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# Elastic, Electronic, Optical and Thermal Properties of $Na_2Po$: An *Ab Initio* Study

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The structural, elastic, electronic, optical and thermodynamic properties of the sodium polonide $Na_2Po$ compound have been studied through the full potential linearized augmented plane wave plus local orbitals (FP-LAPW + lo) and tight-binding linear muffin-tin orbital (TB-LMTO) methods. The exchange–correlation potential was treated within the local density approximation for the TB-LMTO calculations and within the generalized gradient approximation for the FP-LAPW + lo calculations. In addition, Tran and Blaha-modified Becke–Johnson (TB-mBJ) potential and Engel–Vosko generalized gradient approximation were used for the electronic and optical properties. Ground state properties such as the equilibrium lattice constant, bulk modulus and its pressure derivative were calculated and compared with available data. The single-crystal and polycrystalline elastic constants of the considered compound were calculated via the total energy versus strain in the framework of the FP-LAPW + lo approach. The calculated electronic structure reveals that $Na_2Po$ is a direct band gap semiconductor. The frequency-dependent dielectric function, refractive index, extinction coefficient, reflectivity coefficient and electron energy loss function spectra are calculated for a wide energy range. The variations of the lattice constant, bulk modulus, heat capacity, volume expansion coefficient and Debye temperature with temperature and pressure were calculated successfully using the FP-LAPW + lo method in combination with the quasi-harmonic Debye model.

**Key words:** Electronic structure, band gap, optoelectronic, FP-LAPW + lo, TB-LMTO

## INTRODUCTION

The sodium chalcogenides $Na_2A$ (A: S, Se and Te) compounds are narrow direct band gap semiconductors[1,2] crystallizing in the cubic anti-fluorite structure (anti-$CaF_2$-type), space group No. 225.[3] They appear promising for technological application in solid-state batteries, fuel cells, solid-state gas detectors and photo-emissive ultraviolet (UV) light materials.[4–7] Therefore, these materials have been the subject of numerous experimental and theoretical studies. Experimentally, the elastic constants of the $Na_2S$ compound have been determined using an elastic neutron scattering technique at low temperature by Bührer and Bill.[8] Bertheville et al.[9]

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measured the ionic conductivity of $Na_2S$, and showed that this compound exhibits a super-ionic behavior at a temperature close to the melting point, confirming the suggestion of Bührer and Bill.[10] Theoretically, the ground state and high-pressure phases of $Na_2S$ were studied up to a pressure of 100 GPa using Hartree–Fock and density-functional theory.[11] The structural, electronic and elastic properties of sodium chalcogenides $Na_2A$ (A: S, Se and Te) were reported by many authors.[1,10,12–15] The lattice dynamics properties of the $Na_2A$ (A: S, Se and Te) compounds were reported by Kalarasse et al.[16] The structural, electronic and optical properties of alkali metal telluride $Na_2Te$ were investigated in the framework of density functional theory (DFT) within generalized gradient approximation (GGA) by Alay-e-Abbes and Shaukat.[17] Recently, a first-principle study on the lattice dynamics, thermodynamics and elastic properties of $Na_2Te$ under high pressure were performed by Zhang and co-workers[7] using a pseudopotential plane-wave approach based on DFT. These compounds constitute a good example for a homologous series of crystals with predictable physical and physicochemical properties.

Although there has been considerable progress in the theoretical description of the structural and electronic properties of the sodium chalcogenides $Na_2A$ (A: S, Se, Te) compounds, there is a real lack of knowledge about the electronic, elastic, optoelectronic and thermal properties of the fourth member of the series, namely the sodium polonide $Na_2Po$; they are still not investigated experimentally or theoretically, which has prompted us to study them through accurate *ab initio* calculations. Therefore, the present work aims to study the structural, elastic, electronic, optical and thermodynamic properties of $Na_2Po$ in order to provide the data currently lacking for $Na_2Po$.

## COMPUTATIONAL DETAILS

The first part of the present calculations was performed using the full potential linearized augmented plane wave plus local orbitals (FP-LAPW + lo) method[18,19] in the framework of the DFT,[20,21] as implemented in the Wien2K code,[22] which is one of the most accurate and effective methods for the calculation of the ground state properties of materials.[23,24] In this method, the crystal unit cell is partitioned into non-overlapping muffin-tin (MT) spheres which surround each of the atomic and interstitial regions. Inside the MT sphere, which is centered at each atomic nucleus, the electronic wave functions and crystal potential were expanded in a basis set of spherical harmonics, while for the interstitial region, the electronic wave functions were expanded in a basis set of plane waves. The exchange–correlation contribution is treated within the generalized gradient approximation as proposed by Perdew, Burke and Ernzerhof (GGA-PBE)[25] for the calculations of the structural, elastic and thermodynamic properties. On the other hand, for the calculation of the electronic and optical properties, in addition to the GGA-PBE approximation, the Engel–Vosko generalized gradient approximation (EV-GGA)[26] and the recent Tran and Blaha-modified Becke–Johnson potential (TB-mBJ)[27] were also applied. The muffin-tin radii ($R_{MT}$) of 2.0 and 2.25 atomic units (*a.u.*) were used for the Na and Po atoms, respectively. In order to ensure convergence of the computed total energy, the wave functions in the interstitial region were expanded in plane waves with a cut-off $R_{MT}$ $K_{max} = 9$, where $R_{MT}$ denotes the smallest MT radius and $K_{max}$ designate the magnitude of the largest $K$ vector in the plane wave expansion. Inside each MT sphere, the electronic functions were expanded in a basis set of spherical harmonics up to the angular momentum of $l_{max} = 10$. The integrals over the Brillouin zone (BZ) were performed using the $12 \times 12 \times 12$ $k$-point grid for the calculation of the structural and electronic properties, while for the optical properties, a mesh of $20 \times 20 \times 20$ $k$-points was used following the Monkhorst–Pack special $k$-point sampling.[28] The self-consistent iteration process was repeated until the total energy convergence was less than $10^{-5}$ Ry.

The second part of the present calculations was carried by using Andersen's tight-binding version of the TB-LMTO method[29,30] within the local density approximation (LDA) of von Barth and Hedin parameterization[31] to investigate the total energy and electronic structure. The atomic sphere approximation (ASA) has been used where the Wigner–Seitz sphere radii are chosen in such a way that the potential discontinuity at the sphere boundary is a minimum and the charge flow between the atoms is in accordance with the electronegativity criteria. Additionally, the overlaps of the atomic spheres are kept within 16%. The total energy convergence was well-checked by increasing the number of $k$-points where the band structure calculations were performed for 512 $k$-points. In addition, the tetrahedron method of Brillouin zone integration has been used to calculate the density of states (DOS).[32]

The knowledge of specific behaviours of materials when they are under severe constraints, such as in high-pressure and high-temperature environments, is of great importance for technological applications. To address this interest in the present work, the pressure and temperature dependencies of the lattice parameter, bulk modulus, volume expansion coefficient, heat capacity and the Debye temperature of the $Na_2Po$ compound were investigated using the FP-LAPW + lo method combined with the quasi-harmonic Debye model as implemented in the Gibbs code.[33]Further details of this procedure can be found in other published articles.[34,35]