The Chitransh Academic & Research
An International Journal of Multidisciplinary Research

An Online Peer Reviewed / Refereed Journal
Volume 2 | Issue 2 |June 2026
ISSN: 3049-303X (Online)
Website: www.thechitranshacadmic.in

DFT Analysis of the Electronic, Optical, and Mechanical Properties of Ba_2NiWO_6 and Sr_2NiWO_6 Double Perovskite Oxides

Mr. Gururaj R Deshpande
Research Scholar Department of Mechanical Engineering Nirwan University, Jaipur, Rajasthan
Dr. Jaidev Kumbhakar
Department of Mechanical Engineering Nirwan University, Jaipur, Rajasthan
V.V. Potdar
Professor, Department of Mechanical Engineering A.G.Patil Institute of Technology, Solapur, Maharashtra

ARTICLE DETAILS

Research Paper
Received: **06/06/2026**
Accepted: **15/06/2026**
Published: **30/06/2026**

Keywords: Double Perovskite; Ba_2Niwo_6; Sr_2Niwo_6; Density Functional Theory; Optical Response; Elastic Stability.

ABSTRACT

Ba_2NiWO_6 and Sr_2NiWO_6 are ordered nickel-tungstate double perovskites in which A-site size, octahedral rotation, Ni 3d correlation, and W 5d states jointly determine magnetic, electronic, optical, and mechanical behavior. This paper presents a ten-page, literature-anchored density-functional-theory (DFT) analysis and a reproducible computational protocol for comparing the two compounds. Ba_2NiWO_6 is experimentally reported in the cubic Fm-3m structure with a lattice parameter near 8.10875 Å and an optical gap near 3.20 eV, whereas Sr_2NiWO_6 adopts a tetragonal I4/m structure with a = 5.562974 Å, c = 7.919822 Å, and an optical gap near 3.29 eV. Published calculations identify an antiferromagnetic ground state for Ba_2NiWO_6 and type-II antiferromagnetism for Sr_2NiWO_6 . The recommended workflow combines spin-polarized GGA-PBE optimization, magnetic-order screening, projected densities of states, tensor-resolved optical calculations, and finite-strain elastic analysis. The comparison predicts that Sr substitution contracts the lattice and increases octahedral rotation, thereby modifying Ni-O-W hybridization and increasing elastic anisotropy. Because compound-specific elastic tensors were not reported in the source dataset, the mechanical section reports symmetry-complete stability tests and derived-property equations rather than fabricated numbers. The resulting manuscript distinguishes experimental benchmarks, published DFT findings, and calculations that must be performed before claims of original numerical results can be made.

1. Introduction

Ordered double perovskites have the general formula $A_2BB'O_6$, where chemically distinct B and B' cations occupy alternating oxygen octahedra. Rock-salt B-site ordering is favored when the two cations differ strongly in charge and size. This architecture supports systematic control of crystal symmetry, magnetic exchange, dielectric polarization, band-edge chemistry, and mechanical stiffness through substitution at the A, B, or B' sites.

Ba_2NiWO_6 and Sr_2NiWO_6 contain nominal Ba^{2+}/Sr^{2+}, Ni^{2+}, W^{6+}, and O^{2-} ions. The Ni^{2+} ion has a partially occupied $3d^8$ configuration and is the principal source of localized magnetism, while W^{6+} is nominally $5d^0$ and contributes unoccupied states to the conduction region. Oxygen mediates Ni-O-W superexchange and supplies much of the upper-valence-band density. Consequently, structural distortions that change Ni-O and W-O distances or Ni-O-W angles can affect both the magnetic exchange network and the optical transition energies.

Experimental work assigns cubic Fm-3m symmetry to Ba_2NiWO_6 and reports a room-temperature lattice parameter of approximately 8.10875 Å, together with an optical gap of about 3.20 eV [4]. Nanocrystalline samples retain the centrosymmetric cubic structure, although particle size influences magnetic and dielectric response [10]. A first-principles study found the antiferromagnetic phase to be more stable than competing magnetic arrangements and obtained an mBJ gap of 2.48 eV, emphasizing the sensitivity of the predicted gap to exchange-correlation treatment [5].

Sr_2NiWO_6 is structurally less symmetric. Rietveld refinement supports tetragonal I4/m symmetry with $a = 5.562974$ Å and $c = 7.919822$ Å, and diffuse-reflectance analysis gives an optical gap near 3.29 eV [6]. Neutron diffraction and first-principles calculations identify type-II antiferromagnetic ordering at low temperature, with next-nearest-neighbor interactions playing an important role [7]. Comparative magnetic calculations have also treated Ba_2NiWO_6 and Sr_2NiWO_6 within a common electronic-structure framework [8].

Despite this progress, a single transparent framework that connects A-site substitution to structural distortion, orbital-resolved electronic states, optical tensors, and elastic stability remains useful. The objective of this paper is therefore

Corresponding Author: nimmiekka@gmail.com

to define such a framework, synthesize verified literature benchmarks, and specify the calculations needed for a defensible side-by-side DFT study.

Table 1. Literature benchmarks motivating the comparison

Compound	Reported symmetry	Structural benchmark	Optical/electronic benchmark	Magnetic benchmark
Ba_2NiWO_6	Cubic *Fm-3m*	a ≈ 8.10875 Å [4]	Optical gap ≈ 3.20 eV [4]; mBJ gap 2.48 eV [5]	AFM lower than competing phases [5]
Sr_2NiWO_6	Tetragonal *I4/m*	a = 5.562974 Å; c = 7.919822 Å [6]	Optical gap ≈ 3.29 eV [6]	Type-II AFM [7]

Research questions

The analysis addresses four questions: how A-site substitution changes the equilibrium structure; which orbitals form the band edges; how symmetry controls the dielectric and absorption response; and which elastic constants and polycrystalline moduli are required to establish mechanical stability and anisotropy.

2. Computational Methodology

2.1 Electronic-structure calculations

Spin-polarized calculations should be performed with a plane-wave pseudopotential code such as Quantum ESPRESSO [2], VASP, or CASTEP. Exchange and correlation are treated initially with the Perdew-Burke-Ernzerhof generalized-gradient approximation (GGA-PBE) [1]. Because Ni 3d localization and semiconductor band gaps may be poorly represented by semilocal PBE, the baseline results should be cross-checked using PBE+U, mBJ, or a screened hybrid functional. The correction method, U value, pseudopotential family, and valence configurations must be reported explicitly.

Convergence testing is essential. The wave-function cutoff, charge-density cutoff, and k-point mesh are increased independently until the total energy changes by less than 1 meV per atom and key stress components vary negligibly.

Geometry optimization should continue until forces are below 0.01 eV $Å^{-1}$ and residual stress is below approximately 0.1 GPa. Denser meshes are required for the density of states and frequency-dependent optical response.

2.2 Structural and magnetic models

Ba_2NiWO_6 is initialized in the conventional cubic Fm-3m cell with rock-salt Ni/W ordering. Sr_2NiWO_6 is initialized in tetragonal I4/m symmetry, allowing symmetry-compatible octahedral rotation and internal-coordinate relaxation. Ferromagnetic, nonmagnetic, and at least two antiferromagnetic starting states should be compared. For Sr_2NiWO_6, the type-II arrangement reported by neutron diffraction must be included [7]. The ground state is the fully relaxed configuration with the lowest total energy.

$\Delta E_i = E_i$ - Eground

Magnetic comparisons must use identical supercells, k-point density, cutoffs, smearing, and convergence criteria. The local Ni moment should be reported together with the integration convention because moments extracted from atomic spheres, Bader basins, or projector channels are not directly interchangeable.

2.3 Optical and elastic calculations

The independent-particle dielectric tensor is calculated from interband transition matrix elements; the real part follows from the Kramers-Kronig relation [3]. For cubic Ba_2NiWO_6, one diagonal component is sufficient after numerical symmetry checks. For tetragonal Sr_2NiWO_6, $\varepsilon xx = \varepsilon yy$ and εzz should be reported separately. Elastic constants are obtained from small symmetry-adapted strains, preferably using both positive and negative amplitudes to test linearity.

Table 2. Recommended reproducible calculation settings

Item	Ba_2NiWO_6	Sr_2NiWO_6	Acceptance check
Starting symmetry	*Fm-3m*	*I4/m*	No unintended cation disorder
Magnetic states	FM, AFM-I, AFM-II	FM, type-II AFM, alternatives	Same numerical settings
XC baseline	GGA-PBE	GGA-PBE	Functional stated [1]
Gap	PBE+U/mBJ/hybrid	PBE+U/mBJ/hybrid	Method kept

validation			separate
Geometry k mesh	Converged cubic mesh	Converged tetragonal mesh	<1 meV atom^{-1}
Optical tensor	Isotropic check	xx and zz components	Dense unoccupied bands
Elastic strains	±0.3%, ±0.6%, ±1.0%	±0.3%, ±0.6%, ±1.0%	Linear stress response

3. Structural and Magnetic Properties

3.1 A-site size and octahedral geometry

The larger Ba^{2+} ion stabilizes a high-symmetry cubic network in which the NiO_6 and WO_6 octahedra are close to untilted. In contrast, replacing Ba^{2+} with smaller Sr^{2+} reduces the space available at the A site and favors cooperative octahedral rotation. The experimentally observed change from Fm-3m to I4/m symmetry is therefore the central structural distinction between the compounds [4], [6].

A rigorous DFT comparison should report conventional-cell volume, volume per formula unit, mean and symmetry-distinct Ni-O and W-O distances, Ni-O-W angles, and octahedral distortion parameters. Direct comparison of the raw conventional-cell volumes is misleading because the cells contain different numbers and orientations of formula units; normalization per formula unit is required. The tetragonal c/a ratio should also be discussed relative to the chosen cell setting.

The Ni-O-W angle is especially important because it controls the overlap between Ni 3d, O 2p, and W 5d orbitals. A reduction from an idealized 180° path weakens the most direct through-oxygen overlap and can narrow electronic bands. However, the band-gap response is not determined by angle alone: bond-length contraction, crystal-field splitting, exchange splitting, and correlation corrections can act in competing directions.

3.2 Magnetic order

For Ni^{2+} in an octahedral crystal field, the $3d^8$ configuration supports a local magnetic moment primarily associated with the Ni site. The W^{6+} ion is nominally nonmagnetic, so long-range order is mediated through extended Ni-O-W-O-Ni pathways. Published work identifies an antiferromagnetic ground state for cubic Ba_2NiWO_6 [5], while Sr_2NiWO_6 exhibits type-II antiferromagnetic order [7]. These findings require

sufficiently large magnetic cells; a primitive structural cell may be unable to represent all relevant spin arrangements.

Total-energy differences between magnetic states should be reported per formula unit, not per computational cell, and should be compared only after full ionic relaxation or after a clearly stated fixed-structure protocol. A small energy splitting should be accompanied by convergence tests tighter than the splitting itself. Calculated Ni moments lower than the ideal ionic spin-only value would be consistent with Ni-O covalency and spin density transferred to oxygen.

Table 3. Structural and magnetic comparison

Descriptor	Ba_2NiWO_6	Sr_2NiWO_6	Interpretation
Experimental symmetry	*Fm-3m* [4]	*I4/m* [6]	Sr substitution lowers symmetry
Lattice parameters	a ≈ 8.10875 Å [4]	a = 5.562974 Å; c = 7.919822 Å [6]	Different cell settings
Octahedral rotation	Weak/absent in ideal cubic model	Allowed and experimentally required	Greater directional anisotropy
Published ground state	Antiferromagnetic [5]	Type-II antiferromagnetic [7]	Ni-centered exchange network
Key DFT outputs	O coordinate, Ni-O/W-O, ΔE	Tilt angle, distinct bonds, ΔE	Needed for mechanism

Validation criterion

An optimized structure is considered credible only when the symmetry, normalized volume, bond geometry, and magnetic ordering are simultaneously consistent with experiment or with a documented explanation of the discrepancy. Agreement in lattice parameter alone is insufficient.

4. Electronic Properties

4.1 Band-gap assessment

Electronic band structures must be calculated along symmetry-appropriate high-symmetry paths for the cubic and tetragonal Brillouin zones. The valence-band maximum and conduction-band minimum should be identified explicitly, allowing the direct or indirect nature of the gap to be determined. Because antiferromagnetic cells

fold the Brillouin zone, the k-point labels must correspond to the actual magnetic cell rather than to the parent crystallographic cell.

The available benchmarks already show why exchange-correlation choice matters. Ba_2NiWO_6 has an experimental optical gap near 3.20 eV [4], while a published mBJ calculation gives 2.48 eV [5]. The difference should not be treated as a simple error bar: optical measurements may contain excitonic, defect, particle-size, and fitting effects, whereas Kohn-Sham eigenvalue gaps depend strongly on the functional. Sr_2NiWO_6 has a reported optical gap near 3.29 eV [6], but a consistent PBE, PBE+U, mBJ, or hybrid comparison for both compounds is required before a robust substitution trend is claimed.

4.2 Orbital-resolved density of states

Chemical reasoning and published results indicate that Ni 3d and O 2p states dominate the magnetic valence region, while unoccupied W 5d states are important in the conduction manifold. The upper valence band is therefore expected to contain mixed O 2p-Ni 3d character, and the lowest conduction states may contain W 5d with additional Ni 3d weight. Ba or Sr states should occur mainly farther from the band edges, so the A-site substitution affects the gap principally through structure and electrostatics rather than direct frontier-orbital participation.

Projected densities of states should be resolved by spin and, where possible, by crystal-field symmetry. For octahedral Ni^{2+}, separating t2g-like and eg-like contributions helps identify exchange splitting and the role of σ-type Ni-O hybridization. The analysis should integrate the projected density over selected energy windows and compare the result with local magnetic moments, rather than relying only on visual peak labels.

4.3 Expected substitution effects

Sr-driven lattice contraction tends to increase orbital overlap, whereas octahedral rotation tends to reduce the directional Ni-O-W overlap. The net band-gap change is therefore not predetermined. A defensible conclusion should be based on aligned band edges, bond geometry, orbital bandwidths, and a common functional. Any scissor correction used for optical spectra must be applied transparently and must not alter the uncorrected electronic-structure results.

Corresponding Author: nimmiekka@gmail.com

Table 4. Electronic-property reporting checklist

Quantity	Minimum report	Reason
Magnetic cell and path	Cell vectors and k-path labels	Prevents band-folding ambiguity
Band gap	Value, direct/indirect, VBM and CBM	Defines electronic transition
Functional dependence	PBE plus one corrected method	Tests Ni 3d and gap sensitivity
Projected DOS	Ni 3d, W 5d, O 2p, A-site states	Assigns band-edge chemistry
Spin moments	Ni and induced O moments	Connects DOS and magnetism
Band alignment	Common reference or core level	Supports compound comparison

5. Optical Properties

5.1 Dielectric response

The frequency-dependent optical response is derived from the complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The imaginary part reflects allowed interband transitions weighted by dipole matrix elements, while the real part is obtained through the Kramers-Kronig relation [3]. The static electronic dielectric constant $\varepsilon_1(0)$ and the zero-frequency refractive index provide low-energy measures of electronic polarizability.

$$n(\omega) = \{ [\sqrt{(\varepsilon_1^2 + \varepsilon_2^2)} + \varepsilon_1] / 2 \}^{1/2}$$

$$k(\omega) = \{ [\sqrt{(\varepsilon_1^2 + \varepsilon_2^2)} - \varepsilon_1] / 2 \}^{1/2}$$

The absorption coefficient follows from n and k, and reflectivity at normal incidence is calculated from $R = [(n - 1)^2 + k^2] / [(n + 1)^2 + k^2]$. The energy-loss function $L(\omega) = \mathrm{Im}[-1/\varepsilon(\omega)]$ identifies plasma-like resonances. All spectra should state the number of empty bands, broadening, k-point mesh, polarization direction, and whether a gap correction was applied.

5.2 Symmetry and anisotropy

Cubic Ba_2NiWO_6 should be optically isotropic in the ideal bulk crystal, apart from numerical noise. Tetragonal Sr_2NiWO_6 is uniaxially anisotropic, so $\varepsilon xx = \varepsilon yy$ may differ from εzz. Averaging the tensor before analysis can hide physically meaningful

Corresponding Author: nimmiekka@gmail.com

polarization dependence. The onset, principal ε_2 peaks, maximum absorption, low-energy reflectivity, and loss-function peak should therefore be reported separately for in-plane and out-of-plane polarization.

5.3 Interpretation of optical transitions

The absorption edge is expected to involve transitions from O 2p/Ni 3d-derived valence states to W 5d/Ni 3d-derived conduction states. Peak assignments must be made by comparing the initial- and final-state projected densities in the corresponding energy windows. A large density-of-states peak does not necessarily produce a strong optical peak if the transition matrix element is weak or symmetry-forbidden.

The experimental optical gaps of approximately 3.20 eV for Ba_2NiWO_6 and 3.29 eV for Sr_2NiWO_6 place the primary onset near the ultraviolet boundary [4], [6]. Consequently, claims of visible-light activity should distinguish intrinsic band-to-band absorption from defect-assisted absorption, particle-size effects, or alternative experimental gap estimates.

Table 6. Optical quantities and interpretation

Optical quantity	Physical meaning	Required comparison
$\varepsilon_1(0)$	Electronic polarizability	Ba cubic vs Sr xx and zz
ε_2 onset	Lowest allowed interband transition	Band gap and selection rules
Absorption coefficient	Photon attenuation	Edge and strongest energy region
Refractive index	Phase velocity response	Consistency with $\sqrt{\varepsilon_1(0)}$
Reflectivity	Surface optical response	Low-energy and peak values
Loss function	Collective excitation energy	Zero crossing of ε_1

6. Elastic and Mechanical Properties

6.1 Elastic tensors and stability

Mechanical stability must be established from the complete elastic tensor rather than from a bulk modulus alone. Cubic Ba_2NiWO_6 has three independent constants: C_{11}, C_{12}, and C_{44}. Tetragonal Sr_2NiWO_6 has six: C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66}. These are

obtained by fitting stress or total-energy changes under small, symmetry-adapted strains.

Cubic: $C_{11} - C_{12} > 0$; $C_{11} + 2C_{12} > 0$; $C_{44} > 0$

Tetragonal: $C_{11} > |C_{12}|$; $C_{33}, C_{44}, C_{66} > 0$; $2C_{13}^2 < C_{33}(C_{11} + C_{12})$

These conditions are necessary and sufficient for the relevant crystal systems under zero external pressure [11]. Each fit should include multiple positive and negative strain amplitudes. Nonlinearity or asymmetry indicates that the strain is too large, the relaxation protocol is inconsistent, or the stress tolerance is insufficient.

6.2 Polycrystalline moduli

For comparison with ceramic samples, single-crystal constants are converted to Voigt and Reuss bounds and then Hill averages [12]. The bulk modulus B measures resistance to hydrostatic compression, the shear modulus G measures resistance to shape change, and Young's modulus E describes uniaxial stiffness. Poisson's ratio ν reflects transverse contraction.

$BH = (BV + BR)/2$; $GH = (GV + GR)/2$

$E = 9BG/(3B + G)$; $\nu = (3B - 2G)/[2(3B + G)]$

The empirical Pugh ratio B/G is often used as a qualitative ductility indicator; values above about 1.75 are commonly associated with ductile behavior, whereas smaller values suggest brittleness [13]. This threshold is heuristic and should not replace fracture or indentation measurements. The universal anisotropy index $AU = 5GV/GR + BV/BR - 6$ equals zero for an isotropic material.

6.3 What can be concluded without fabricated numbers

Symmetry alone predicts that Sr_2NiWO_6 can exhibit stronger elastic anisotropy than cubic Ba_2NiWO_6, because tetragonal symmetry permits distinct axial and basal stiffnesses. It does not determine whether Sr_2NiWO_6 is stiffer, harder, more ductile, or more brittle. Those claims require the calculated Cij values. Accordingly, this paper provides the complete mechanical protocol and stability criteria but does not insert unsupported elastic constants.

Table 7. Mechanical outputs required for an original DFT study

Output	Ba_2NiWO_6	Sr_2NiWO_6	Decision enabled
Independent Cij	C_{11}, C_{12}, C_{44}	C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66}	Born stability
Hill moduli	B, G, E, ν	B, G, E, ν	Polycrystalline stiffness
Pugh ratio	B/G	B/G	Ductile/brittle tendency
Anisotropy	AU and directional E	AU and directional E	Texture sensitivity
Fit quality	Strain linearity and residuals	Strain linearity and residuals	Numerical credibility

7. Comparative Structure-Property Relationships

7.1 Coupled effect of Ba-to-Sr substitution

The clearest experimentally established substitution effect is the symmetry reduction from cubic Ba_2NiWO_6 to tetragonal Sr_2NiWO_6 [4], [6]. This change is consistent with a smaller A-site cation and stronger octahedral rotation. The structural perturbation propagates into three property families. First, it changes Ni-O-W overlap and therefore the width and relative energy of Ni 3d, O 2p, and W 5d bands. Second, it introduces optical birefringence and polarization-dependent absorption. Third, it permits a larger number of independent elastic constants and direction-dependent stiffness.

The magnetic response is also connected to geometry. Ni moments communicate through long Ni-O-W-O-Ni pathways, so exchange strengths can depend strongly on bond angles and orbital orientation. The type-II antiferromagnetic state of Sr_2NiWO_6 indicates that interactions beyond the nearest Ni pair are important [7]. A meaningful DFT analysis should therefore compare several magnetic configurations and, where possible, map their energy differences onto an exchange model.

7.2 Property selection for applications

For dielectric components, desirable features include a stable insulating gap, moderate electronic polarizability, low optical absorption in the operating range, and mechanical integrity. For ultraviolet optoelectronics or photocatalysis, the absorption edge, carrier-effective masses, defect tolerance, and absolute band-edge positions become more important. Mechanical stiffness can improve dimensional stability, but

excessive brittleness or anisotropy may complicate sintering, film growth, or thermal cycling.

Neither compound can be declared superior for all applications from the available evidence. Ba_2NiWO_6 offers higher crystallographic symmetry and an experimentally reported ultraviolet-scale gap. Sr_2NiWO_6 offers a distinct tetragonal crystal field, type-II antiferromagnetism, and potentially useful anisotropic response. Application selection should be based on a multidimensional property map rather than on band gap alone.

Table 8. Evidence-based comparative assessment

Property axis	Ba_2NiWO_6	Sr_2NiWO_6	Evidence strength
Crystal symmetry	Cubic *Fm-3m*	Tetragonal *I4/m*	Strong: experiment [4], [6]
Optical gap	≈3.20 eV	≈3.29 eV	Moderate: diffuse reflectance [4], [6]
Magnetic order	Antiferromagnetic	Type-II antiferromagnetic	Strong: calculation/neutron [5], [7]
Optical anisotropy	Ideally isotropic	Uniaxial tensor expected	Strong from symmetry; magnitude uncalculated
Elastic anisotropy	Cubic constraints	More independent directions	Strong from symmetry; magnitude uncalculated
Mechanical ranking	Not established	Not established	Requires converged Cij

Recommended decision rule

A claim of substitution-driven improvement should be accepted only when the same functional, pseudopotential quality, magnetic treatment, convergence thresholds, and property definitions are used for both compounds. Otherwise, methodological differences may be larger than the chemical trend.

8. Limitations, Reproducibility, and Conclusions

8.1 Limitations

The principal limitation of the present paper is that it synthesizes literature benchmarks and specifies a complete DFT workflow but does not include newly executed calculation files. The reported lattice parameters, optical gaps, and magnetic conclusions are therefore attributed to their original sources [4]-[8]. Compound-specific elastic constants and derived moduli are intentionally omitted because they were not available in the supplied evidence. This distinction is essential for research integrity.

A second limitation is the sensitivity of Ni-containing oxides to exchange-correlation treatment. Semilocal PBE may underestimate the gap and may over-delocalize Ni 3d states. PBE+U can improve localization but introduces a parameter; mBJ can improve band gaps but is not a universal total-energy functional; hybrids are more expensive and may still require convergence checks. Results from different approaches should be presented in parallel rather than combined into a single unlabeled dataset.

Optical spectra calculated in the independent-particle approximation neglect excitonic effects and may depend on broadening and unoccupied-band convergence. Mechanical calculations are sensitive to residual stress, strain amplitude, and whether internal coordinates are relaxed for each strain. Experimental ceramic moduli may also differ from ideal-crystal DFT values because of porosity, grain boundaries, texture, and defects.

8.2 Reproducibility package

A publishable original study should archive the starting crystallographic files, pseudopotential identifiers, code version, input files, convergence curves, magnetic supercells, relaxed structures, k paths, density-of-states grids, optical settings, strain matrices, stress outputs, and scripts used to derive moduli. Reported tables should be generated directly from machine-readable outputs to reduce transcription errors.

8.3 Conclusions

Ba_2NiWO_6 and Sr_2NiWO_6 provide a useful pair for examining how A-site size couples structure to functional properties in ordered nickel-tungstate double perovskites.

Ba_2NiWO_6 is reported as cubic Fm-3m with a lattice parameter near 8.10875 Å and an optical gap near 3.20 eV [4]. Sr_2NiWO_6 is tetragonal I4/m with a = 5.562974 Å, c = 7.919822 Å, and an optical gap near 3.29 eV [6]. Published work supports antiferromagnetism in both compounds, including a type-II ground state for Sr_2NiWO_6 [5], [7].

The most defensible electronic picture places mixed O 2p-Ni 3d states near the valence edge and W 5d/Ni 3d states in the conduction region. Sr substitution increases structural anisotropy and should produce polarization-dependent optical and elastic responses. However, the direction of the band-gap shift and the ranking of mechanical stiffness cannot be inferred from symmetry alone.

The proposed calculation protocol resolves these uncertainties through matched magnetic, electronic, optical, and finite-strain calculations. Its key methodological conclusion is simple: structural, optical, and mechanical claims must be made from a single converged computational framework, while experimental and previously published values remain clearly labeled.

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