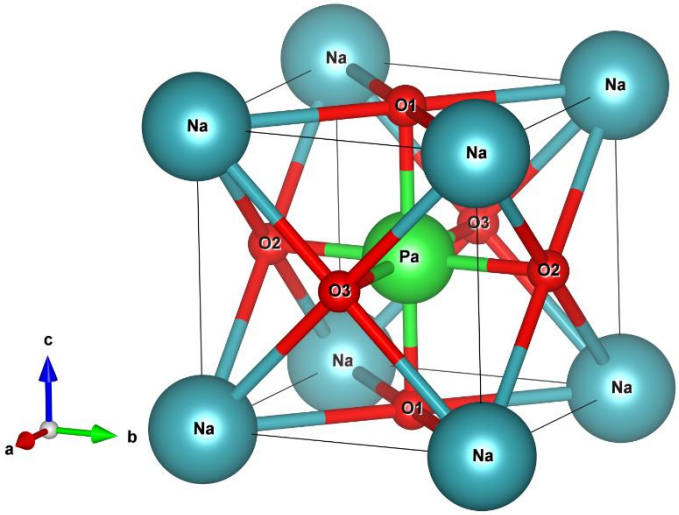

Figure 1. The unit cell of $NaPaO_3$ compound drawn by Vesta [21].

After the volume optimization we draw the unit cell by using Vesta computer programme as given in Figure 1. As seen from the Fig. 1, $NaPaO_3$ is a perovskite.

In order to understand the electronic features, we calculated and plotted the electronic band structure (Fig.2) and partial and total density of states graphs (Fig. 3). The band diagram is obtained throughout $\Gamma - X - M - \Gamma - R - X$ high symmetry points. As seen from Fig. 2 and 3, The Fermi level is aligned with 0 eV. Below the Fermi level, there are valance energy bands (12) and above the Fermi level there are conduction energy bands (8). The three of the valance bands are belond to core energy levels which are occurred approximately -15 eV. The band gap is 2.052 eV with indirect transition. Therefore, $NaPaO_3$ is a semiconductor.

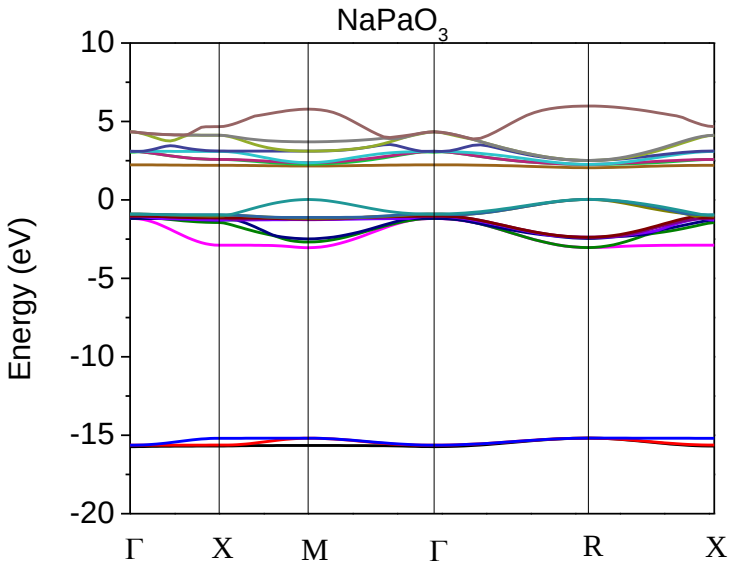

Figure 2. The electronic band structure of $NaPaO_3$.

PDOS and DOS graphs are consistent with each other and the electronic band structure graph. The contributions of each atoms in the unit cell of $NaPaO_3$ to the total density of states, that is partial (PDOS) and the total density of states (DOS) are given in Fig.3. The main contribution of Na atom is to the conduction bands with its s state. However the contribution of Na atom is very low (6 a.u.) when compared to other atoms (between 300-600 a.u.) in $NaPaO_3$ compound. Additionally, the participation of Pa atoms in the conduction bands is facilitated by their f state. The contributions of O atoms are very similar to each other. Most of their contributions are to the valance bands. The core energy contributions are also comes from the O atoms with s state as seen from Fig. 3. The rest of the contributions are from their p states. The total density of states graph is in close agreement with the electronic band structure.

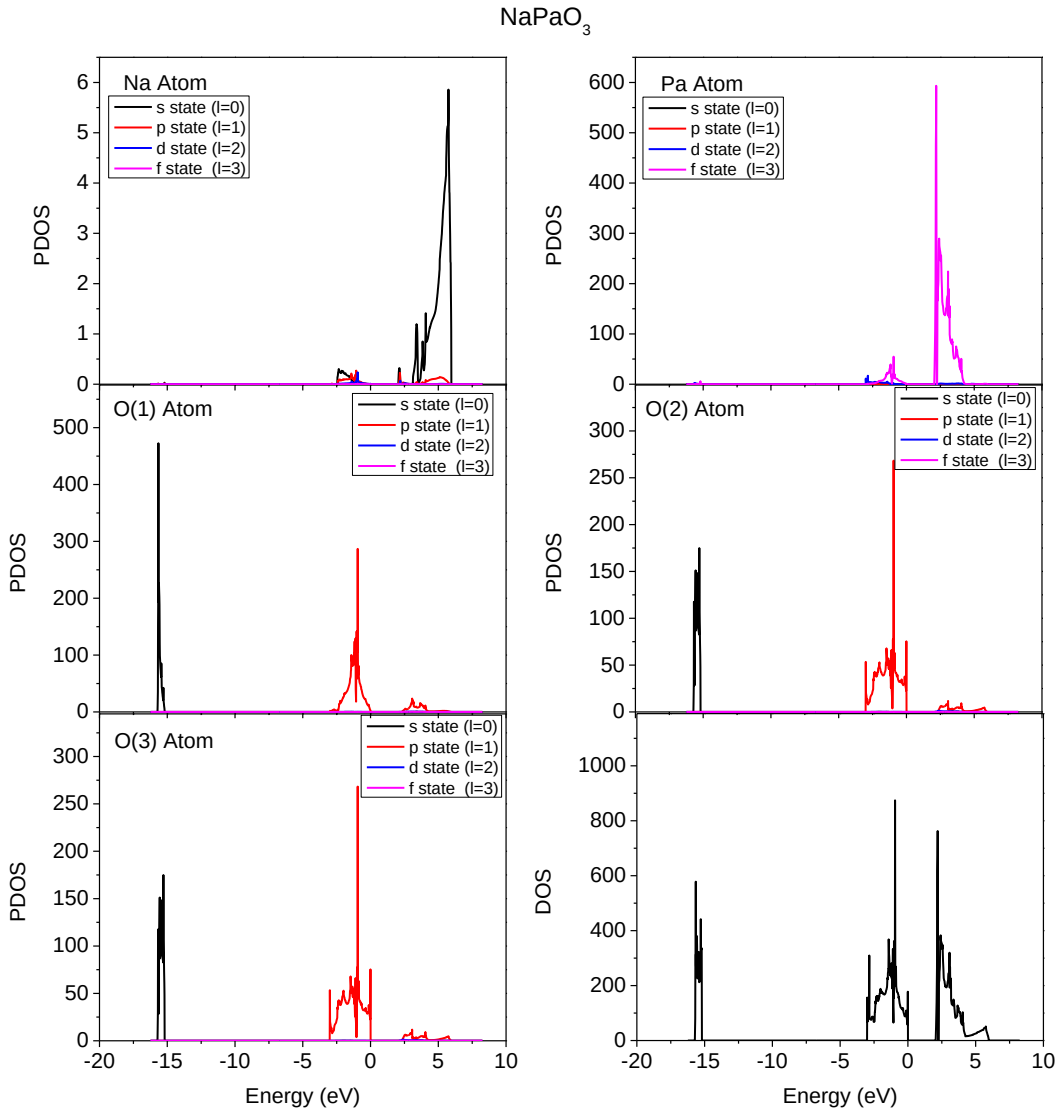

Figure 3. The partial and the total density of states graphs of $NaPaO_3$.

This study also examines the elastic properties of NaPaO3. In order to calculate the bulk, shear, and Young moduli, the Poisson ratio, flexibility coefficient, and Debye temperature, the elastic stiffness constants were calculated. Elastic stiffness constants

have 36 components in the matrix notation. However, because of the symmetry and cubic structure properties the number of the components decreases to 12. Additionally out of 12, 3 of them are (C_{11}, C_{12}, C_{44}) independent components (Table 1).

Table 1. Elastic stiffness constants of $NaPaO_3$

Elastic Stiffness Constants (GPa)	**$NaPaO_3$**
$C_{11}(=C_{22}=C_{33})$	360.6
$C_{12}(=C_{13}=C_{21}=C_{23}=C_{31}=C_{32})$	24.5
$C_{44}(=C_{55}=C_{66})$	27.1

The mechanically stability conditions are $C_{11}+2C_{12}>0$, $C_{44}>0$, $C_{11}>C_{12}$, $C_{11}>0$ and $C_{12}<Bulk\ Modulus<C_{11}$ [22]. Since $NaPaO_3$ meets with these conditions, this compound is mechanically stable.

Table 2. Elastic properties of $NaPaO_3$

Elastic Properties (Units)	Units	$NaPaO_3$
Bulk Modulus	B (GPa)	138.250
Shear Modulus	G (GPa)	81.407
Young Modulus	E (GPa)	155.653
Poisson Ratio	*v* (-)	0.312
Flexibility Coefficient	$K=B_{VRH}/G_{VRH}$ (-)	2.331
Debye Temperature (K)	Θ_D (K)	134.541
Zener Anisotropy Factor	A(-)	0.2

As seen from Table 2, Bulk and Young modulus are close to each other as expected. Poisson ratio and Flexibility coefficient gives information about the elasticity of a compound. The specific value of Poisson ratio is 0.26 and the specific value of the Flexibility coefficient is 1.75. If the calculated values of those are higher than those specific values, the material is said to be elastic, if lower than those specific values than material is a fragile material. Since the calculated value of Poisson ratio is 0.312 and the calculated value of Flexibility coefficient is 2.331, $NaPaO_3$ is an elastic material. The Debye temperature is correlated with the thermal conductivity. The calculated Debye temperature is 134.541 K, which shows that this compound has a high thermal conductivity when compared to the literature [23, 24]. Zener anisotropy factor shows how elastically isotropic a material is. If the Zener anisotropy factor is equal or very close to 1, than that material is elastically isotropic. The calculated value of Zener anisotropy factor for $NaPaO_3$ is 0.2, so this compound is not elastically isotropic material.

CONCLUSIONS

Within this research, the structural, electronic and elastic properties of $NaPaO_3$ are investigated. The ground state lattice parameter and total energy are calculated. The unit cell of this compound is sketched by using Vesta programme. The calculations on electronic properties have shown that $NaPaO_3$ is a semiconductor. Its band gap is 2.052 eV with indirect transition. The electronic band structure and all DOS graphs are compatible with each other. The contributions of atoms that is partial density of states

are calculated and plotted. Is is also obtained that $NaPaO_3$ is an elastic material and it is mechanically stable but it is not elastically isotropic.

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