

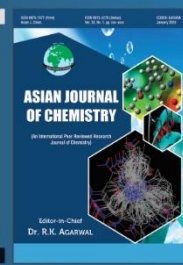


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Novel Ba-Based Oxynitride Perovskites Synthesized via Sol-gel Method for High-Performance Solar Cell Applications

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Novel barium based oxynitride perovskites (BaCuO_2N , BaCoO_2N and bimetallic $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$) were successfully synthesized by a cost-effective sol-gel method. The XRD patterns were indexed to a triclinic crystal system for the single-metal compositions, whereas the mixed Cu–Co composition was indexed to a monoclinic system. FESEM and AFM analyses revealed nanoscale grains with distinct surface morphologies, while optical characterization showed broad absorption across the UV-visible region. Thermal analysis indicated that the major mass-loss events occurred below approximately 350 °C. The investigated materials exhibited p-type semiconducting behaviour. Among the studied compositions, BaCoO_2N showed the highest measured power conversion efficiency (PCE) of 15.77%, compared with 10.60% for BaCuO_2N and 10.86% for $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ under the applied measurement conditions. The higher PCE of BaCoO_2N suggests that its composition and associated structural and optoelectronic characteristics may be favourable for photovoltaic performance.

Keywords: Perovskite oxynitrides, Composite, Sol-gel technique, Perovskite solar cells.

INTRODUCTION

High efficiency photovoltaic technologies are considered a key enabler for sustainable decarbonization and have been subject of intensive research efforts due to the critical global need for clean energy harvesting [1,2]. The metal halide perovskite solar cells (PSCs) have gained tremendous scientific interest due to their exceptional optoelectronic properties such as high absorption coefficient, wide tunable bandgap, long carrier diffusion length, low-temperature solution processability, etc. [3,4]. As a result, the power conversion efficiencies (PCEs) of single-junction PSCs have quickly risen from 3.8% in 2009 to more than 26.95% [5] and silicon-perovskite tandem cells have reached more than 34% [6]. Although these unparalleled performance milestones, the commercial use of conventional organic–inorganic halide perovskites is still inherently limited by the serious thermal, moisture-induced and structural degradation and by the volatility of ionic migration under operational bias [7].

In order to overcome these stability constraints while maintaining the excellent optoelectronic properties, recent studies have focused on the development of stable perovskite

crystal lattice, namely transition metal oxynitride structures (ABO_2N) [8]. The introduction of N into the oxide framework reduces the fundamental bandgap by the hybridization of N-2p and O-2p orbitals and the introduction of multivalent transition metals (e.g. Co and Cu) at the B-site allows the electronic band structure, charge carrier density and localized d-d orbital transitions to be tuned [9].

Moreover, the ability to prepare these oxynitrides at the nanoscale using liquid-phase chemical synthesis methods like sol-gel processing provides higher surface-to-volume ratios [10] and lower charge transport pathways and non-radiative recombination losses [9]. However, the synergistic effect of mixed transition-metal substitutions on the optical harvesting, electrical transport and photovoltaic conversion parameters of oxynitride perovskites is not well explored.

Novel transition-metal oxynitride perovskites, namely BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$, were synthesized by sol-gel method and systematically studied to assess their optoelectronic properties. To understand the effects of Cu/Co substitution on the optical bandgap, electrical transport behaviour and extraction of the photogenerated charge-carriers, a comprehensive characterization was performed by combining

optical spectroscopy, Hall effect measurements and current density–voltage (J-V) analysis of fabricated solar cells. The results offer insights into the structure–property relationships of these oxynitride perovskites and suggest their potential for photovoltaic applications.

EXPERIMENTAL

Synthesis: The nanoparticles of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ oxynitride perovskite were synthesized by using a urea assisted sol-gel method. The metal nitrate precursors were dissolved in 100 mL of deionized water with continuous magnetic stirring. BaCuO_2N and BaCoO_2N were prepared by using 0.3 M of $\text{Ba}(\text{NO}_3)_2$, and 0.3 M $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$, and 0.3 M $\text{Ba}(\text{NO}_3)_2$ and 0.3 M $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, respectively. For $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$, $\text{Ba}(\text{NO}_3)_2$, $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ and $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ were used at 0.3, 0.15 and 0.15 M, respectively. Citric acid was added with a citric acid/metal ratio of 1:1 and urea was added with a ratio of 10:1.

The precursor mixtures were stirred at 50 °C until homogeneous and subsequently heated to 110 °C to induce gel formation and self-combustion, producing porous precursor powders. The powders were finely ground in an agate mortar and pestle and transferred to covered alumina crucibles. The thermal treatment was carried out in a laboratory muffle furnace without an external gas flow. The samples were heated at a rate of 5 °C min⁻¹ to 400 °C and maintained at this temperature for 2 h, followed by heating at the same rate to 700 °C and holding for 3 h. Excess urea was employed as the combustion fuel and was also intended to provide an *in situ* N₂ source during the thermal treatment. After completion of the 700 °C treatment, the furnace was switched off and the covered crucibles were allowed to cool naturally to room temperature.

For each composition, 50 mg of the oxynitride nanoparticles was dispersed in 10 mL of DMSO and ultrasonicated for 60 min before the commercial 2 cm × 2 cm n-type silicon substrates were sequentially cleaned with deionized water, ethanol, acetone and dried. The suspensions were sonicated for a short time prior to deposition to re-suspend settled particles. An amount of about 150 µL of each suspension was dropped on the center of the substrate and spin-coated for 60 s at 2000 rpm. 5 cycles of coating/drying were performed at 100 °C for 10 min. The films were then left at 100 °C for 30

min and allowed to cool down to room temperature without any further treatment at high temperature.

Fabrication and photovoltaic evaluation of oxynitride/n-Si heterojunctions: The positive Hall coefficients indicated p-type semiconducting behaviour of the synthesized oxynitride nanoparticles which has been exploited to form oxynitride/n-Si heterojunctions using the synthesized oxynitride films deposited on the n-type Si substrates. After deposition of the oxynitride films on the silicon substrates, Al electrodes were deposited onto the surface of the oxynitride films using a dedicated mask for solar-cell fabrication. Copper wires were then connected to the electrodes using a thin layer of conductive silver adhesive to establish electrical contact. The photovoltaic characteristics of the fabricated oxynitride-based devices were evaluated from current density–voltage (J-V) measurements using a Keithley 2400 source-measure unit. A tungsten halogen lamp was used as the light source and the incident light intensity was set to 100 mW cm⁻². The voltage was swept from 0 to 1 V. The J-V characteristics were used to determine the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), maximum current density (J_{max}), maximum voltage (V_{max}), fill factor (FF) and power conversion efficiency (PCE).

The fill factor was calculated using eqn. 1:

$$\text{Fill factor} = \frac{J_{\max} \times V_{\max}}{J_{sc} \times V_{oc}} \quad (1)$$

The power conversion efficiency was calculated using (eqn. 2):

$$\text{PCE (\%)} = \frac{J_{sc} \times V_{oc} \times \text{FF}}{P_{in}} \times 100 \quad (2)$$

where P_{in} is the incident optical power density.

RESULTS AND DISCUSSION

XRD studies: The XRD diffractograms of the synthesized BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ nanoparticles oxynitride are shown in Fig. 1. It can be observed that BaCuO_2N exhibited several diffraction reflections with the maximum diffraction peak at $2\theta = 23.47844^\circ$ ($d = 3.78602$ Å). BaCoO_2N also exhibited several diffraction reflections with the maximum diffraction peak at $2\theta = 23.93842^\circ$ ($d = 3.71430$ Å). On the other hand, $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ exhibited several

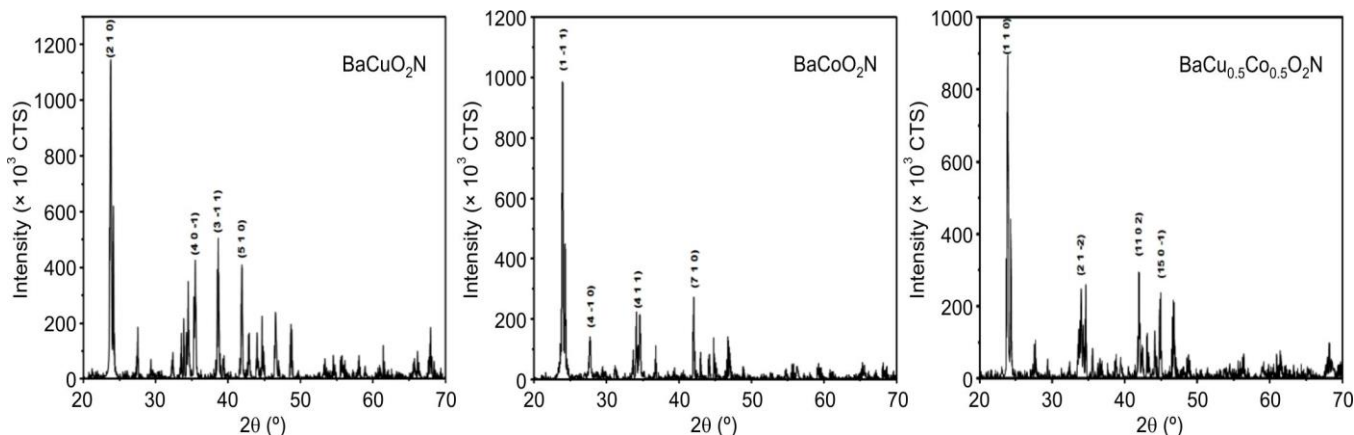


Fig. 1. X-ray diffraction patterns of the synthesized BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ oxynitride perovskites

diffraction reflections with the maximum diffraction peak at $2\theta = 23.89408^\circ$ ($d = 3.72110 \text{ \AA}$). The diffraction patterns obtained for all samples exhibited well-defined reflections, indicating the crystalline nature of the synthesized materials.

The indexing results indicated a triclinic crystal system with $P1$ space group for BaCuO_2N and BaCoO_2N , whereas $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ was indexed to a monoclinic crystal system with $P2/m$ space group. The three compositions produced de Wolff M20 values of 11-15, which are consistent with the reliability of the corresponding indexing solutions. The indexed diffraction reflections, together with their corresponding 2θ and d -spacing values, are listed in Table-1.

TABLE-1
SELECTED INDEXED DIFFRACTION REFLECTIONS
OF THE SYNTHESIZED BARIUM-BASED
NANO-PEROVSKITE OXYNITRIDES

Compound	2θ ($^\circ$)	d ($\text{\AA}$)	$h k l$
BaCuO_2N	23.47844	3.78602	(2 1 0)
BaCuO_2N	38.62171	2.32933	(3 $\bar{1}$ 1)
BaCuO_2N	41.72803	2.16283	(5 1 0)
BaCoO_2N	23.93842	3.71430	(1 $\bar{1}$ 1)
BaCoO_2N	27.75222	3.21193	($\bar{4}$ 1 0)
BaCoO_2N	34.10702	2.62662	(4 1 1)
BaCoO_2N	41.95372	2.15172	(7 1 0)
$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$	23.89408	3.72110	(1 1 0)
$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$	33.99224	2.63523	(2 1 $\bar{2}$)
$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$	41.72836	2.16281	(11 0 2)
$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$	44.93538	2.01562	(15 0 $\bar{1}$)

The indexing results were used to calculate the unit-cell dimensions and the corresponding crystal systems and space groups were identified. Since there were no diffraction patterns for the investigated compositions of the series of Ba-based transition-metal oxynitrides corresponding to the ones under study, the structural assignments were based on the experimental diffraction patterns and on the indexing results. Thus, the XRD data provide structural information based on the indexing results.

The obtained lattice parameters and unit-cell volumes are summarized in Table-2. The lattice angles for BaCuO_2N and BaCoO_2N are not exactly 90° , which is in correspondence with the triclinic symmetry of the indexing procedure. However, the monoclinic structure obtained from the indexing procedure is consistent with $\alpha = \gamma = 90^\circ$ and $\beta = 94.33^\circ$ for

$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$. The observed differences in the lattice parameters and unit-cell volumes reflect structural variations among the investigated compositions. The calculated crystallographic densities of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ were 3.57 g cm^{-3} , 3.15 g cm^{-3} and 3.03 g cm^{-3} , respectively. The variation in density is associated with the differences in crystal symmetry and unit-cell parameters among the synthesized compounds.

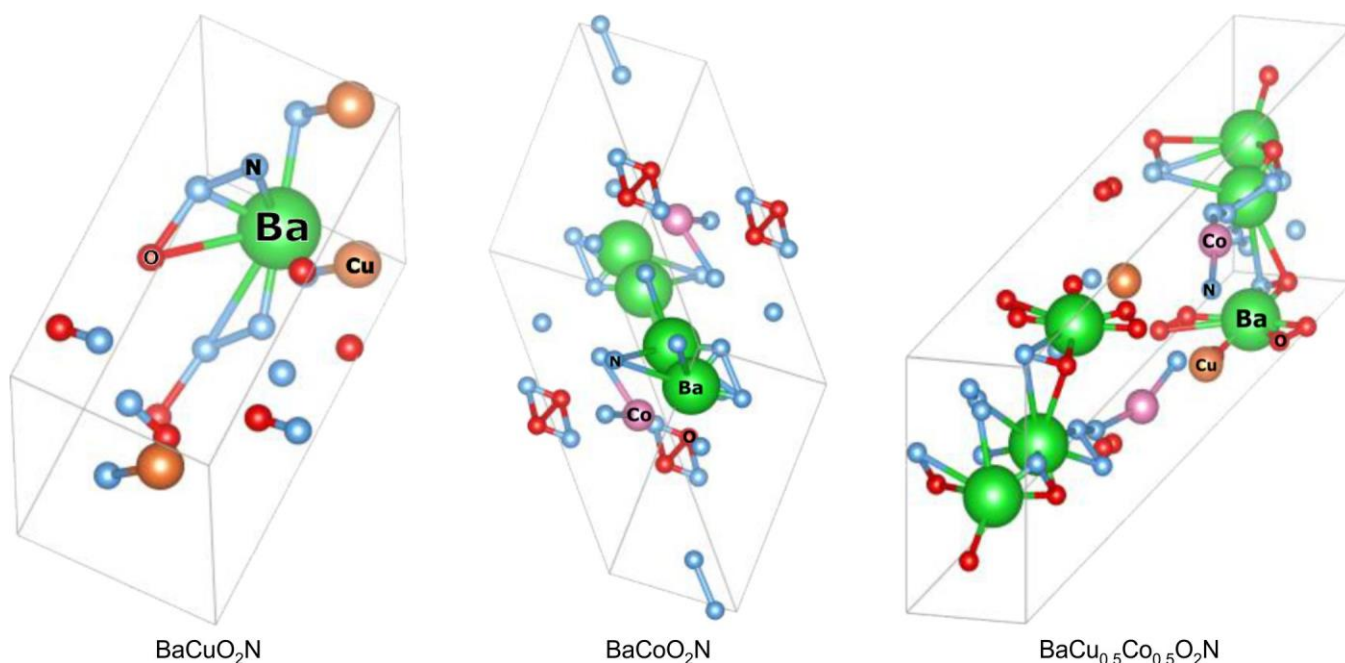
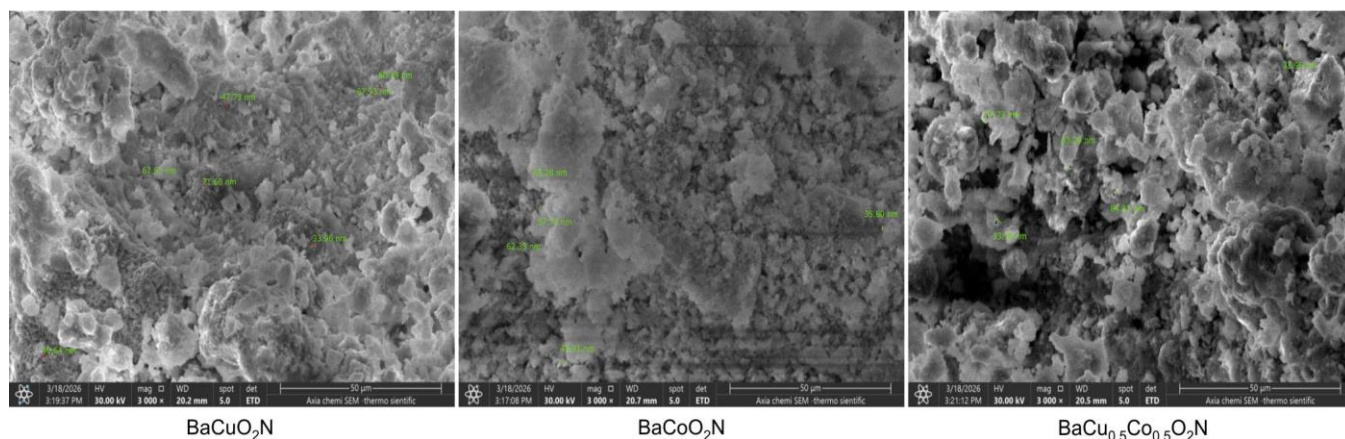
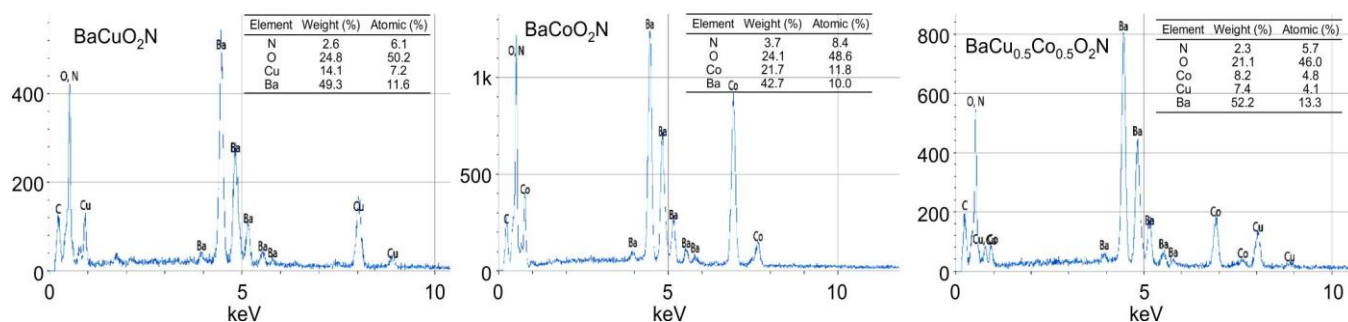
The crystallographic models obtained by indexing are shown in Fig. 2. The arrangement of the atoms (Ba, Cu, Co, O and N) inside the corresponding unit cells is displayed in the models using the crystallographic parameters derived in the indexing analysis. The differences in the structural representations between the single-metal and mixed compositions correspond to differences in the indexed lattice parameters and unit-cell volumes. The atomic arrangement within the crystal lattice plays an important role in determining the physical, electronic and optical properties of perovskite oxynitride materials [11,12].

FESEM studies: The FESEM images (Fig. 3) of the synthesized nanoparticles of barium oxynitride BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ show different surface topologies with highly agglomerated nanoparticles which are found to have irregular geometric shapes [13]. The agglomeration observed might relate to the high surface energy of nanoscale particles and particle coalescence during the high temperature calcination procedure. The microstructural estimation from the direct grain size measurements is in good agreement with the fact that the measured grain sizes ranged from approximately 35 to 67 nm [14]. In addition, there are some intergranular pores and micro-voids were also observed within the aggregated clusters.

EDS studies: Energy-dispersive X-ray spectroscopy (EDS) was employed to identify the constituent elements and evaluate their elemental distribution in the synthesized oxynitride samples. In the EDS spectrum for BaCuO_2N (Fig. 4a), the presence of Ba, Cu, O and N, with atomic concentrations of 11.6%, 7.2%, 50.2% and 6.1%, respectively. The detection of nitrogen provides elemental evidence for the presence of N in the synthesized material; however, the EDS results alone cannot be used to establish the exact O/N stoichiometric ratio or phase purity. For BaCoO_2N , the EDS spectrum (Fig. 4b) revealed Ba, Co, O and N as the major detected elements, with atomic concentrations of 10.0%, 11.8%, 48.6% and 8.4%, respectively. The simultaneous detection of Ba and Co is con-

TABLE-2
INDEXED LATTICE PARAMETERS AND CALCULATED UNIT-CELL CHARACTERISTICS OF
 BaCuO_2N , BaCoO_2N AND $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ NANO-PEROVSKITE OXYNITRIDES

Parameters		BaCuO_2N	BaCoO_2N	$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$
Space group		$P1$	$P1$	$P2/m$
Cell parameters	α	104.71	95.66	90.00
	β	100.74	96.98	94.33
	γ	82.59	80.07	90.00
	a ($\text{\AA}$)	11.98	15.27	30.82
	b ($\text{\AA}$)	4.78	8.39	3.75
	c ($\text{\AA}$)	4.03	4.43	7.52
Cell volume ($\text{\AA}^3$)		218.56	554.53	865.86
Density (g cm^{-3})		3.57	3.15	3.03

Fig. 2. Structural models derived from the indexed crystallographic parameters of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ Fig. 3. FESEM micrographs of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ nano-perovskite oxynitridesFig. 4. EDX spectra of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ nano-perovskite oxynitrides

sistent with the intended elemental constituents of the BaCoO_2N composition. The detected nitrogen signal supports the presence of nitrogen in the material, although EDS alone does not provide definitive confirmation of the exact oxynitride stoichiometry or nitridation efficiency.

For $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$, the EDS spectrum (Fig. 4c) simultaneously detected Ba, Cu, Co, O and N, with atomic concen-

trations of 13.3%, 4.1%, 4.8%, 46.0% and 5.7%, respectively. The simultaneous detection of Cu and Co is consistent with the intended incorporation of both transition-metal cations in the mixed composition. However, the measured elemental ratios show deviations from the nominal stoichiometric composition, which may arise from the limitations of EDS quantification, particularly for light elements such as nitrogen.

Therefore, the EDS results are interpreted as qualitative-to-semi-quantitative evidence of elemental composition rather than definitive proof of exact stoichiometry or phase purity [15].

AFM studies: The two-dimensional (2D) and three-dimensional (3D) deflection maps (Fig. 5) display of the surface over the scanning area of ($2.5 \times 2.5 \mu\text{m}^2$) show clear morphological differences with the introduction of the transition

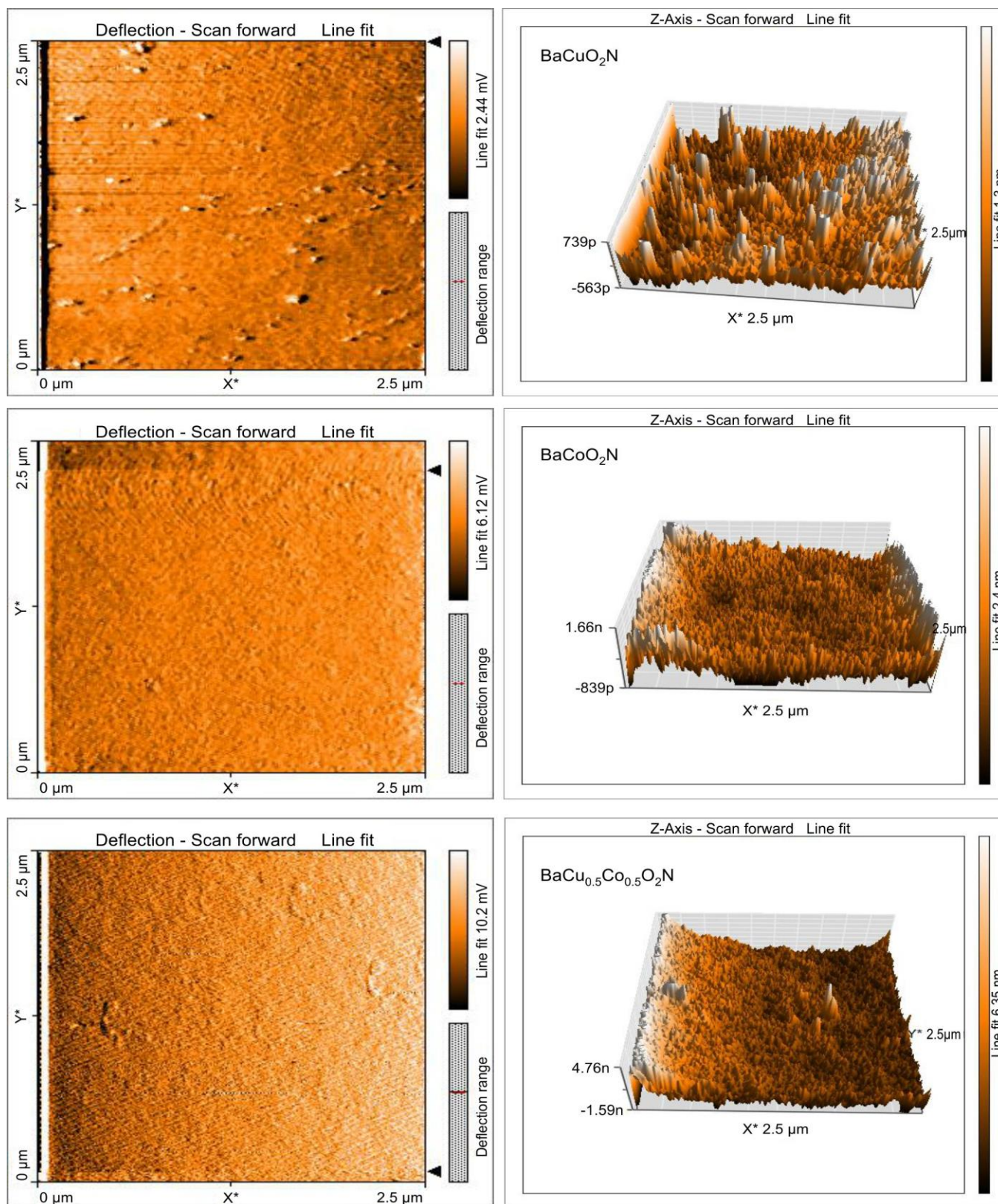


Fig. 5. AFM images of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ nano-perovskite oxynitrides

elements [16]. The topographic 3D profile of the pure BaCuO_2N sample shows an irregular topography with sharp peaks and a set of isolated, very small nanostructures with interesting high vertical structures. The BaCuO_2N sample exhibits an irregular surface topography with pronounced height variations and sharp surface features.

BaCoO_2N showed a relatively more uniform and densely packed granular morphology. In contrast, $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ exhibited more pronounced nanoscale surface features and larger height variations. These observations are consistent with the roughness parameters (Table-3), where the mixed Cu–Co composition exhibited the highest R_a , R_q and R_t values. However, the AFM results alone do not establish the mechanisms responsible for grain growth, lattice strain or charge-carrier transport.

TABLE-3 AFM DATA OF BaCuO_2N , BaCoO_2N AND $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ NANO-PEROVSKITE OXYNITRIDES			
Perovskites oxynitride	R_a (nm)	R_q (nm)	R_t (nm)
BaCuO_2N	0.269	0.652	6.12
BaCoO_2N	0.452	0.797	8.787
$\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$	1.451	4.763	59.292

UV-Vis studies: The electronic UV-Vis absorption spectra of the BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ oxynitride perovskites prepared by the sol-gel method are shown in Fig. 6. The absorption coefficient (α) was determined from the

measured absorbance using $\alpha = 2.303A/t$, where t is the sample thickness and A is the absorbance. The optical band gaps were estimated by extrapolating the linear portion of the plots of $(\alpha h\nu)^2$ versus $h\nu$ to $(\alpha h\nu)^2 = 0$ using the Tauc relation for direct allowed transitions, $(\alpha h\nu)^2 = B(h\nu - E_g)$. The direct allowed transition was adopted for the Tauc analysis as the absorption-edge region showed good linearity in the plots of $(\alpha h\nu)^2$ versus $h\nu$ (Fig. 7).

The estimated optical band gaps were 2.77 eV, 2.04 eV and 1.63 eV for BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$, respectively. The progressive decrease in the optical band gap from BaCuO_2N to BaCoO_2N and then to the mixed Cu–Co composition, which indicates a shift of the optical absorption edge toward lower photon energies with B-site transition metal substitution. $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ exhibited a lower band gap and an optical response extending toward longer wavelengths, which may be related to changes in the electronic structure caused by Cu/Co co-incorporation.

Thermal studies: Thermal stability and decomposition of the BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ oxynitride perovskites synthesized by sol-gel were studied up to 550 °C by TGA and DTG as shown in Fig. 8. For all three oxynitride materials, the total mass loss up to 550 °C was less than 0.25 wt.%. The TG thermograms and their derivatives (DTG) exhibited three main mass-loss stages below 350 °C, followed by an approximately stable plateau. For BaCuO_2N , the mass losses in the ranges of 25–100, 100–200 and 200–350 °C were

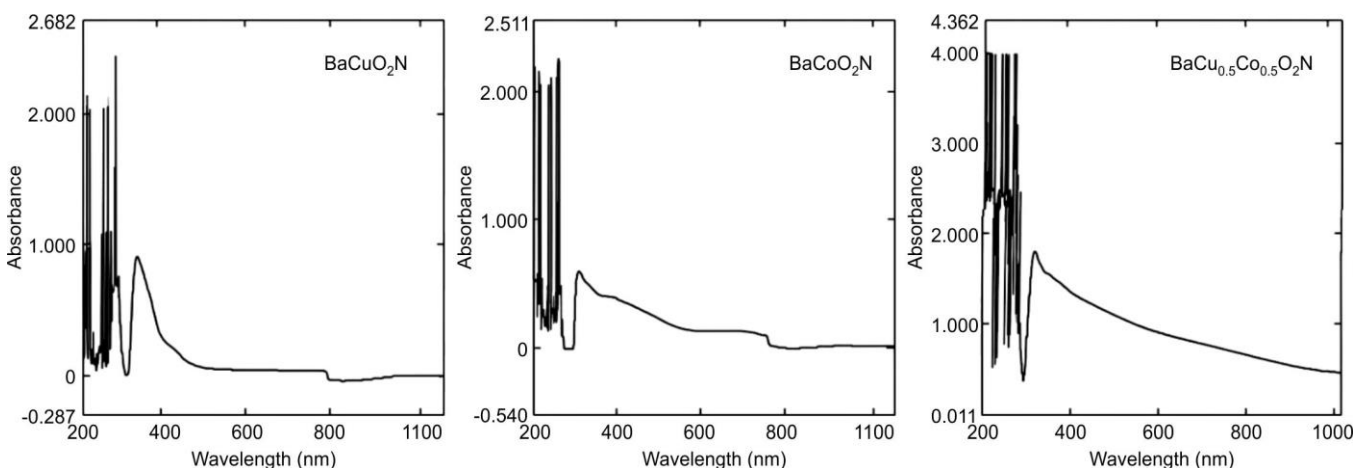


Fig. 6. Electronic spectra of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$ nano-perovskite oxynitrides

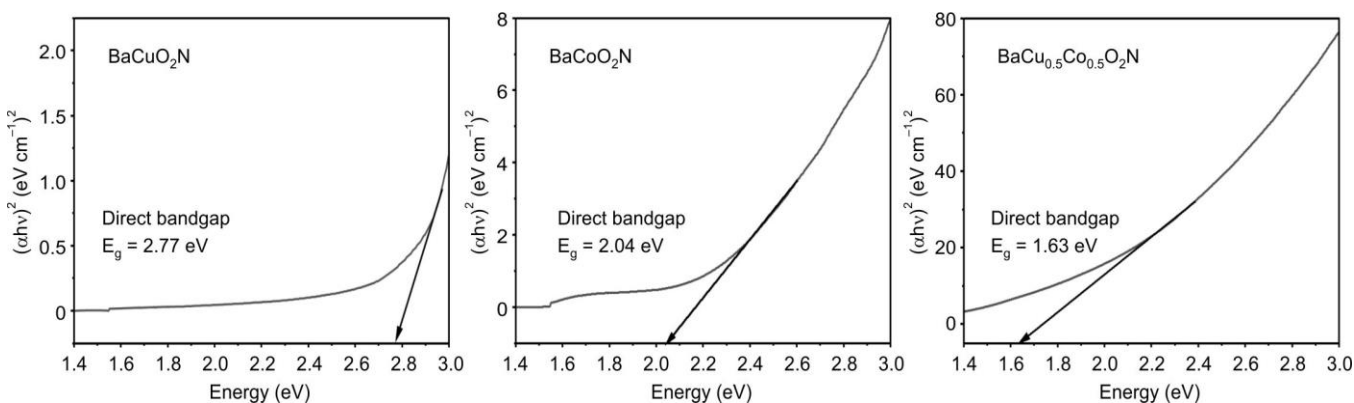


Fig. 7. Tauc plots of BaCuO_2N , BaCoO_2N and $\text{BaCu}_{0.5}\text{Co}_{0.5}\text{O}_2\text{N}$

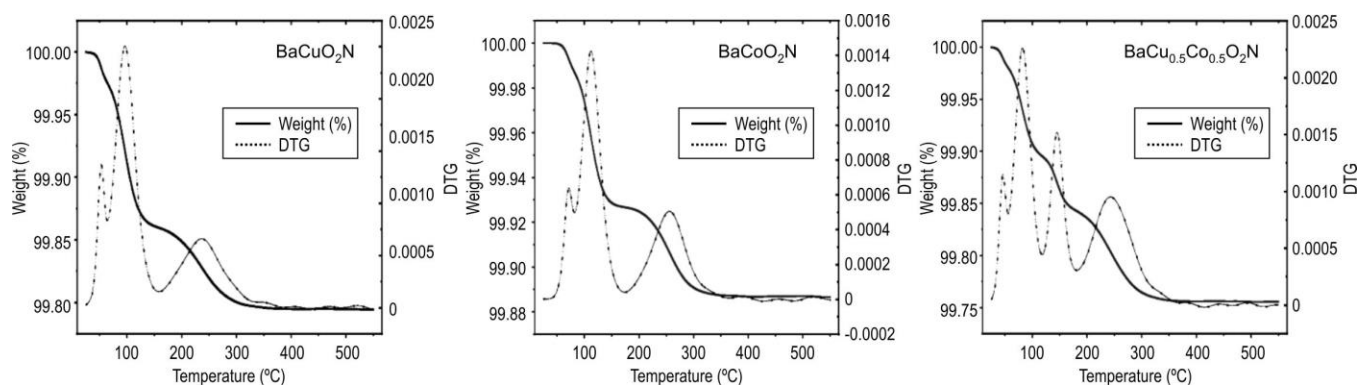


Fig. 8. TGA-DTG thermograms of BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N nano-perovskite oxynitrides

approximately 0.088, 0.063 and 0.053 wt.%, respectively, giving a total mass loss of about 0.205 wt.% up to 550 °C. For BaCoO₂N, the corresponding mass losses were approximately 0.026, 0.049 and 0.037 wt.%, respectively, with a total mass loss of about 0.113 wt.%.

For BaCu_{0.5}Co_{0.5}O₂N, the individual mass losses were approximately 0.092, 0.071, and 0.079 wt.%, exhibiting a total mass loss of about 0.244 wt.%. The initial mass decrease below 100 °C together with the DTG peak observed around 50-80 °C, which can be attributed to the removal of physically adsorbed moisture and other weakly bound surface species [17]. A subsequent thermal event occurred between 100 and 200 °C is accompanied by a distinct DTG peak. This region can be assigned to the removal of trapped solvent molecules and hydration water associated with the porous sol-gel network.

The mass loss observed between 200 and 350 °C is likely related to the decomposition of residual nitrate species and incompletely combusted organic components originating from the precursor system. Above 350 °C, the samples exhibited negligible additional mass changes up to 550 °C. The corresponding mass losses were approximately 0.002, 0.001, and 0.001 wt.% for BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N, respectively. The thermal profile therefore suggests that most of the precursor-derived volatile species were removed below 350 °C, with little further decomposition within the remaining temperature range examined.

The DTG profile of BaCu_{0.5}Co_{0.5}O₂N also exhibited partially resolved peaks between 100 and 250 °C. Such peak splitting may arise from overlapping thermal processes involving different residual species present in the mixed-metal precursor, although assignment of the individual events would require additional thermal or evolved-gas analysis.

Thermodynamic studies: The thermodynamic parameters of the non-isothermal reactions of the BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N were obtained from the TGA data and calculated by the Coats-Redfern method and are summarized

in Table-4. The bimetallic BaCu_{0.5}Co_{0.5}O₂N exhibited the lowest activation energy (112,582.9 J/mol), followed by BaCuO₂N (115,965.6 J/mol) and BaCoO₂N (117,699.6 J/mol) [18]. The corresponding enthalpy values were 113,486.7, 115,220.8 and 110,104.1 J/mol for BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N, respectively. All samples show positive activation entropy ($\Delta S = 63.4$ to 87.5 J/K mol). The positive ΔS values suggest an increase in entropy from the reactant state to the activated state [19].

Perovskites oxynitride	(ΔE_a) (J/mol)	(ΔH) (J/mol)	(ΔS) (J K ⁻¹ mol ⁻¹)	(ΔG) (J/mol)
BaCuO ₂ N	115965.6	113486.7	87.4518	87413.03
BaCoO ₂ N	117699.6	115220.8	63.39724	96318.90
BaCu _{0.5} Co _{0.5} O ₂ N	112582.9	110104.1	81.33369	85854.46

Photovoltaic studies: Table-5 summarizes the electrical transport parameters obtained from Hall effect measurements for BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N oxynitride perovskites synthesized via the sol-gel method. The electrical conductivity increased from 6.90 S cm⁻¹ for BaCuO₂N to 8.05 S cm⁻¹ for BaCoO₂N, while BaCu_{0.5}Co_{0.5}O₂N exhibited an intermediate conductivity of 7.33 S cm⁻¹. BaCoO₂N exhibited the highest electrical conductivity (8.05 S cm⁻¹) and carrier mobility (311 cm² V⁻¹ s⁻¹) among the investigated compositions. For BaCu_{0.5}Co_{0.5}O₂N, the conductivity (7.33 S cm⁻¹), carrier concentration (2.05×10^{17} cm⁻³), mobility (223 cm² V⁻¹ s⁻¹) and Hall coefficient (30.4 cm³ C⁻¹) were intermediate relative to the corresponding single-metal compositions. The positive Hall coefficient values observed across all synthesized samples indicate p-type semiconducting behaviour, with holes as the dominant charge carriers.

The photovoltaic characteristics of the synthesized oxynitride perovskite nanomaterials were evaluated by J-V mea-

Perovskites oxynitride	Conductivity (S cm ⁻¹)	Bulk concentration (cm ⁻³)	Mobility (cm ² V ⁻¹ s ⁻¹)	Hall coefficient (cm ³ C ⁻¹)
BaCuO ₂ N	6.90E+00	2.15E+17	2.01E+02	2.91E+01
BaCoO ₂ N	8.05E+00	1.62E+17	3.11E+02	3.86E+01
BaCu _{0.5} Co _{0.5} O ₂ N	7.33E+00	2.05E+17	2.23E+02	3.04E+01

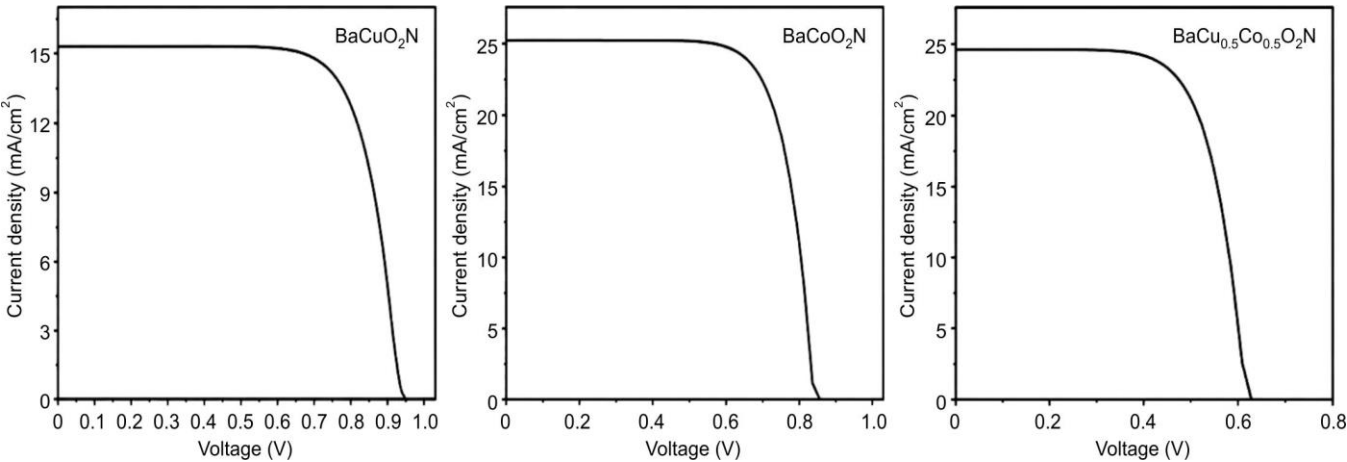


Fig. 9. J-V curves of BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N nano-perovskite oxynitrides

surements (Fig. 9). The measured J-V characteristics showed different photovoltaic parameters for BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N. The corresponding power conversion efficiencies were 10.60%, 15.77% and 10.86%, respectively, as summarized in Table-6.

TABLE-6 PHOTOVOLTAIC PARAMETERS OF BaCuO ₂ N, BaCoO ₂ N AND BaCu _{0.5} Co _{0.5} O ₂ N SOLAR CELLS			
Parameter	BaCuO ₂ N	BaCoO ₂ N	BaCu _{0.5} Co _{0.5} O ₂ N
J _{sc} (mA/cm ²)	15.30	25.15	24.45
V _{oc} (V)	0.93	0.85	0.63
J _{max} (mA/cm ²)	14.07	23.42	22.18
V _{max} (V)	0.75	0.67	0.49
FF	0.738	0.734	0.705
PCE/efficiency (%)	10.60	15.77	10.86

The observed variation in photovoltaic performance is associated with differences in the short-circuit current density (J_{sc}) and fill factor (FF). The photocurrent density (J_{sc}) varied considerably among the investigated materials, with values of 15.30, 25.15, and 24.45 mA cm⁻² for BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N, respectively. BaCoO₂N exhibited the highest J_{sc}, while BaCuO₂N showed the lowest value. The observed differences in photocurrent response can be associated with variations in light absorption and charge generation and collection within the respective materials. BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N exhibited higher J_{sc} values than BaCuO₂N, which indicate the differences in their photovoltaic response under the measurement conditions. These differences may be associated with variations in the optical absorption and charge-generation characteristics of the investigated materials. BaCuO₂N exhibited the highest open-circuit voltage (V_{oc} = 0.93 V), whereas BaCoO₂N showed the highest measured PCE (15.77%). The photovoltaic response varied among the investigated compositions under the applied measurement conditions.

Conclusion

In conclusion, novel Ba-based oxynitride perovskites, BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N, were successfully synthesized through a cost-effective sol-gel route. Structural

analysis established triclinic symmetry for the single-metal compositions and monoclinic symmetry for the Cu-Co mixed composition, while FESEM and AFM confirmed nanoscale grains with distinct surface features. The materials exhibited broad UV-visible absorption and p-type semiconducting behaviour. Thermal analysis revealed that the major mass loss processes occurred below ~350 °C, primarily due to residual moisture, solvents, nitrate species and organic residues. Among the investigated compositions, BaCoO₂N exhibited the highest electrical conductivity (8.05 S cm⁻¹) and carrier mobility (311 cm² V⁻¹ s⁻¹), with an activation energy of 117.7 kJ mol⁻¹. The optical band gaps were 2.77, 2.04, and 1.63 eV for BaCuO₂N, BaCoO₂N and BaCu_{0.5}Co_{0.5}O₂N, respectively. The corresponding p-oxynitride/n-Si heterojunctions achieved PCE values of 10.60%, 15.77%, and 10.86% under 100 mW cm⁻² illumination, with BaCoO₂N reaching the highest PCE (15.77%) and BaCuO₂N delivering the highest V_{oc} (0.93 V). These findings establish a clear relationship between the composition and the structural, optical, electrical and photovoltaic characteristics of the investigated oxynitrides and support their further investigation as materials for photovoltaic applications.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

DECLARATION OF AI-ASSISTED TECHNOLOGIES

During the preparation of this manuscript, the authors used an AI-assisted tool(s) to improve the language and no data, results or scientific conclusions were generated by AI. All analyses, interpretations and conclusions are the authors' own. The authors reviewed and edited the content and take full responsibility for the published work.

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