

Review

A Review of Synthesis, Characterization, Properties, and Applications of Double Perovskite Oxides

Pablo V. Tuza ^{1,*}  and Mariana M. V. M. Souza ² 
¹ Facultad de Ciencia e Ingeniería en Alimentos y Biotecnología, Universidad Técnica de Ambato, Ambato 180216, Ecuador

² Escola de Química, Universidade Federal do Rio de Janeiro (UFRJ), Rio de Janeiro 21941-909, RJ, Brazil; mmattos@eq.ufrj.br

* Correspondence: pablo.tuza.alvarado@gmail.com; Tel.: +593-2400987

Abstract

Double perovskites are represented by the formula $A_2BB'O_6$ and $AA'BB'O_6$. These materials have been synthesized using the solid-state reaction, sol–gel, Pechini, and hydrothermal methods. X-ray fluorescence, X-ray diffraction, magnetic measurements, transmission electron microscopy, X-ray photoelectron spectroscopy, temperature-programmed reduction, synchrotron X-ray diffraction, neutron powder diffraction, extended X-ray absorption fine structure, and Raman spectroscopy have been used for the characterization of double perovskites. X-ray diffraction, synchrotron X-ray diffraction, and neutron powder diffraction coupled with the Rietveld method determine the crystal structure of a sample. These materials present various properties and applications. The present review aims (i) to report a process to determine the symmetry, apparent size, and apparent strain using the Rietveld method; (ii) show how experimental characterization techniques complement each other in the investigation of double perovskites; (iii) describe how the synthesis method can help in the uncovering of double perovskites with improved properties; and (iv) exemplify some of the main applications of double perovskites.

Keywords: double perovskites; synthesis; X-ray diffraction; Rietveld method; characterization; applications



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1. Introduction

Perovskites are mixed oxides represented by the formula ABO_3 , where A is an alkali earth or rare earth metal, and B can be a transition metal [1]. The crystalline structure of this material can be represented using octahedra sharing corners. The oxygen atoms are positioned at the octahedra vertices, the octahedra centers are occupied by B cations, and the A cations are placed in the cavities between the octahedra, as depicted in Figure 1, which was drawn using the Vesta software (version 3.90.0a) [2].

Double perovskites (DPs) can be represented by the formula $A_2BB'O_6$ or $AA'BB'O_6$ [3], where the apostrophe symbol indicates a DP containing distinct metal ions with the same molar composition. There are three types of B-cation arrangement for DPs: random, rock salt, and layered [3], which are indicated in Figure 2. For the case of the random arrangement, the octahedra are randomly distributed in the structure. In the rock salt ordering case, the octahedra are ordered as the sodium and chloride ions in the NaCl structure. As indicated in its name, in the layered DP, BO_6 , and $B'O_6$ octahedra layers are intercalated between them. It is worth mentioning that ABO_3 perovskites with B cations with a molar ratio different from 0.5 mol can be represented using the DP random arrangement.

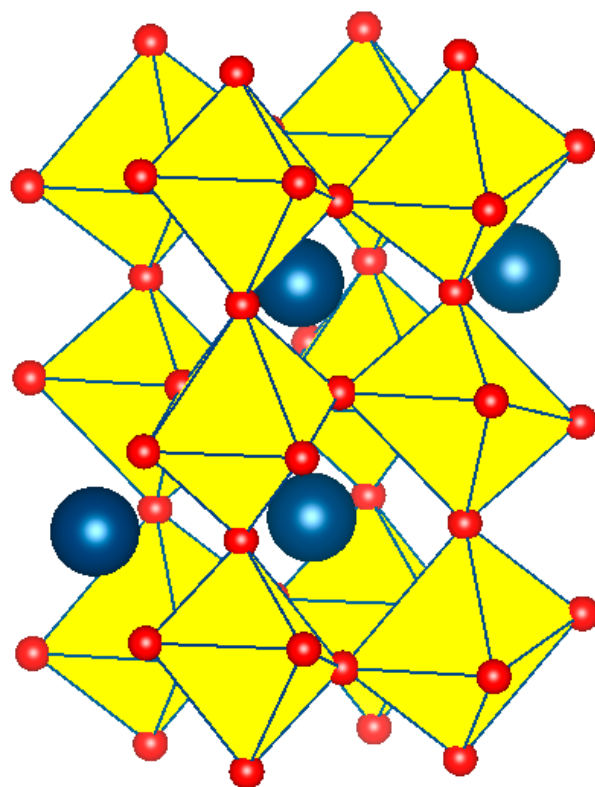


Figure 1. Perovskite crystal structure, where the A cation and oxygen ions are dark-blue and red spheres, and the B cation is in the octahedral center.

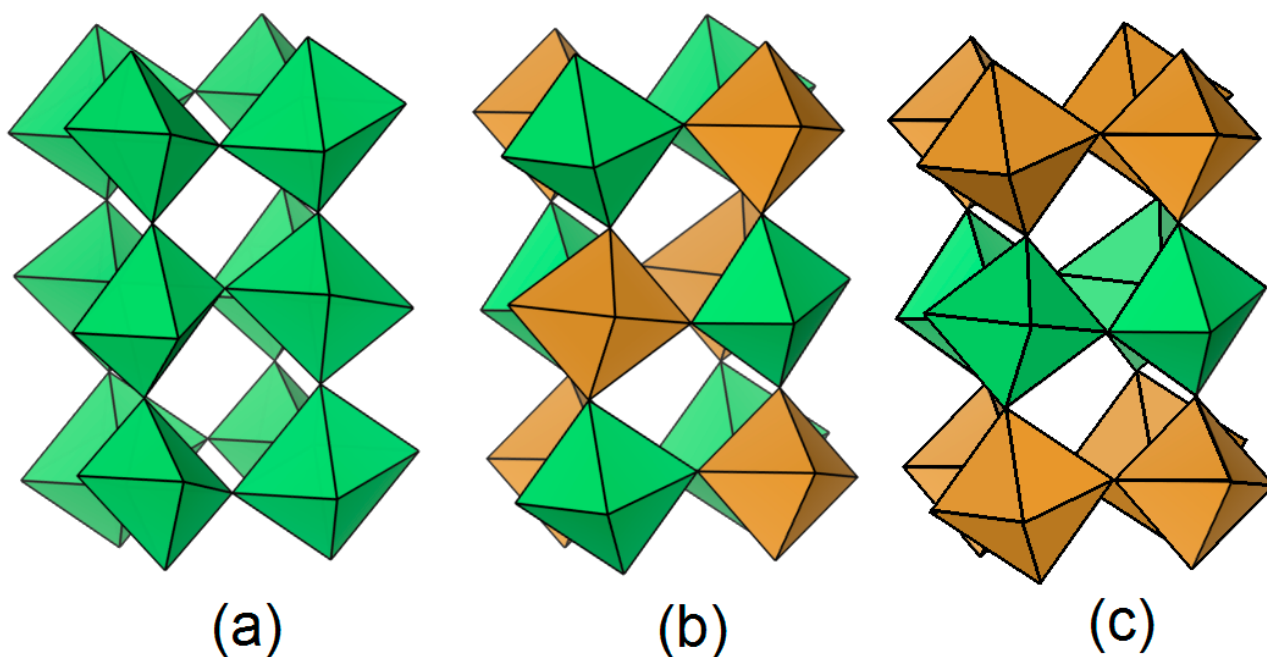


Figure 2. (a) Random, (b) rock salt, and (c) layered arrangements for DPs. For the random arrangement, both BO_6 and $\text{B}'\text{O}_6$ octahedra are depicted in green. In contrast, for the rock-salt and layered orderings, BO_6 octahedra are shown in green, while $\text{B}'\text{O}_6$ octahedra are depicted in light brown.

Surface exchange and diffusion of oxygen ions, conductivity enhancement [4], and improvement of catalytic properties are advantages of DPs over ABO_3 materials. For example, $\text{La}_2\text{NiTiO}_6$, which contains LaNiO_3 and LaTiO_3 , shows stable catalytic activity for the steam reforming of methane compared to the low-stable Ni or the inactive Ti perovskite,

as the DP presents enhanced metal–support interaction compared to the conventional perovskites [5].

B and B' cation arrangement in DPs mostly depends on B and B' valence differences [6], but it also may be influenced by B and B' ionic radius differences, as occurs for the $\text{Bi}_2\text{AlGaO}_6$ and $\text{Bi}_2\text{AlInO}_6$ [7]. Furthermore, the calcination time may influence the arrangement, as La-Ni-Ti-containing DPs with random ordering changed to a rock-salt arrangement by modifying the calcination step from 17 h at 800 °C to 135 h at 1000 °C [8].

2. Synthesis

DPs can contain B cations with mixed valences, and this allows for the design of several mixed oxides in accord with the octet rule and the preparation. Four preparation methods are mostly used to prepare these mixed oxides: the solid-state reaction, the sol–gel, the modified Pechini, and the hydrothermal methods.

2.1. Solid-State Reaction Method

The solid-state reaction is the most employed method to synthesize DPs. It consists of mixing adequate amounts of oxide [9] or carbonate [10] precursors of DPs. Then, the mixture is calcined at high temperatures, like 1400 °C [11], for diffusion and chemical reaction of the starting materials. It is worth noting that oxide diffusion is so low at 500 °C [12]. Similarly, higher pressures employed during the synthesis process ensure high diffusion rates [13], and this warrants the formation of the DP phase.

The ball-milling period of the precursors prior to their heating influences the morphology. Zouridi et al. [14] established that the mechanochemical step influences the particle size and produces a spherical nanometric single-phase $\text{La}_{0.5}\text{Sr}_{0.5}\text{Ti}_{0.5}\text{Mn}_{0.5}\text{O}_{3-\delta}$. Moreover, the perovskite phase can form during the ball-milling process, as observed for the $\text{La}_{1-x}\text{Sr}_x\text{Ti}_{1-y}\text{Mn}_y\text{O}_{3\pm\delta}$ [15]. Furthermore, the microstrain depends on the ball-milling time, as described for the SrTiO_3 [16].

An oxygenless atmosphere can influence the formation of DPs. Włodarczyk et al. [13] established that the Ar atmosphere inhibits cation oxidation during the preparation of the Ba_2CeWO_6 . Moreover, the final calcination step for the formation of the single-phase $\text{Sr}_2\text{FeMoO}_6$ was 1500 °C for 12 h in 2% H_2/Ar , followed by 1500 °C for 6 h [17], whereas it was 1074 °C for 4 h in 3% H_2/Ar [18]. It is worth noting that the last sample contained about 2 wt% impurities of Fe and SrMoO_4 .

The sintering temperature affects the coherent length [16], but this condition also affects other properties. Nadig et al. [19] indicated that the $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ calcined from 900 °C to 1200 °C presented the optimal oxygen content for the sample heated to 1100 °C, and this oxygen amount affects its cooling power.

2.2. Sol–Gel Method

The sol–gel method, also known as the citrate sol–gel method [20], is widely used for the preparation of DPs. In this method, nitrates [21], oxides, organometallic compounds [22], and metals [23] of DPs are used as starting materials. As can be found in work by Valdés et al. [24], all precursors are mixed, including the citric acid, in pH-adjusted water using NH_4OH at 80 °C. The resulting mixture was transformed into a gel at 90 °C for 24 h after evaporation at 80 °C. Finally, this last solid was calcined and then reduced.

The sol–gel method can be used to obtain DPs at temperatures lower than those employed in the solid-state reaction method. To illustrate this, Valdés et al. [24] used the sol–gel method for the synthesis of $\text{Sr}_2\text{FeMoO}_6$ and employed a reducing atmosphere. The maximum temperature used in this work was 1200 °C, and this is less than that used in the solid-state synthesis for the same material (1500 °C, [17]).

Although the sol–gel method followed by ball milling has not been reported in the literature for DPs, this additional step may improve the mixed oxide properties. For instance, Bartoletti et al. [25] reported that the sol–gel synthesis of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$, before a ball-milling process, increased its number of defects compared to the same material without the mechanochemical step, and this additional step in the synthesis method improved the $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ catalytic activity.

Some technological differences in the sol–gel method that influence the DP properties have been reported in the literature. For instance, Xu et al. [26] reported the effect of polyvinyl alcohol (PVA) on the synthesis of $\text{La}_2\text{CoMnO}_6$. The final calcination temperature was lower compared to that reported without PVA (700 °C, Xu et al. [26] vs. 900 °C, Yousif et al. [27]). Martinez-Rodriguez et al. [28] prepared the $\text{Pr}_{1-x}\text{Ba}_x\text{MnO}_{3-\delta}$ using EDTA and ethylene glycol (EG) in the preparation method. These authors reported that the sol–gel EDTA synthesis produced a sample with the highest proportion of cubic phase compared to the sol–gel EG preparation for $x = 0.5$, as the first method produces a better thermally stable sample.

Environmentally friendly fuels, such as lactose, fructose, maltose, sugar, and an organic compound-based powder called liquorice, as well as other types of fuels like oxalic acid, maleic acid, green coffee powder, and pomegranate paste, were employed for the preparation of $\text{Tb}_2\text{ZnMnO}_6$ [29] and $\text{Tb}_2\text{FeMnO}_6$ [30], respectively. These authors claimed homogeneous and smaller particle sizes for the case of maltose fuel used to synthesize the Zn-containing DP, while the best results in size and morphology corresponded to the maleic acid addition to obtain the Fe-containing DP. Additionally, the grape juice used as fuel can modulate the particle size, as reported for the Y_2CrMnO_6 [31].

2.3. Pechini Method

The Pechini method, also known as Pechini sol–gel [32], is characterized by producing a metal-containing polymer. This method is usually carried out in four stages: (i) metal solution preparation, (ii) chelate production through attachment of solution-containing cations and an organic acid like citric acid, (iii) resin production through chelate polymerization, by employing an alcohol such as the EG, and (iv) synthesis of DPs after multiple thermal treatments.

In the first step, precursor solubilization is required. Some low-cost precursors, such as titanium species produced through titanium isopropoxide evaporation, are not water-soluble. Nitric acid can be employed to help solubilize this titanium precursor, like 3.4 mol/L nitric acid [33].

Moreover, the addition of ammonia hydroxide can be carried out in the first step or to adjust the pH after the third step [34]. The addition of ammonia promotes the production of a foam-like structure. For example, Córdova-Calderón et al. [8] reported the formation of this structure after calcining the resin at 450 °C during $\text{La}_2\text{NiTiO}_6$ preparation, and this was not claimed by Pérez-Flores et al. [35] in the same sample produced from the calcination of an NH_4OH -free resin.

Some technical differences in the method include ball-milling of the powder from resin calcination [36] or the use of ethylenediaminetetraacetic acid with citric acid as complexing agents [37]. Related to the CoFe_2O_4 preparation, Cheraghi et al. [38] used lemon juice, whereas Al-Wasidi and Abdelrahman [32] employed tartaric acid as a source of complexing agents. This last acid may provide small crystallite sizes, as in the synthesis of MgAl_2O_4 [39].

Moreover, the EG may be replaced by another alcohol. For instance, dos Santos et al. [40] employed glycerol instead of EG in the synthesis of SiO_2 . These authors claimed a higher surface area for the higher weight alcohol, as a result of the polymeric matrix

influence in the product. Cheraghi et al. [38] reported a mixture of sucrose and EG, while Al-Wasidi and Abdelrahman [32] used 1,2-propanediol.

The resin calcination can be performed using a heating rate of 2 °C/min, which may help maintain low gas production from this polyester decomposition. Bataliotti et al. [41] described that the polymer containing Te ions presented three steps of degradation, and these processes accounted for about 90% weight loss and gas production.

2.4. Hydrothermal Method

The hydrothermal method is carried out by employing nitrates and ammonium salts [42], chlorides [43], and organometallic compounds [44] of double-perovskite-containing metals. To begin with, a solution is obtained from the precursors, and then it is placed in a Teflon-lined stainless-steel autoclave for thermal treatment. Finally, the products are washed and dried.

The hydrothermal method has influenced the structure of DPs. Yi et al. [45] claimed that the dielectric behavior of $\text{La}_2\text{FeCrO}_6$ is related to its oxygen vacancies. Irfan et al. [46] reported that the $\text{Ce}_2\text{NiCrO}_6$, $\text{Pr}_2\text{NiCrO}_6$, and $\text{Nd}_2\text{NiCrO}_6$ presented agglomerated particles related to the synthesis method. Valdés et al. [24] reported lower particle sizes of $\text{Sr}_2\text{FeMoO}_6$ compared to those from the microwave sol-gel method by providing uniform heating in the particle production. Zhang et al. [47] reported that the hydrothermal method promotes the stabilization of the NiO_6 and MnO_6 structures, which are influenced by the size of R^{3+} ions in the R_2NiMnO_6 .

The materials containing DPs prepared using the hydrothermal method have shown better catalytic properties than the conventional catalysts. McGuire et al. [48] used Y_2CoMnO_6 and Y_2NiMnO_6 as supports for the Pt catalyst in performing methanol oxidation. Pt/ Y_2CoMnO_6 provided a better performance compared to the commercial Pt/C and the Pt/ Y_2NiMnO_6 , as it has a stronger metal-to-support interaction. These authors also stated that the Y_2CoMnO_6 was more active and stable than the Y_2NiMnO_6 and the commercial IrO_2 for oxygen evolution reaction (OER). Additionally, Y_2CoMnO_6 is a bifunctional catalyst, as it is also active for the oxygen reduction reaction.

The hydrothermal method has been used to prepare DP-containing composites. Sharma et al. [49] observed that the reduced graphite oxide $\text{Sr}_2\text{TiMnO}_6$ ($\text{Sr}_2\text{TiMnO}_6\text{-rGO}$), prepared by mixing graphite oxide and the DP and then aging the blend using the hydrothermal method, presented activity for the Rhodamine B dye due to its absorbance range and bandgap value. The $\text{Sr}_2\text{TiMnO}_6$ was prepared following the solid-state reaction method. Moreover, Khan et al. [50] indicated that the LSTN@NiMn-LDH , where LSTN and LDH are LaSrTiNiO_6 and lamellar double hydroxides, were prepared by the hydrothermal method and used as a catalyst for the OER and hydrogen evolution reaction (HER). The authors reported that OER occurs because of the interaction between oxygen species and the catalyst, whereas the HER activity is due to a synergistic effect between LSTN and NiMn-LDH .

3. Characterization

3.1. X-Ray Fluorescence

The chemical composition of DPs can be determined through X-ray fluorescence (XRF) using a spectrometer. The results can be expressed on an oxide or a metal basis. Popov et al. [51] reported that the experimental chemical composition of the $\text{Ba}_2\text{CoNbO}_6$ on a metallic basis was 2(0.03):1(0.03):0.998(0.03) for Ba:Nb:Co; hence, the composition was within the interval formed by the mean value of the corresponding experimental chemical composition and the standard deviation. The chemical composition and the presence of impurities were established using the X-ray fluorescence method. A value of 5.4 for oxygen

mols in the $\text{Sr}_2\text{CoNbO}_{6-\delta}$ and impurities in the sample was determined using XRF and confirmed by magnetization measurements [52]. Jin et al. [53] indicated that the Al:Fe experimental molar ratio for the $\text{La}_2\text{FeAlO}_6$ prepared using glucose and citric acid was about 1, and these values were obtained using X-ray fluorescence. Also, the chemical composition quantified using X-ray fluorescence indicates mixed valences of Mn in the $\text{Sr}_2\text{MnNbO}_{6-\delta}$ [54].

3.2. X-Ray Diffraction (XRD)

XRD can be used to determine the crystal structure, the crystallite size, and the phase composition of DPs. XRD is performed in a diffractometer, and its operating parameters are the 2θ range, step size, and count time. The intensity of the main reflection of the XRD pattern should be at least 10,000 a.u., as reported for the XRD of NdCaFeSnO_6 [55].

This characterization technique is largely employed to determine the crystal structure. Fabrelli et al. [56] reported that the $\text{La}_{2-x}\text{Ba}_x\text{CoMnO}_6$ presented an evolution from orthorhombic ($Pnma$) to rhombohedral ($R\bar{3}c$), and then to hexagonal ($P6_3/mmc$) as Ba content increases (Figure 3). Zaraq et al. [57] established that the $\text{Sr}_2\text{Co}_{0.75}\text{Fe}_{0.25}\text{TeO}_6$, $\text{Sr}_2\text{Co}_{0.5}\text{Fe}_{0.5}\text{TeO}_6$, and $\text{Sr}_2\text{Co}_{0.25}\text{Fe}_{0.75}\text{TeO}_6$ present monoclinic symmetry and space group $I2/m$ at room temperature. The symmetry was maintained, but the space group changed to $P2_1/n$ at temperatures below 100 K, whereas the symmetry and the space group changed to tetragonal ($I4/m$) and then to cubic ($Fm\bar{3}m$) at high temperatures up to 1100 K. Córdova-Calderón et al. [8] indicated two different symmetries for the La-Ni-Ti DP as a function of the calcination temperature (Figure 4), fostering the synthesis of DPs with desired crystal structures.

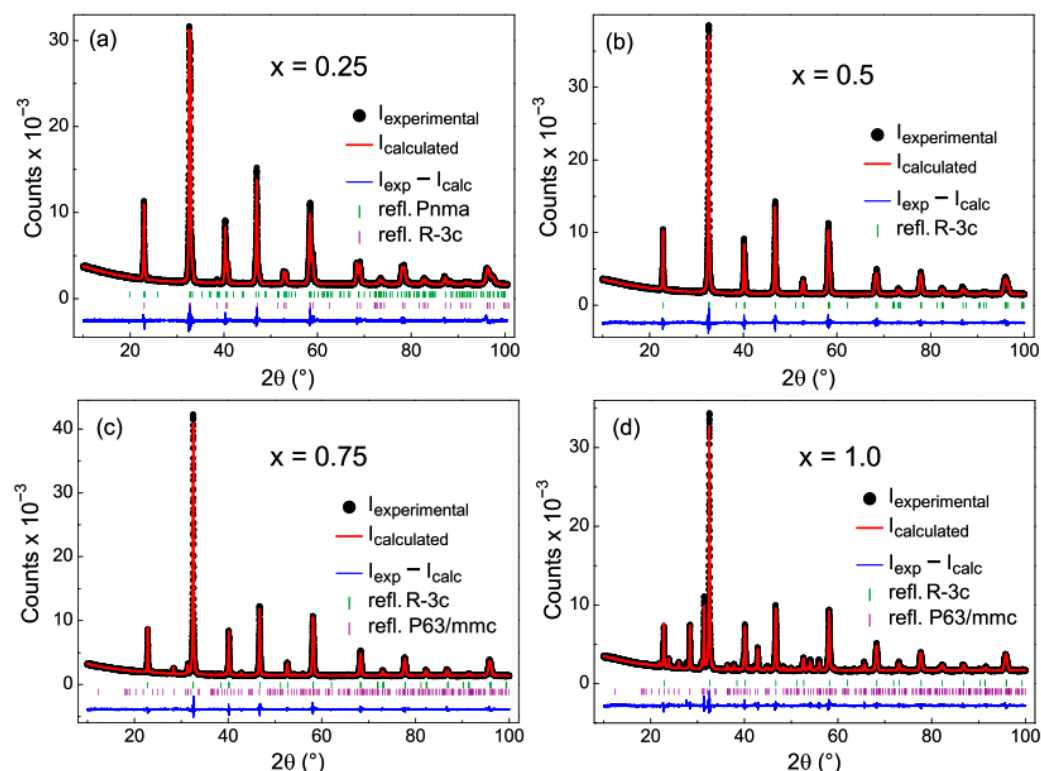


Figure 3. Observed, calculated, and difference XRD patterns of the $\text{La}_{2-x}\text{Ba}_x\text{CoMnO}_6$ for x of (a) 0.25, (b) 0.5, (c) 0.75, and (d) 1. Reprinted with permission from Ref. [56]. Copyright 2025, Elsevier.

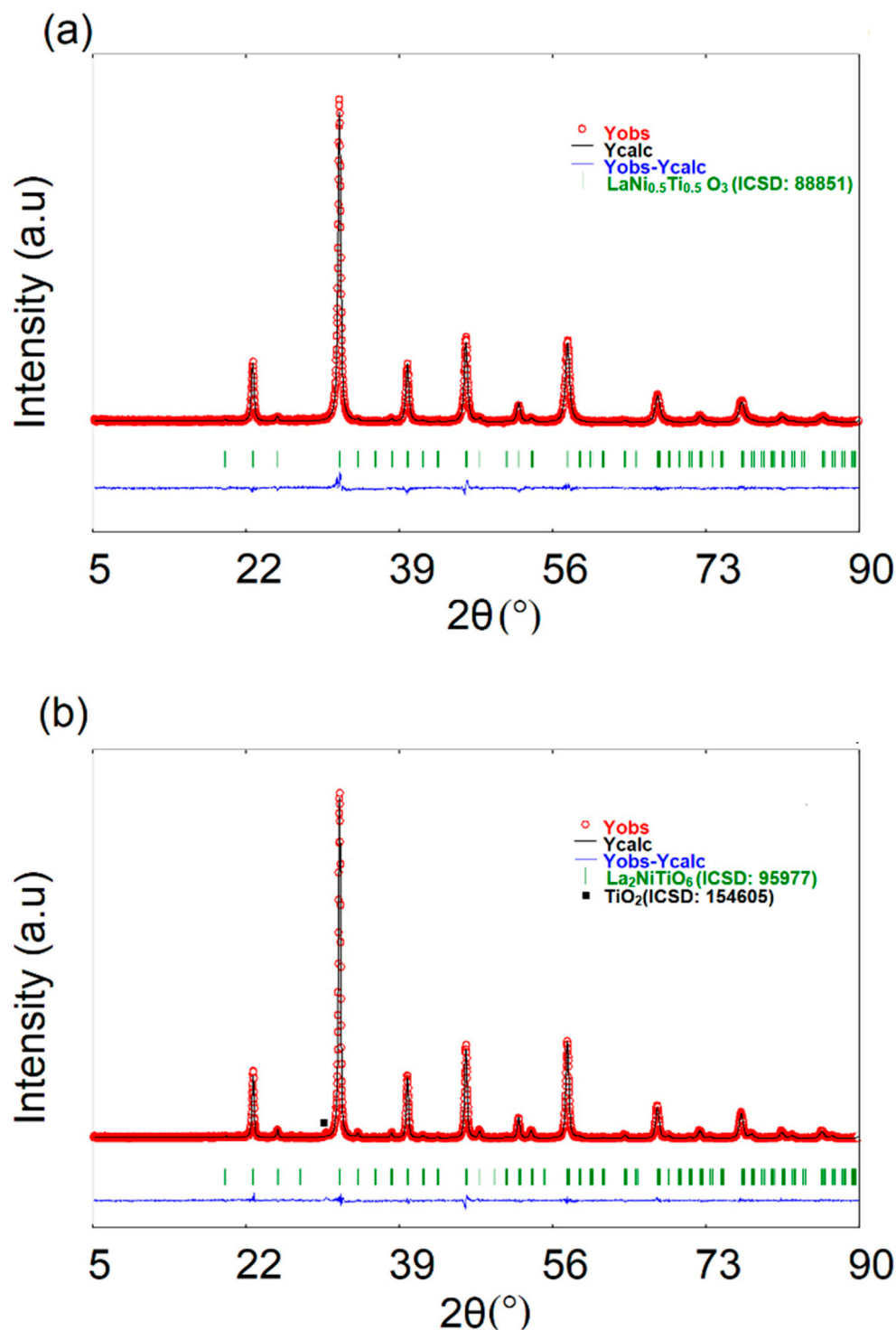


Figure 4. Observed, calculated, and difference XRD patterns of (a) $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ and (b) $\text{La}_2\text{NiTiO}_6$. Reprinted from Ref. [8].

3.2.1. Crystal Structure Determination

Crystal structures are determined using the Rietveld method, which is implemented in various programs, such as Fullprof [58]. This free and reliable package has been extensively used to refine crystal structures through cyclic steps where the convergence must be achieved.

Free databases like the Crystallographic Open Database share crystallographic information of materials through CIF files. The operator obtains a crystal structure template in a PCR file through the default crystal structure simulation option by opening the CIF file

with the PCR tool of Winplotr [59] and then saving it. The PCR file will be saved in the same CIF file folder. Steps 2 and 3 of Figure 5 depict this procedure, whereas the default and written parameters in a PCR file showing hypothetical values are presented in Table S1. It is important to note that the written parameters in Table S1 should be immediately placed after their prior default row. For instance, row 3 must be added to the PCR file after row 2. In addition, two rows of zeros in rows 8 and 12–17 of Table S1 represent values (top row) and codewords (bottom row) for each parameter, where the codeword enables the parameter refinement. Finally, for the case of the refinement of various parameters in each row, if not specified in the refinement process, the refinement proceeds from left to right.

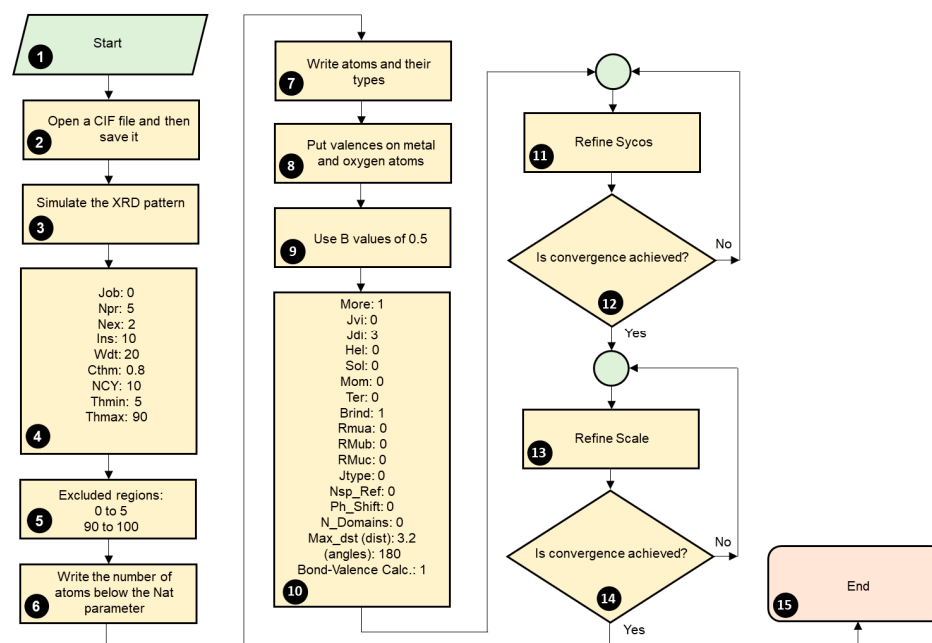


Figure 5. Initial procedure for refining the structure of a DP.

The Rietveld refinement process using the PCR file may be described as five steps: (i) parameter setting, (ii) background, (iii) unit cell parameters, (iv) peak shape parameters, and (v) atomic coordinates refinement.

In the parameter-setting step, an operator changes from simulation to refinement by altering the Job parameter value in row 1 of Table S1 from 2 to 0. Then, the peak shape function is selected and added below the Npr parameter from rows 1 and 9 of Table S1. There are seven different peak functions in Fullprof (version 3.0), and the pseudo-Voigt function is chosen and presented in Table S1. However, other authors prefer the Thompson–Cox–Hastings pseudo-Voigt convoluted with the axial divergence asymmetry function [60]. The suitable function provides better values for the criteria’s parameters to judge the quality of refinement.

Next, the researcher specifies the number of excluded 2 θ ranges by writing a value for the Nex parameter in row 1 of Table S1 through adding code, depicted in row 6 of Table S1. For instance, if the operator performs the instructions in step 5 of Figure 5, the order-ascending range-containing values, i.e., the lowest and the highest values, replace each row of zeros in row 6 of Table S1.

Moreover, the format of the experimental data, the cut-off of peak profile tails, the monochromator polarization correction, the maximum number of iterations per refinement, the minimum, and the maximum 2 θ values are specified through the Ins, Wdt, Cthm, NCY, Thmin, and Thmax parameters in rows 2, 4, and 5 of Table S1.

Furthermore, the operator should add the number of atoms, the atoms, and their valences describing the researched material, as depicted in steps 6 to 8 of Figure 5. The number of atoms (Nat) parameter comprises row 9 of Table S1, whereas the atoms, their types, and valences should be written one above another at row 12 of Table S1. Similarly, the researcher should write literature-based values to isotropic displacement parameters (Biso) for investigations where these values are not refined, as presented by our group [61], and indicated in step 9 of Figure 5. The Biso parameter is contained in row 12 of Table S1.

Additionally, the operator should write 1 for the More parameter located in row 9 of Table S1 and write the code to calculate bond distances and angles, as indicated in row 10 of Table S1. This procedure is shown in step 10 of Figure 5.

Also, the Sycos parameter that accounts for the largest systematic aberration in the Bragg–Brentano geometry [62] and Scale parameters located in rows 7 and 13 of Table S1 are refined, as presented in steps 11 to 14 of Figure 5. In step 11, the operator should select the experimental data saved in the DAT file previously placed in the PCR file folder. Silva et al. [63] refined the Zero parameter in row 7 of Table S1 instead of Sycos. It is worth noting that if the goniometer of the diffractometer is correctly aligned, the Zero parameter should not be refined.

In the background refinement step, four parameters describing the background located in row 8 of Table S1 are refined to ensure convergence is achieved in the program, as depicted in Figure 6.

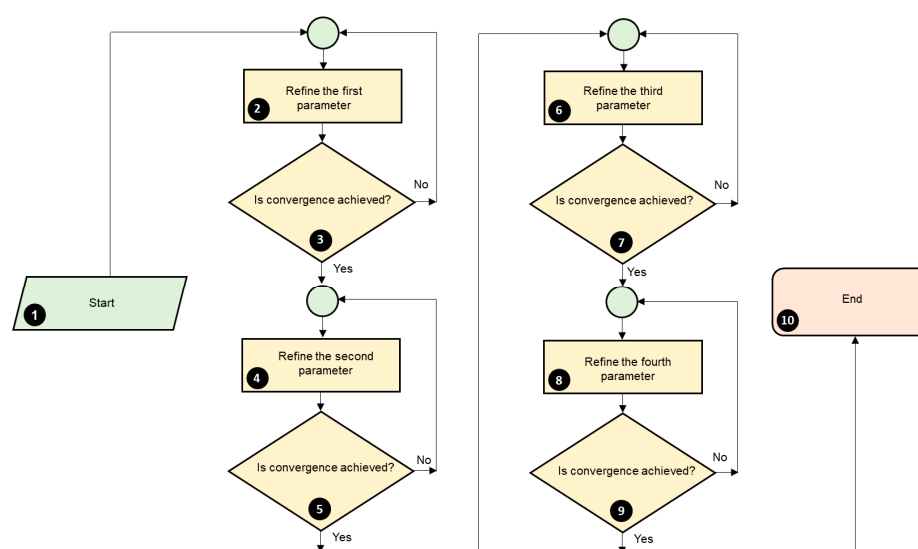


Figure 6. Background refinement through a trial-and-error method.

In the refinement of the unit cell parameters, the operator should refine the unit cell parameters in row 15 of Table S1, as presented in Figure 7, for an orthorhombic symmetry. If the symmetry enables an angle to be refined, like the β angle in the symmetry monoclinic, this angle should be refined after the c parameter (Figure 7), and followed by a convergence verification step, similar to step 7 in Figure 7.

In the refinement step of the peak shape parameters, the operator should refine U , V , W , and X parameters for the peak shape function that are depicted in row 14 of Table S1. It should be observed whether peak shape models enable the refinement of other parameters, like the so-called Shape1; these parameters should be refined right after the X parameter. The procedure of peak shape parameter refinement is presented in Figure 8.

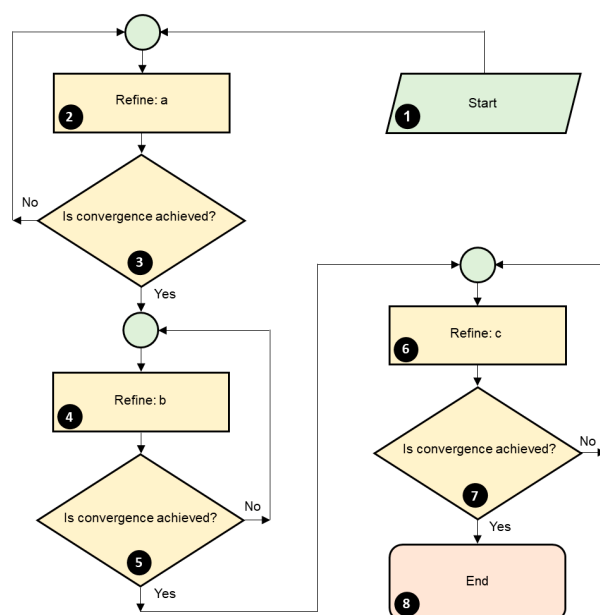


Figure 7. Refinement of unit cell parameters.

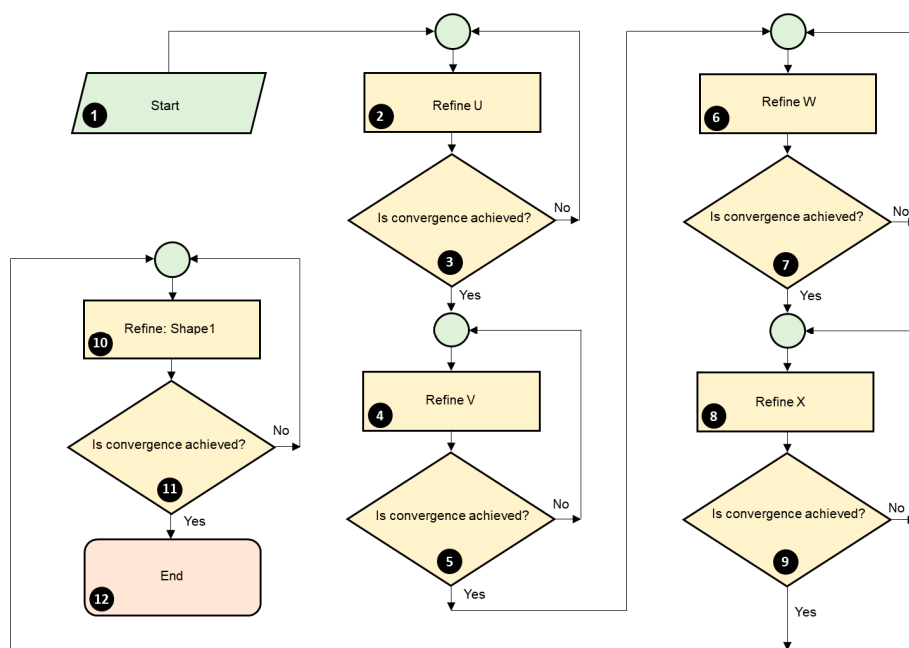


Figure 8. Order of refinement of U, V, W, and X parameters.

The last refinement step involves the atomic coordinates: X, Y, and Z parameters shown in row 14 of Table S1 are refined, as depicted in Figure 9 for a material containing La, Ni, Ti, and O, with orthorhombic symmetry. After the operator has refined all of the atomic coordinates, other parameters, such as Biso and Occ parameters, should be refined.

Furthermore, if the sample powder is packed on a depression of the sample holder prior to the experimental data collection, as recommended by the diffractometer manufacturer, and the diffraction peaks are symmetric, the preferred orientation (Pref1 and Pref2) and asymmetry parameters (Asy1 to Asy4) in row 16 of Table S1 should not be refined. Otherwise, each parameter should be refined after step 16 of Figure 9, following the order of refinement shown in this figure. For this last case, the last 2θ value should be placed under AsyLim located in row 4 of Table S1, to enable the refinement of asymmetry parameters.

It is worth mentioning that preferred orientation is a source of error, as it modifies the diffraction peak intensities [64], and it may occur in compressed samples [65].

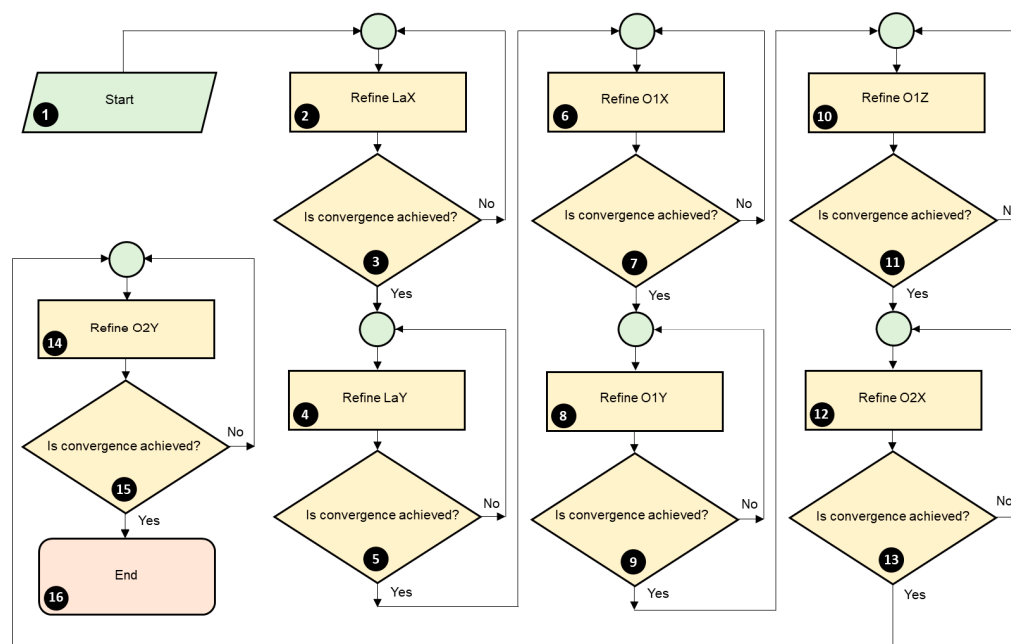


Figure 9. Order of refinement of atomic coordinates for a material containing La, Ni, Ti, and O and an orthorhombic symmetry.

Finally, other authors have refined most of the parameters presented in this work. Silva et al. [63] refined the scale factor, background coefficients, zero-point error, asymmetry, atomic coordinates, Biso, Occ parameters, and unit cell parameters, although they did not describe the order of refinement.

3.2.2. Graph of the Observed and Calculated XRD Pattern

A graph for the observed, calculated, and difference in XRD patterns is presented after finishing the Rietveld refinement method. Bhuyan et al. [66] reported that this graph showed no secondary phase for the $\text{Gd}_2\text{FeCrO}_6$ sample. Hosen et al. [20] established the absence of long-range ordering of B cations through the refinement of the crystal structure of $\text{Gd}_2\text{CoCrO}_6$ nanoparticles as a result of a peak absence around 20° . However, the graph showed background noise in this sample, which is characteristic of particle sizes at the nanoscale. Guo et al. [67] claimed that the $\text{La}_2\text{NiRuO}_6$ -calculated pattern corresponds to its experimental profile, as observed in the difference between the data, which is represented below these profiles in the graph. Zaraq et al. [57] reported that the monoclinic $\text{Sr}_2\text{Co}_{0.5}\text{Fe}_{0.5}\text{TeO}_6$ presents (111) and $(11\bar{1})$ reflections in the 2θ range 23.5° to 25.5° and (311) ($\bar{3}11$) (131) ($\bar{1}31$) reflections in the 2θ range 51° to 53° characterizing the $P2_1/n$ at 100 K; hence, they ensured that the Sr-Co-Fe-Te DP cannot be assigned the space group $I2/m$.

Steps 1 to 5 of Figure 10a present a graph generation procedure for the observed and calculated XRD patterns through the Winplotr tool of the Fullprof package. Step 6 of Figure 10a depicts the edition step, where the operator adds a format to the patterns. Some usual procedures are indicated in Table S2. Step 7 of Figure 10a indicates the export file procedure. This graph is in a BMP file that can be edited in other image-editing programs like Paint.

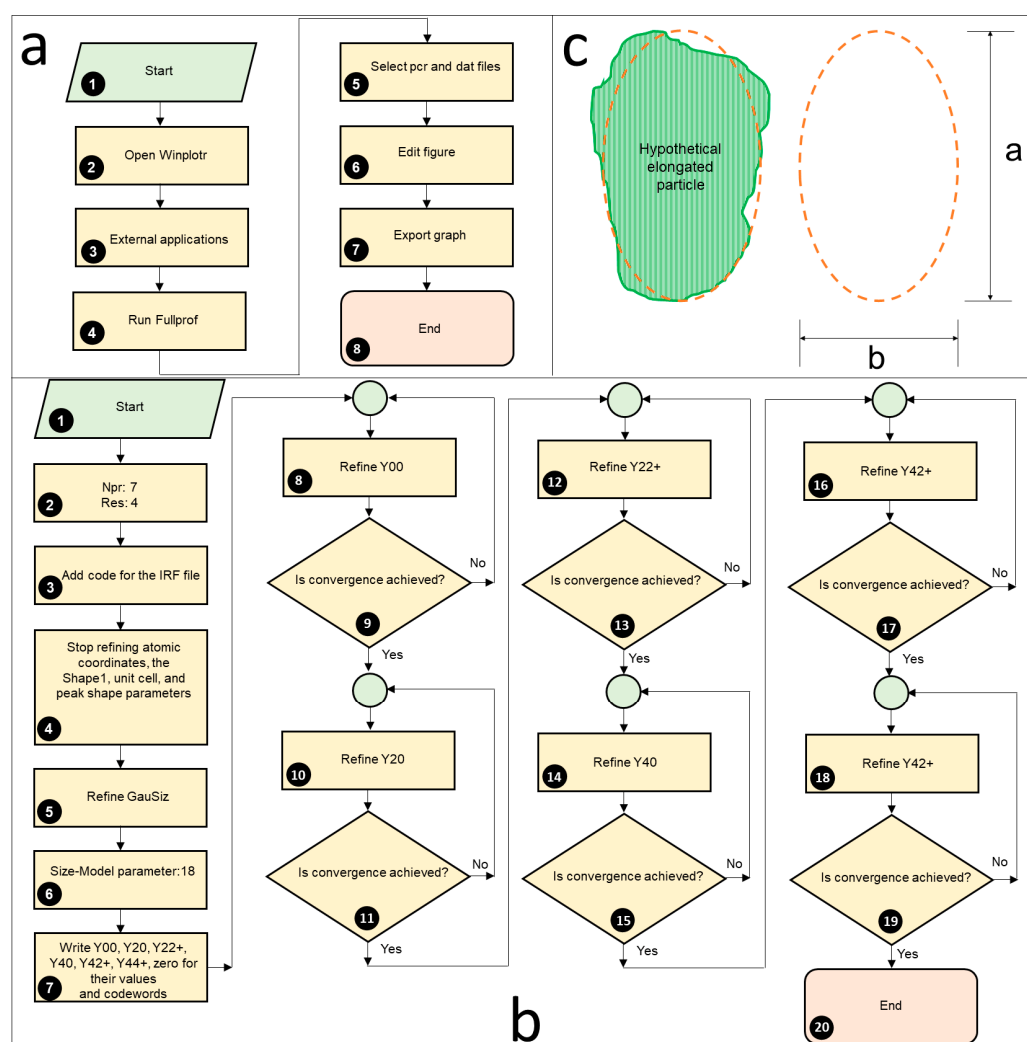


Figure 10. (a) Graph generation for the observed and calculated XRD pattern using Fullprof (version 3.0). (b) Crystallite size and strain procedure in a PCR file for an orthorhombic symmetry with space group *Pbnm*. (c) The a- and b-axes of the orange-dashed ellipse correspond to the axes of the elongated hypothetical particle.

3.2.3. Criteria for Judging the Quality of the Refinement

Several factors, like R_p , R_{wp} , R_{exp} , and χ^2 , have been used to quantify the quality of a crystal structure refinement. However, there is no consensus on a range of parameter-accepted values. For example, R_p and R_{wp} values of 21.4 and 26.8 were reported by our group in the refinement of La, Ni, Ti, and Co perovskites [61]. El Hachmi and Sadoune [68] reported values of 4.61 and 5.99 for these same parameters of the crystal structure of the $\text{SrLa}_2\text{NiFeNbO}_9$.

The R factors should be presented along with bond distances to address the quality of the refinement. For instance, Córdova-Calderón et al. [8] reported Ni-O and Ti-O distances from the structure refinement of $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ and $\text{La}_2\text{NiTiO}_6$ and compared them with previously reported values in the literature to assess the quality of the refinement.

Moreover, the R factors and χ^2 help assign the symmetry and space group for a sample with the same chemical composition but different B cation arrangements. Our group verified that the symmetry and space group for $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ provided higher R-factor and χ^2 values when used to describe the $\text{La}_2\text{NiTiO}_6$ [8].

3.2.4. CIF File Generation

CIF files contain crystallographic sample information that other researchers can use to simulate the XRD pattern using the Fullprof program and then refine the crystal structures of their own samples, as shown in Figures 5–10a. Additionally, they can even draw an image of the crystal structure of the sample using other packages, such as the Vesta software (version 3.90.0a). If the operator has completed the procedures outlined in Figures 5–10a and then enters a codeword of -1 for the Rpa [69] parameter in row 2 of Table S1, the Fullprof program will generate the CIF file for the sample.

3.2.5. Apparent Crystallite Size and Apparent Strain

The apparent crystallite size and apparent strain can be determined through a microstructural analysis in the Fullprof program. Both parameters depend on the full width at half maximum, but the apparent strain is also derived from the Stokes–Wilson apparent strain. Figure 10b presents a summary of the procedure in determining the apparent crystallite size and apparent strain for an orthorhombic structure and space group *Pbnm*. The analysis is performed using the Fullprof program and the default Thompson–Cox–Hastings pseudo-Voigt convoluted with axial divergence asymmetry peak function [70], i.e., Npr of 7, located in rows 1 and 9 of Table S1. The IRF file is derived from a refinement of a standard, such as the CeO₂, and its name and extension are included in the PCR file, as depicted in row 3 of Table S1. A value of 4 for the Res parameter (row 1, Table S1) can describe the information format for this resolution file [62].

Moreover, parameters located from row 12 to 15 of Table S1 should be unchanged by writing zero for their codeword, except for the Scale and the GauSiz. Furthermore, the symmetry and space group should be specified in the Size-Model parameter. For instance, the orthorhombic symmetry with space group *Pbnm* corresponds to a value of 18 [70]. Additionally, the operator should write the crystallite size and strain parameters particular to a crystal structure and space group, as described in steps 7 to 20 of Figure 10b. For example, the parameters shown in row 17 of Table S1 were manually written, and these parameters describe an orthorhombic symmetry, with space group *Pbnm*. As a matter of fact, each symmetry presents its own set of size and strain parameters [70], and these parameters should be refined following the method presented in Figure 10b. On the other hand, it is worth noting that row 17 should replace row 18 in the PCR, and this last row will appear automatically at step 9 of Figure 10b. An MIC file containing the apparent size and apparent strain will be created and saved in the PCR file folder.

3.3. Magnetic Measurements

Magnetic measurements, such as temperature-dependent magnetization in zero-field-cooled (ZFC) and field-cooled (FC) modes at various magnetic fields, can be conducted using a magnetometer. DPs can show various magnetic behaviors. Almadhi et al. [71] demonstrated that (Ca_{0.5}Mn_{0.5})₂MnTeO₆ is a spin glass, whereas Shibuya et al. [72] synthesized Ba₂(Cd_{1-x}Ca_x)ReO₆ and observed that canted antiferromagnetic (AFM) order and quadrupolar order can be observed for $0 \leq x \leq 0.6$, AFM order and quadrupolar order correspond to $0.6 \leq x \leq 0.9$, and AFM order can be verified for $0.9 \leq x \leq 1$. Agarwal et al. [73] demonstrated different valences and ionic radius mismatches among Co, Cr, and Mn in La₂Co_(1-x)Cr_(x)MnO₆ by increasing the Cr amount through magnetic measurements. This influence reduced the Curie temperature, coercive field, and remanence.

Macchiutti et al. [74] showed the magnetization vs. temperature (*M*(*T*)) curves in ZFC and FC modes, the inverse of the magnetic susceptibility vs. temperature (*(T)*), and the Curie–Weiss law fit for the La_{1.5}Sr_{0.5}CoMnO₆ calcined at various temperatures. The authors

observed that a decrease in the $M(T)$ values occurs due to the increase in boundaries, as the number of antiphase domains increases with the grain size [74].

Zhang et al. [75] depicted the ZFC and FC magnetization curves, the first derivative of ZFC curves, the variation in the Curie temperature (T_C), and the glass transition temperature (T_g) as a function of the Ga content for the $\text{La}_{1.5}\text{Sr}_{0.5}\text{Co}_{1-x}\text{Ga}_x\text{MnO}_6$. It could be observed that the T_g is practically imperceptible for $x \geq 0.3$ due to the dilution effect of the Ga ions in the sample [75].

An important interfacial effect is the Exchange Bias (EB) [76], and it depends essentially on magnetic interactions in the sample. Qiu et al. [77] claimed that an EB field of 1200 Oe at 10 K for the $\text{Sr}_2\text{FeReO}_6$ - LaFeO_3 may be attributed to the B cations arrangement and ferrimagnetic (FiM) nature of the DP interfacing the G-type AFM FeO_6 -containing perovskite. Pal et al. [78] contended that the EB results from atoms not occupying their sites and competition of ferromagnetic (FM), AFM, and spin glass interactions in the $\text{Sr}_2\text{FeRuO}_6$. Deng et al. [79] described that the EB depends on the spin-orbit coupling on Ir and AFM behavior of the B and B' cations for the Y_2NiIrO_6 . Kush and Srivastava [80] established that the EB depends on surface spins in interfacial frozen glassy states at the FiM particle's interface. Datta et al. [81] indicated that the EB phenomenon results from the competing FiM and AFM interactions for the NdSrCoIrO_6 . Moreover, while Mahalle et al. [82] reported that the EB is influenced by the applied field for the $\text{Gd}_2\text{CoRuO}_6$, Li et al. [83] stated that the EB depends on the FM layer thickness in the $\text{Bi}_{0.5}\text{Sr}_{0.5}\text{Fe}_{0.5}\text{Cr}_{0.5}\text{O}_3$.

The FM, AFM, FiM, and paramagnetic nature are determined using magnetic scans. While these characteristics are typical of DPs, the AFM behavior is related to B cation ordering. For instance, Córdova-Calderón et al. [8] reported NiO_6 and TiO_6 random ordering in $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ and a Néel temperature (T_N) of 15 K. Moreover, these authors stated the $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ Curie-Weiss temperature and the effective magnetic moment by fitting the inverse susceptibility to the Curie-Weiss law. Furthermore, a T_N of 80 K from magnetic measurements is due to the NiO_6 and MoO_6 AFM ordering in the $\text{Sr}_2\text{NiMoO}_6$, whereas a T_N of 60 K is related to MoO_6 substitution by the WO_6 [84]. Additionally, a magnetization vs. magnetic field curve justifies FM and AFM domains [20] and indicates multiferroic [85] and ferromagnetic properties [86]. Moreover, the FiM nature in the $\text{Ba}_2\text{FeMnO}_6$ depends on the double-exchange interaction of the B and B' cations through the oxygen [87].

Magnetic susceptibility values derived from magnetization values also present magnetic transitions, as shown by Zaraq et al. [88] for $\text{Sr}_2\text{FeTeO}_6$, $\text{Sr}_2\text{Fe}_{0.75}\text{Ni}_{0.25}\text{TeO}_6$, $\text{Sr}_2\text{Fe}_{0.5}\text{Ni}_{0.5}\text{TeO}_6$, $\text{Sr}_2\text{Fe}_{0.25}\text{Ni}_{0.75}\text{TeO}_6$, and $\text{Sr}_2\text{NiTeO}_6$. The Curie temperature showed magnetic transitions, and its change with x in $\text{Sr}_{2-x}\text{Ce}_x\text{Fe}_{1+x/2}\text{Mo}_{1-x/2}\text{O}_6$ was identified using magnetic susceptibility measurements [89].

Some structural studies can be performed through magnetic measurements. The progressive Pr substitution in $\text{Sr}_{2-x}\text{Pr}_x\text{FeTiO}_{6-\delta}$ from $x = 0.2$ to $x = 0.8$ promoted a transition from AFM to FM [90]. A glassy phase is produced by adding W in $\text{Sr}_2\text{NiMo}_{1-x}\text{W}_x\text{O}_6$ ($0 \leq x \leq 1$), as indicated in the ZFC and FC curves at low temperatures [84].

3.4. Transmission Electron Microscopy

Transmission electron microscopy (TEM) provides sample images at the nanometric scale, containing information about the sample morphology and particle size. Guo et al. [67] employed the ImageJ [91] package in the exsolution process of Ni-Ru particles from $\text{La}_{1.85}\text{NiRuO}_6$ reduced using 3% H_2O -wetted 5% H_2/Ar at 350 °C, finding Ni-Ru particle sizes of about 2.2 nm (Figure 11). Also, these authors measured the interplanar spacing and angles using fringe patterns through the DigitalMicrograph and the ImageJ program. Moreover, these authors manually selected the particles for their size determi-

nation through ImageJ, using a time-consuming procedure. Dara et al. [92] reported that $\text{Tb}_2\text{CoMnO}_6$ presented agglomerated particles at the nanoscale, as depicted in Figure 12.

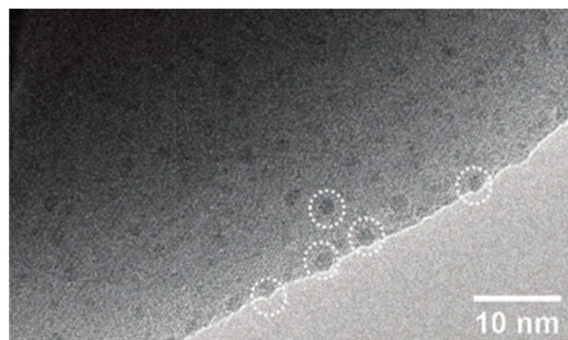


Figure 11. TEM micrograph of reduced $\text{La}_{1.85}\text{NiRuO}_6$. Reprinted from Ref. [67]. The white-dashed circles indicate Ni-Ru nanoparticles.

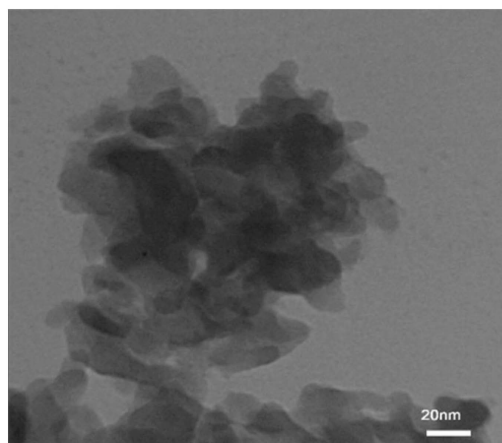


Figure 12. TEM image of $\text{Tb}_2\text{CoMnO}_6$. Reprinted from Ref. [92].

The diameter of a spherical particle describes its size. For the case of an elongated particle, its size is the mean of the ellipse axis simulating its shape [93]. Figure 10c presents these axes for a hypothetical particle. Additionally, particle sizes should be equal to or higher than the crystallite size obtained using Size and Strain Analysis from Fullprof, as a particle can be constituted of one or many crystallites. For instance, the $\text{Lu}_2\text{FeMnO}_6$'s TEM's particle size was 55 nm, whereas its crystallite size was 25.2 nm (Figure 13) [94].

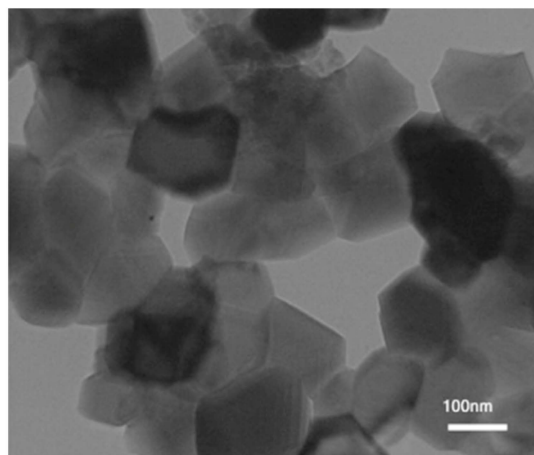


Figure 13. TEM micrograph of the $\text{Lu}_2\text{FeMnO}_6$. Reprinted from Ref. [94].

3.5. X-Ray Photoelectron Spectroscopy

X-ray photoelectron spectroscopy (XPS) provides structural information from the surface of the analyzed material, approximately 10 nm deep [95], and indicates the oxidation states of each ion [96]. For example, Ali et al. [97] reported surface Mn^{3+}O_6 and Fe^{3+}O_6 in $\text{La}_2\text{MnFeO}_6$ and surface Mn^{3+}O_6 and Co^{3+}O_6 in $\text{La}_2\text{MnCoO}_6$ using XPS, thereby verifying the structure of a DP in their samples. Sharmili et al. [42] claimed that $\text{La}_2\text{NiMnO}_6$ presents a uniform distribution of its constituents. Hosen et al. [20] determined mixed valences for Co and Cr cations in the $\text{Gd}_2\text{CoCrO}_6$ through XPS; thus, this DP presents short-range ordering of B cations. Kush and Srivastava [80] established defects in the $\text{La}_2\text{FeCoO}_6$ through the analysis of their B cations by using the XPS technique. Bhattacharjee et al. [98] indicated that some $\text{Fe}^{2+}\text{-O-Fe}^{2+}$ and $\text{Fe}^{2+}\text{-O-Fe}^{3+}$ interactions for the Ba_2FeVO_6 and Ca_2FeVO_6 were identified through XPS. Zhang et al. [11] reported the La 3d, Mn 2p, and Ni 2p spectra for the $\text{La}_2\text{MnNiO}_6$ (Figure 14) that resemble the perovskite characteristic through XPS.

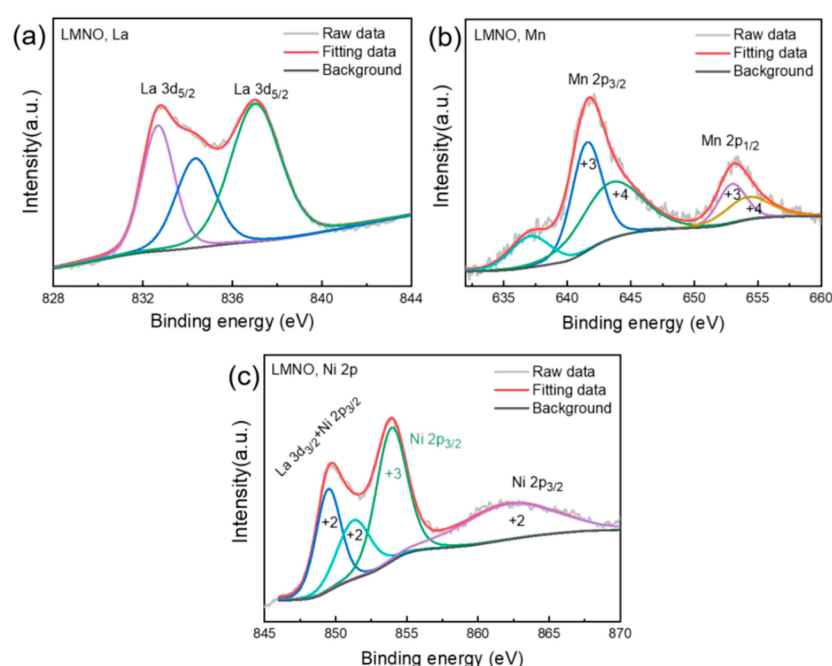


Figure 14. XPS survey scan of the $\text{La}_2\text{MnNiO}_6$. XPS spectra of (a) La 3d, (b) Mn 2p, and (c) Ni 2p. Reprinted/adapted with permission from Ref. [11].

Furthermore, XPS provides the surface chemical composition of a sample. For instance, Raji et al. [99] reported that the experimental surface molar ratios for Ba, Co, W, and O in Ba_2CoWO_6 measured through XPS were 1.9, 0.9, 0.85, and 5.8.

Additionally, XPS states the presence of atoms with different valences. For instance, Tang and Zhu [100] reported mixed valences for Fe and Re and two types of oxygen in $\text{La}_2\text{FeReO}_{6+\delta}$: lattice and adsorbed oxygen. Also, this characterization technique was used to report oxygen vacancies, as in the NdBaFeTiO_6 [101]. Additionally, Ghorbani and Ehsani [102] established that the mean oxygen valence of the $\text{Ba}_2\text{FeMoO}_6$ was -1.59 . Kumar et al. [103] reported an increase in the adsorbed oxygen with a decrease in the Sr content for $\text{Sr}_{2-x}\text{FeCoO}_{6-\delta}$, as determined by core-level XPS, due to an increase in the number of oxygen vacancies. Furthermore, Ghorbani and Ehsani [104] claimed the generation of mixed valences in $\text{Ba}_{2-x}\text{Ag}_x\text{FeMoO}_6$ for x of 0.025, prepared using the sol–gel method. Yi et al. [105] indicated Cr^{3+} , Cr^{4+} , Ni^{2+} , and Ni^{3+} , lattice and adsorbed oxygen in the $\text{La}_2\text{CrNiO}_6$. Moreover, Solanki et al. [106] reported that the ratio of $\text{Co}^{2+}/\text{Co}^{3+}$ depends on x up to 0.2 for the $\text{La}_2\text{CoTi}_{1-x}\text{Ni}_x\text{O}_6$.

3.6. Temperature-Programmed Reduction

The temperature-programmed reduction (TPR) can be carried out in conventional equipment with a TCD or mass detector. Initially, the sample is pretreated to eliminate adsorbed water by heating it under a flow of an inert gas like Ar. Subsequently, the sample is reduced under a flowing reduction mixture like H_2/Ar .

TPR is used to determine surface oxygen species and reduction processes in the sample. $\text{La}_2\text{AlFeO}_6$, prepared using glucose and citric acid, demonstrated two peaks: one peak stating the reduction of Fe^{3+} to Fe^{2+} and another peak at high temperatures describing the Fe^{2+} reduction to Fe^0 . More Fe^{3+} species are present in the material prepared using glucose, and this was determined through the TPR peak area. Moreover, the mixed oxide prepared using glucose was reduced at lower temperatures than the same material prepared using citric acid [53].

Roosbahania et al. [107] stated that the $\text{La}_2\text{NiMnO}_6$ presented two peaks in the TPR profile: the first peak at 378 °C represents the reduction of (i) surface oxygen species, (ii) Mn^{4+} to Mn^{3+} , and (iii) Ni^{3+} to Ni^{2+} . The second peak (at 466 °C) depicts the reduction of (i) lattice oxygen and (ii) Ni^{2+} reduction to Ni^0 . These authors also claimed that for $\text{La}_2\text{CoMnO}_6$, there was one peak (at 409 °C) showing the reduction of (i) Mn^{4+} to Mn^{3+} and (ii) Co^{3+} to Co^{2+} .

Guamán-Ayala et al. [33] reported that $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ DP presented two TPR peaks. One peak at low temperatures described the reduction of surface oxygen and Ni^{3+} to Ni^{2+} , whereas the peak at high temperatures indicated the reduction of Ni^{2+} to Ni^0 . The peak at high temperatures was confirmed through quantitative phase analysis using the Rietveld method. There is a more delayed H_2 consumption in the $\text{La}_2\text{NiTiO}_6$ compared to the $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ [108].

3.7. Synchrotron X-Ray Diffraction (SXRD)

Synchrotron X-ray powder diffraction measurements can be collected through Debye–Scherrer cameras [109]. Before the data collection, the sample is packed into a capillary, and the measurements can be collected at low temperatures using a cryostat and a blower [110].

These scans can be used to determine the symmetry and space group of a sample. Zhao et al. [111] reported that $\text{Pb}_2\text{NiMoO}_6$ presented a monoclinic symmetry with space group Pc using synchrotron X-ray powder diffraction dataset. Liang et al. [112] claimed a triclinic crystal structure for Ca_2CuWO_6 with space group $P\bar{1}$ among 100 to 1000 K.

Moreover, these patterns have been used to verify crystal structure stabilities with temperature. da Cruz Pinha Barbosa et al. [113] contended that $\text{Ba}_2\text{ZnReO}_6$ presents a transition from cubic to tetragonal at 23 K by using synchrotron radiation. Silva et al. [114] claimed that SmSrCoFeO_6 and EuSrCoFeO_6 maintain the orthorhombic crystal structure and $Pnma$ space group from 9 to 300 K, as stated using a synchrotron X-ray powder diffraction dataset. Morimura and Yamada [109] argued that the CoO_6 and RuO_6 octahedra arrangement in $\text{La}_2\text{CoRuO}_6$ changed from rock-salt to random ordering by pressing the sample using 8 GPa and 1373 K, as confirmed by SXRD.

The refinement of the crystal structure can be performed using the Fullprof program, and most of the parameters proposed in this work for the Rietveld method using XRD patterns are fitted in the Rietveld refinement coupled to the SXRD dataset, but following a different refinement strategy. For instance, the unit cell, overall isotropic displacement (Bov, row 13 Table S1), scale, peak shape of the pseudo-Voigt, atomic coordinates, asymmetry, and the background parameters were refined for the $\text{Ce}_{1-x}(\text{Nd}_{0.74}\text{Ti}_{0.26})_x\text{O}_{2-x/2}$, where several background points were previously selected, A and B cations were fixed, and the order of refinement is not reported [115].

3.8. Neutron Powder Diffraction (NPD)

The symmetry, space group, and B cation arrangements at low temperatures have been determined using NPD measurements. Ni and Ir moments present ordering below 74 K, as confirmed through 1.5 to 90 K neutron thermodiffractogram [116]. Naveen et al. [117] reported that the $\text{Ca}_{2-x}\text{La}_x\text{FeRuO}_6$ presents orthorhombic symmetry and space group $Pbnm$; hence, these DPs present random ordering of FeO_6 and RuO_6 at temperatures lower than 3 K. The crystal structure and space group at 150 K for CaMnCoWO_6 were determined, making use of a neutron-derived fit [118]. Almadhi et al. [71] reported no apparent long arrangement of spins in $(\text{Ca}_{0.5}\text{Mn}_{0.5})_2\text{MnTeO}_6$ at 1.6 K. $\text{Sr}_2\text{MnNbO}_{6-\delta}$ presents the $Pbnm$ space group from 4 to 300 K as established via the NPD method [54].

Magnetic properties can also be studied through neutron diffraction data. Short-range spin orders in CaMnFeTaO_6 were verified by the absence of magnetic diffraction peaks in the neutron diffraction patterns [119]. A ferromagnetic order between Mn and Cr in CaMnCrSbO_6 was observed through neutron diffraction [120]. Moreover, neutron diffraction patterns of the CaMnCoWO_6 revealed magnetic peaks that disappeared through heating from 15 to 20 K [118]. The absence of a magnetic peak at 1.5 K using neutron diffraction was observed for the CaMnMnWO_6 , and this was related to a spin glass transition at 8 K [121]. A magnetic phase separation for $\text{Sr}_2\text{CuTe}_{0.3}\text{W}_{0.7}\text{O}_6$ and $\text{Sr}_2\text{CuTe}_{0.2}\text{W}_{0.8}\text{O}_6$ was observed through neutron diffraction measurements [122].

The investigation of the structure has been carried out using neutron diffraction profiles. The amount of Er in $\text{La}_{2-x}\text{Er}_x\text{NiMnO}_6$ preserved the monoclinic symmetry, as verified through Rietveld refinement of neutron diffraction data [123]. Pal et al. [124] stated that the $\text{Pr}_{1.5}\text{Sr}_{0.5}\text{CoMnO}_6$ presented a CoO_6 and MnO_6 random arrangement composed of two symmetries, monoclinic ($P2_1/n$) and orthorhombic ($Pbnm$). Almadhi et al. [71] claimed accurate cation Occ parameters using the contrast in neutron-scattering lengths. Copper sites were partially substituted by iron in CaCuFeReO_6 , as indicated by the refinement of the mixed oxide crystal structure [125]. Moreover, these authors reported magnetic diffraction peaks in the neutron diffraction patterns collected from 5 to 500 K. To research oxygen positions in $\text{Sr}_2\text{Ga}_{1-x}\text{Mn}_x\text{SbO}_6$, the Rietveld refinement of NPD data was employed [126]. Oxygen diffusion paths in the $\text{La}_2\text{Ge}_{1-x}\text{Cr}_x\text{MgO}_{6-\delta}$ structure are described through neutron diffraction measurements [127].

The refinement can be performed using the Fullprof program. López et al. [127] reported that in the refinement of the crystal structure of $\text{La}_2\text{Ge}_{1-x}\text{Cr}_x\text{MgO}_{6-\delta}$ using NPD, the pseudo-Voigt function was selected, and the scale, background, zero, peak shape, asymmetry, unit cell, and isotropic displacement parameters were refined. The authors also reported the use of scattering lengths in the refinement. The scattering length of oxygen is detectable through NPD [128], compared to XRD, where oxygen cannot be well detected [126]. Similarly, the Ni and Ti in the $\text{La}_2\text{NiTiO}_6$ are more detectable in NPD than in XRD, as their scattering lengths are different [108].

3.9. Extended X-Ray Absorption Fine Structure (EXAFS)

EXAFS provides information about the symmetry and the structure. Jeevanandham et al. [129] observed defects in the $\text{La}_2\text{Ni}_{0.2}\text{Cu}_{0.8}\text{MnO}_6$. Majumder et al. [130] reported the concentration and distribution of antisite disorders in $\text{Sm}_2\text{NiMnO}_6$. Kavaliuk et al. [131] established that the bond length difference between values obtained from EXAFS and XRD are of 0.2 Å in the $\text{BaLn}_8\text{Co}_2\text{O}_{6-\delta}$, $\text{BaLn}_{10}\text{Co}_2\text{O}_{6-\delta}$, $\text{BaLn}_{12}\text{Co}_2\text{O}_{6-\delta}$, and $\text{BaLn}_{14}\text{Co}_2\text{O}_{6-\delta}$, where Ln can be La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu, as XRD provides an average value for this parameter.

3.10. Raman Spectroscopy

The crystal structure of DPs has been investigated using Raman spectroscopy. Murthy et al. [132] synthesized the $\text{SrLa}_{1-x}\text{Mn}_x\text{LiTeO}_6$ and claimed the same symmetry for all samples and the Mn inclusion in the perovskite structure. The Cr-O and Fe-O bond lengths in $\text{Gd}_2\text{FeCrO}_6$ were calculated using the Raman spectrum and compared to those calculated through XRD, and the difference was 0.04 Å [66]. Chahla et al. [55] indicated that the NdCaFeSnO_6 showed bands in the Raman spectrum related to the bending and stretching modes of SnO_6 and FeO_6 . Moreover, they reported that the unit cell expansion with the temperature was observed through a peak displacement around 350 cm^{-1} in the Raman spectrum.

Khan et al. [133] established that A-site ordering and anti-site disorder in Gd-doped Y_2CoMnO_6 influence the Raman spectra. Meena et al. [134] stated that $\text{La}_{2-x}\text{Ca}_x\text{FeMnO}_6$ presents improper ordering of FeO_6 and MnO_6 by Raman scattering spectroscopy. Boudad et al. [10] indicated five band shifts in the LaBaFeTiO_6 Raman spectrum compared to that of EuBaFeTiO_6 . Wlodarczyk et al. [13] reported that Ba_2CeWO_6 decomposed in air above 573 K, whereas Silva et al. [135] contended that $\text{La}_2\text{CoMnO}_6$ showed phonon energy behaviors associated with short-range Co and Mn ferromagnetic clusters through Raman spectroscopy measurements.

4. Properties and Applications

DPs present several properties like FM [136], magnetoresistance effect [137], ferroelectric [138], AFM [139], FiM [140], multiferroic [141], metal–insulator transition [142], magnetocaloric effect [143], luminescent [144], magnetic [53], optical, electrical, and mechanical [145], semiconducting [146], and half-metallic FM [147].

Some material properties are related to magnetic properties. BaBiFeTiO_6 presents ferroelectric properties with remanent polarization, as depicted by the polarization vs. electric field hysteresis loop [138]. The FiM behavior of $\text{Sr}_2\text{CrHfO}_6$ was observed at 2 K [140]. $\text{Gd}_2\text{CrFeO}_6$ exhibits magnetic entropy changes and refrigerant capacity similar to those of other materials with magnetocaloric effects [143]. The magnetic moments of $\text{La}_2\text{BB}'\text{O}_6$ ($\text{BB}' = \text{CrCo}, \text{CrNi}, \text{ScNi}, \text{VNi}, \text{VSc}$) confirm their properties [147].

Other properties are related to their bandgap values. $\text{Ba}_2\text{GdBiO}_6$ can be used in ultraviolet and infrared absorption due to its bandgap [145]. The bandgap of the semiconducting $\text{Sr}_2\text{FeMnO}_6$ is 1.38 eV [146], whereas the direct bandgap of the semiconducting $\text{Gd}_2\text{CoCrO}_6$ justifies its optical property [20]. Other DPs for optoelectronic applications are LaBaFeTiO_6 and EuBaFeTiO_6 , which present high bandgap values [10], whereas the bandgaps of $\text{Sr}_2\text{InSbO}_6$ and $\text{Ba}_2\text{InSbO}_6$ are 2.55 eV and 1.75 eV [148].

DPs can be used in memory devices [138], sensors [141], cooling [143], LED [144], energy storage and photonics [149], catalytic [53], biomedical [150], photocatalytic [20], electronic, spintronic, optoelectronic, and magnetic [147], solar cell, thermoelectric, and transport [148] applications.

Several characteristics make DPs appealing for their applications. Transport parameters determine the $\text{Sr}_2\text{PrSnO}_6$ applications in spintronics [136]. The electronic, magnetic, optical, and mechanical properties foster the photovoltaic applications of the $\text{Ca}_2\text{TaNiO}_6$, $\text{Sr}_2\text{TaNiO}_6$, and $\text{Ba}_2\text{TaNiO}_6$ [139]. The strain-influenced properties promote the LaSrNiReO_6 and $\text{LaSr}_{0.5}\text{Ca}_{0.5}\text{NiReO}_6$ for memory devices [142]. Sm-doped $\text{Sr}_2\text{LaSbO}_6$ presents excitation at 406 nm, suitable for LED applications [144]. $\text{La}_2\text{CoMnO}_6$ exhibits appealing absorption behavior and superior supercapacitor performance, making it suitable for applications in photonics and energy storage [149]. Fe^{2+} from the reduction of surface Fe^{3+} in the $\text{La}_2\text{FeAlO}_6$ through artificial light is active for OH production from H_2O_2 in the Fenton reaction [53], a catalytic application of DPs. The Seebeck coefficient and UV

response in the $\text{Sr}_2\text{NdNbO}_6$ appeal for its biomedical applications [150]. The magnetoresistance effect, along with the mixed oxide AFM nature, fosters $\text{Mn}_2\text{CoReO}_6$ spintronic applications [137]. The FM arrangement, insulating behavior, and ferroelectricity promote the $\text{Dy}_2\text{MnCoO}_6$ -sensing application [141]. The Ce-doped $\text{Ba}_2\text{TiMoO}_6$ degrades methylene blue, which may be related to its capacity to absorb UV radiation that can be used for photocatalytic reactions [151]. The $\text{Sr}_2\text{FeMoO}_6$ prepared using the sol–gel method at a pH of 8 and irradiated for 35 min converted methylene blue completely, which can be related to its absorption of UV and VIS radiation and a higher amount of surface oxygen [152]. The $\text{Lu}_2\text{CrMnO}_6$ can be used for hydrogen storage, as it presents nanostructures with appealing hydrogen sorption and oxidation-reduction processes [153].

5. Summary

Double perovskites (DP), represented by the formula $\text{A}_2\text{BB}'\text{O}_6$ and $\text{AA}'\text{BB}'\text{O}_6$, present three arrangements (random, rock salt, and layered). They can be synthesized using the solid-state reaction, sol–gel, Pechini, and hydrothermal methods, and characterized using XRF, XRD, magnetic measurements, TEM, XPS, TPR, SXRD, NPD, EXAFS, and Raman spectroscopy.

The Rietveld method was coupled to XRD, SXRD, and NPD and implemented in the Fullprof program. Several options are available in the Winplotr tool of the Fullprof package to draw the Rietveld refinement results. A CIF file can be generated from the sample after refinement of the crystal structure. The results of the Rietveld method can be used to determine the apparent size and apparent strain.

The results from the characterization techniques complement those obtained from the Rietveld method. For the case of $\text{La}_2\text{NiTiO}_6$, XRF verifies the occupation number of La, Ni, and Ti in the crystalline structure determined from the Rietveld method coupled to XRD, SXRD, or NPD. Magnetic measurements can verify the Ni and Ti arrangement and symmetry. The apparent crystallite size of the $\text{La}_2\text{NiTiO}_6$ can be contrasted with TEM information. The adsorbed oxygen on the surface can be verified by the XPS and the TPR. The Ni–O and Ti–O bond length distances from EXAFS and Raman spectroscopy can complement the results of the Rietveld refinement.

The synthesis method can have an important role in investigating DPs with enhanced properties. Green chemicals in the sol–gel method have been reported to provide DPs with an appealing particle size. The ball-milling step can introduce defects in the sample. NH_4OH can produce a structure-like foam after the resin calcination using the Pechini method. DPs-containing composites have been prepared using the hydrothermal method.

The combination of magnetic, electronic, optical, and catalytic properties makes DPs highly versatile for applications in spintronics, photovoltaics, memory devices, sensors, LEDs, cooling systems, energy storage and photonics, catalysis, photocatalysis, biomedicine, thermoelectric, and hydrogen storage.

6. Outlook and Challenges

Several DPs have been reported in the literature; however, more research on this type of mixed oxides is required. First of all, additional studies should be carried out on cheap ion-containing DPs like Fe, Co, or Cu, as these metals present catalytic properties to produce ammonia, hydrocarbons, or hydrogen. These systems may be designed using active metals with non-active ions to improve the metal–support interaction, as demonstrated for the $\text{La}_2\text{NiTiO}_6$. Furthermore, cheap, active, and stable supports like core shell structures should be studied to favor the cost–benefit ratio to implement DPs materials in catalytic applications.

The calcination temperature may influence the oxygen content, as observed in the solid-state reaction method, or the symmetry, as stated for the Pechini method. The partial substitution of B cations may produce vacancies (Pechini method) or mixed valences in the structure (sol–gel). In the sol–gel synthesis, the inclusion of a milling step may modulate the properties of DPs. In the Pechini method, alternative carboxylic acids or alcohols to the citric acid and ethylene glycol may influence the morphology of the samples.

Moreover, more fundamental knowledge about cost-effective systems, such as materials containing DPs and activated carbon, is required to develop technologies for separating, purifying, and storing hydrogen.

Finally, biomedical items may be a new extensive application of DPs, as a result of DP properties, and this new horizon may be fostered by meeting customer needs with starting materials through extensive DP characterization. Therefore, additional research is required on DPs, especially on cost-effective materials and preparation methods, promoting catalytic processes, biomedical applications, and renewable energies.

Supplementary Materials: The following supporting information can be downloaded at <https://www.mdpi.com/article/10.3390/inorganics13110372/s1>: Table S1: Default (black) and written (blue) parameters in a portion of a PCR file using the Fullprof program with hypothetical values; Table S2: Procedures in the edition step for the observed and calculated XRD pattern.

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Abbreviations

The following abbreviations are used in this manuscript:

AFM	Antiferromagnetic
DP	Double perovskite
BMP	File containing a figure of a crystal structure
CIF	Crystallographic information file
DAT	File containing observed X-ray diffraction data
EB	Exchange Bias
EG	Ethylene glycol
EXAFS	Extended X-ray absorption fine structure
FC	Field-cooled mode
FiM	Ferrimagnetic
FM	Ferromagnetic
HER	Hydrogen evolution reaction
IRF	File for an instrumental resolution function containing information of a standard like CeO ₂
LED	Light-Emitting Diode
M	Magnetization

MIC	File containing the apparent size and apparent strain
OER	Oxygen evolution reaction
PCR	A tool of the Fullprof program that generates editing files used during the refinement of a crystal structure, called PCR files
PVA	Polyvinyl alcohol
NPD	Neutron Powder Diffraction
SXRD	Synchrotron X-ray diffraction
T	Temperature
T _C	Curie Temperature
TEM	Transmission electron microscopy
T _g	Glass transition temperature
T _N	Néel temperature
TPR	Temperature-programmed reduction
XPS	X-ray photoelectron spectroscopy
XRD	X-ray Diffraction
XRF	X-ray Fluorescence
ZFC	Zero-field cooled mode
χ	Magnetic susceptibility

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