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Properties and Applications of Perovskite-Type Oxides Structure, Properties and Preparation of Perovskite-Type Compounds **Fundamentals of Perovskite Oxides** Anionic Substitution in Perovskite-type Oxides *Perovskite Materials* Structures and Relationships of Some Perovskite-type Compounds **Ferroelectricity and the Chemical Bond in Perovskite-type Oxides** *Perovskites and Related Mixed Oxides* Anionic Substitution in Perovskite-type Oxides Tuning Structural and Physical Properties Via A-site Doping in Perovskite-type Transition Metal Oxides Perovskite Oxide for Solid Oxide Fuel Cells Air Separation with Perovskite-type Oxide Membranes Perovskites **Energetics of Perovskite-type Materials Applied in Solid Oxide Fuel Cells (SOFCs) Investigation of Structural and Magnetic Properties of Perovskite Type Oxides Containing 5d Ions Crystal structure and phase transition studies in perovskite-type oxides using powder-diffraction techniques and symmetry-mode analysis Crystal Structure and Phase Transition Studies in Perovskite-type Oxides Using Powder-diffraction Techniques and Symmetry-mode Analysis Perovskite Materials, Devices and Integration Oxides other than Perovskite-type and LiNbO3 family** *Structure and reactivity of perovskite-type oxides* Perovskite-type Layered Cuprates (High-Tc Superconductors and Related Compounds) **Perovskite-type Oxides and LiNbO3 Family Revolution of Perovskite Perovskite-type Oxides and LiNbO3 Family** Perovskite-type Layered Cuprates (High-Tc Superconductors and Related Compounds) **Perovskite** *Synthesis and Characterization of Cobalt-containing Perovskite-type Oxides* **Solution Based Preparation of Perovskite-type Oxide Films and Powders Perovskite Materials for Energy and Environmental Applications Catalysis by Metals on Perovskite-Type Oxides** A Study of Pentavalent Molybdenum in Perovskite Type Compounds **Optical Properties and Electronic Band Structures of Perovskite-Type Ferroelectric and Conductive Metallic Oxide Films** The Form of Solemnization of Matrimony. With Introduction and Notes *Hybrid Perovskite Composite Materials* **Mixed Ionic Electronic Conducting Perovskites for Advanced Energy Systems Perovskites** *Structure, Properties, and Preparation of Perovskite-type Compounds, by Francis S. Galasso* **Studies on the Solid State Chemistry of Perovskite-type Oxides for Oxygen Separating Membranes Perovskite-type Metal Oxides Electrical Conductivity and Structure Heterogeneous Ferroelectric Solid Solutions**

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"A model for crystallographic transitions in perovskites is proposed. The model consists of regular octahedra sharing corners and topologically able to rotate without distortion around their three-fold axes. This model, with R3c symmetry (18e position) can be described in terms of a continuous rotation of angle, w, of octahedra from two ideal symmetry forms: the hexagonal close-packed and the cubic face-centered configurations. A parametric relation is derived between w and the rhombohedral cell angle, [alpha], or the corresponding hexagonal axial ratio c/a . A wide range of atomic structures based on a framework of regular or slightly distorted octahedra sharing corners can be derived from this model. A number of compounds of composition ABX3 are examined. In all of these the anion X lies exactly or approximately in 18e position of the R3c space group with the cation B midway between the AX3 layers. The site of the cation A may be vacant, as in the case where X is fluorine. These pseudosymmetric compounds can be viewed also as being generated by an array of linear chains of rigid octahedra sharing corners . Along this chain, [phi], the bond angle (cation B - anion X - cation B) is related to the bimolecular rhombohedral cell angle, [alpha], or equivalently, to the variable parameter, x, of the anions [x, 0, 1/4], (hexagonal set, R3c.) These theoretical relationships are compared graphically to some crystallographic data for a trifluoride-type series, BF3, (B = Ru, Co, V, Fe, Ti) and a perovskite-type series, AB03 (A = Bi, Pb, La, Li, and B =Fe, Zr-Ti, Co, Al, Nb, Ta). The experimental data for all of these compounds are in excellent agreement with the theoretical relationships. The atomic positions of the perovskite-type compounds PbZr0.9Ti0.1O3 and BiFe03 were determined using X-ray and neutron diffraction. Their octahedral framework can be considered as an early stage of a continuous trigonal rotation which is fully developed in LiNb03 and LiTaO3. In this isomorphous ferroelectric series, the B cation shifts from the ideal perovskite positions and are related to the A cation shifts and the spontaneous polarization. The symmetry is then reduced to the non-centrosymmetric space group, R3c. In all of these compounds the distortion of the octahedra is a second order effect compared to the trigonal rotation. Such deformations, in agreement with the theoretical data, generate superstructure reflections which depend only on the oxygen position, and the intensity of these reflections can be correlated

with the trigonal rotation, w. The temperature dependence of w for the low temperature phase of PbZr0.9Ti0.1O3 is consistent with the existence of an unstable phonon mode at the (1/21/21/2) point at the Brillouin zone corner, as in LaAlO3. One of the most significant aspects of this work has been to relate certain phase transitions in ferroelectric materials, such as PbZr0.9Ti0.1O3, with intensively studied transitions in some non-ferroelectric perovskites, such as LaAlO3 and SrTiO3"--Abstract, pages ii-iv. Perovskite-type oxides are widely explored in a number of environment and energy related research fields. This Special Issue Book "Catalysis by Metals on Perovskite-Type Oxides" provides updates on the recent advances in the catalytic applications of transition metals dispersed on perovskite-type oxides and their working structure. Perovskites have attracted great attention in the fields of energy storage, pollutant degradation as well as optoelectronic devices due to their excellent properties. This kind of material can be divided into two categories; inorganic perovskite represented by perovskite oxide and organic-inorganic hybrid perovskite, which have described the recent advancement separately in terms of catalysis and photoelectron applications. This book systematically illustrates the crystal structures, physic-chemical properties, fabrication process, and perovskite-related devices. In a word, perovskite has broad application prospects. However, the current challenges cannot be ignored, such as toxicity and stability. Optical Properties and Electronic Band Structures of Perovskite-Type Ferroelectric and Conductive Metallic Oxide Films. Perovskite is a calcium titanium oxide mineral species composed of calcium titanate. This book discusses perovskite thin films, which are widely employed in today's advanced technology. The broad range of physical properties in such category of materials has offered various functionalities in devices ranging from dynamic random access memories and ferroelectric nonvolatile memories to piezoelectric and optical devices. The structural, magnetic and electron transport properties of ordered-disordered perskovite cobaltites is discussed as is perovskite-type oxides, ferroelectric PbTiO3 from a single-domain state to composite components, and others. The magnetic properties of oxides with perovskite, corundum, ilmenite and amorphous structures have been compiled in subvolume 27F. Part 27F2, published in 1994, presents magnetic data on perovskite-type layered cuprates which were discovered to show superconductivity with critical temperatures above 40 K (high-Tc superconductors). The present volume 27F2S is an update and extension of 27F2 with more precise data on high quality single crystals and some new effects and phenomena, covering the literature of the period 1991-2000. In this book, the authors present current research in the study of the crystallography, chemistry and catalytic performance of perovskites. Topics discussed include the defect structure and defect-induced expansion of perovskite oxides; perovskite-based catalysts for transformation of natural gas and oxygenates into syngas; Bi containing multiferroic perovskite oxide thin films; perovskites as catalysts for environmental remediation; microwave-assisted synthesis and characterisation of perovskite oxides; perovskite and lead based ceramic materials; photocatalytic properties of perovskite-type layered oxides; structure of perovskite electron-ionic conductors; and distorted perovskites. The book deals with perovskite-type ferroelectric solid solutions for modern materials science and applications, solving problems of complicated heterophase/domain structures near the morphotropic phase boundary and applications to various systems with morphotropic phases. In this book domain state–interface diagrams are presented for the interpretation of heterophase states in perovskite-type ferroelectric solid solutions. It allows to describe the stress relief in the presence of polydomain phases, the behavior of unit-cell parameters of coexisting phases and the effect of external electric fields. The novelty of the book consists in (i) the first systematization of data about heterophase states and their evolution in ferroelectric solid solutions (ii) the general interpretation of heterophase and domain structures at changing temperature, composition or electric field (iii) the complete analysis of interconnection domain structures, unit-cell parameters changes, heterophase structures and stress relief. Data on ferroelectric and antiferroelectric behaviour of pure compounds and solid solutions are critically

evaluated and in addition all other properties relevant to the characterization of these crystals are presented in tables and figures. Subvolume A is for oxides and B for non-oxides including liquid crystals. This subvolume consists of a printed version and an electronic version on CD-ROM. All the compiled data can be found on the CD-ROM. The abundance and diversity of the data, however, make an overview of the relevant research field difficult, and thus the printed version is designed to survey the present status of ferroelectrics research and to grasp the contents of CD-ROM. About 6% of tables and 28% of figures in CD-ROM are selected and presented in the printed version. Volume III/27 covers the magnetic properties of non-metallic inorganic compounds based on transition elements. It can therefore be considered as a supplement supplement to volumes III/4 and III/12 "Magnetic and Other Properties of Magnetic Oxides and Related Compounds" which appeared in 1970 and in the period 1978-1982 respectively. The magnetic properties of the oxides with curundum, ilmenite and perovskite-type crystal structure and amorphous oxides are given in volume 27f. The present subvolume III/27f2 contains a comprehensive survey of the perovskite-type layered cuprates, i.e. the high-Tc superconductors and related compounds, and will therefore also be of great interest for all those working on the understanding and the development of high-Tc superconductors. Uniquely describes both the crystallography and properties of perovskite related materials. Practical applications in solar cells, microelectronics and telecommunications Interdisciplinary topic drawing on materials science, chemistry, physics, and geology Contains problems and answers to enhance knowledge retention The focus of this thesis work is to explore the exotic magnetism in perovskite type oxide materials containing 5d transition metal. Strong spin orbit coupling and extended 5d orbitals lay the foundation of unique orbital and spin interactions between 5d ions. Understanding the physics of 5d ions is not only of fundamental interests, but important in the search for new phases of matter such as topological insulators, Weyl semimetals and quantum spin liquids. Chapter 2 and 3 discuss the magnetic behavior of 5d1 and 5d2 ions on a face-centered cubic lattice embedded in the double perovskite structure. The crystal structure, transport and magnetic properties of double perovskites Ba2BReO6 (B=Cd, Zn, Sc, In, Lu, La), Sr2LuReO6 and Ca2ScReO6 are characterized by X-ray diffraction, neutron diffraction, dc electric conductivity, dc magnetometry and heat capacity. Ferromagnetic ground states are prevalent in 5d1 systems. Orbital degree of freedom dominates the magnetic behavior over a wide temperature range before the magnetic ordering, resulting in changing effective moments with temperature and artificial negative Weiss constants. The ground state is a delicate balance sensitive to factors such as spin orbit coupling, metal-oxygen covalency, and subtle structural details. On the other hand, 5d2 systems are dominated by antiferromagnetic ground states. Filling d orbitals on the diamagnetic ion tends to destroy long range magnetic ordering in compounds with cubic symmetry. Strong distortion of the octahedral environment of 5d2 ions can result in ionic singlet states, which is not possible in 5d1 systems. Chapter 4 investigates the superexchange coupling between 5d ions and 3d ions in ordered double perovskites Sr2-xCaxCoOsO6. The crystal structures and magnetic properties are characterized using X-ray diffraction, neutron diffraction and magnetometry. Independent magnetic ordering of Co and Os sublattices are found in Sr-heavy compounds with less structural distortions, stabilized by Co-Co interactions (Co-O-O-Co and Co-O-Os-O-Co superexchange coupling) and Os-Os interactions (Os-O-O-Os and Os-O-Co-O-Os superexchange coupling), respectively. The Os-Os interactions are more sensitive to structural distortions than the Co-Co interactions. As a result, magnetic ordering of the Os sublattice disappear at lower Ca doping level than that of the Co sublattice. The strength of Co-Os superexchange coupling increases as the structure gets more distorted, resulting in ferrimagnetic ordering between Co and Os sublattices on the Ca-heavy compound. Complex glassy behavior is present in a wide compositional range in between due to the presence of competing magnetic interactions. Data on ferroelectric and antiferroelectric behaviour of pure compounds and solid solutions

are critically evaluated and in addition all other properties relevant to the characterization of these crystals are presented in tables and figures. Subvolume A is for oxides and B for non-oxides including liquid crystals. This subvolume consists of a printed version and an electronic version on CD-ROM. All the compiled data can be found on the CD-ROM. The abundance and diversity of the data, however, make an overview of the relevant research field difficult, and thus the printed version is designed to survey the present status of ferroelectrics research and to grasp the contents of CD-ROM. About 6% of tables and 28% of figures in CD-ROM are selected and presented in the printed version. Data on ferroelectric and antiferroelectric behaviour of pure compounds and solid solutions are critically evaluated and in addition all other properties relevant to the characterization of these crystals are presented in tables and figures. Subvolume A is for oxides and B for non-oxides including liquid crystals. This subvolume consists of a printed version and an electronic version on CD-ROM. All the compiled data can be found on the CD-ROM. The abundance and diversity of the data, however, make an overview of the relevant research field difficult, and thus the printed version is designed to survey the present status of ferroelectrics research and to grasp the contents of CD-ROM. About 6% of tables and 28% of figures in CD-ROM are selected and presented in the printed version. This thesis investigates the structure-property relationship of two important classes of transition metal oxides (the perovskite-type A-site substituted titanates (Sr[sub 1-x-y]Ca[sub x]Nd[sub y])TiO[sub 3] and manganites (Sr[sub 1-x]Ba[sub x])MnO[sub 3]). A thorough evaluation is provided of their potential for prospective technological applications in heat recycling and information technology by examining the thermoelectric and multiferroic prop- erties, respectively. In the titanate compounds, we doped on the A-site with small rare earth ions in order to generate mixed valent transition metals to increase band filling while the Ca doping maintained fixed levels of distortions. In the case of the manganites, A-site Sr ions were substituted with large Ba ions for the purpose of increasing the materials strain and to promote ferroelectricity. Crystal structure was investigated using high-resolution neutron powder diffraction as a function of temperature and Nd/Ba doping. In the titanates, two series were synthesized and designed to have a nominally constant tolerance factor at room temperature. We determine the room temperature structures as tetragonal I4/mcm and orthorhombic Pbnm for the Sr-rich and Ca-rich series, respectively. Three low temperature orthorhombic structures, Pbnm, Ibmm and Pbcm were also observed for the Sr-rich series; whereas, the symmetry of the Ca-rich series remained unchanged throughout the full measured temperature range. Thermoelectricity in ternary (Sr[sub 1-x-y]Ca[sub x]Nd[sub y])TiO[sub 3] perovskites was investigated. The double substitution at the A-site maintained a fixed crystal distortion while Nd3+ doping modified the electronic properties of the materials via increased band filling. Unique compositions of cations allowed for increased A-site atomic mass disorder and the lattice thermal conductivity was significantly suppressed to values as low as ~ 1.5 W/K.m in some samples, approaching amorphous Silicon limit. Charge doping via balanced formation of Ti^3+ at the B-site has transformed materials into n-type semi-conductors. I examined the range of applicability of various conduction models, viz., variable range hopping, semiconductor-type conductivity across band gap, and small polaron hopping for the best description of the temperature variation of measured resistivity. We succeeded in achieving a relatively high figure of merit ZT=0.07 at ~ 400 K in the Sr-rich Sr[sub 0.76]Ca[sub 0.16]Nd[sub 0.08]TiO[sub 3] composition which is comparable to that of the best n-type TE SrTi[sub 0.80]Nb[sub 0.20]O[sub 3] oxide material reported to date. With an enhanced Seebeck coefficient at elevated temperatures and reduced thermal conductivity, we predict that Sr[sub 0.76]Ca[sub 0.16]Nd[sub 0.08]TiO[sub 3] and similar compositions have the potential to become some of the best materials in their class of thermoelectric oxides. We also report the structure-property phase diagram of unique single-ion type-1 multiferroic pseudocubic Sr1-xBaxMnO3 perovskites. Employing a specially designed multi-step reduction-oxidation synthesis technique, we have synthesized previously unknown Sr[sub 1-

x]Ba[sub x]MnO[sub 3] compositions in their polycrystalline form with a significantly extended Ba solubility limit that is only rivaled by a very limited number of crystals and thin films grown under non-equilibrium conditions. Understanding the multiferroic interplay with structure in Sr[sub 1-x]Ba[sub x]MnO[sub 3] is of great importance as it opens the door wide to the development of newer materials from the parent (AA')(BB')O3 system with enhanced properties. To this end, using a combination of time-of-flight neutron and synchrotron x-ray scattering techniques, we determined the exact structures and quantified the Mn and oxygen polar distortions above and below the ferroelectric Curie temperature TC and the Neel temperature TN. In its ferroelectric state, the system crystalizes in the noncentrosymmetric tetragonal P4mm space group which gives rise to a large electric dipole moment PS, in the z-direction, of 18.4 and 29.5 microC/cm2 for x = 0.43 and 0.45, respectively. The two independently driven ferroelectric and magnetic order parameters are single-handedly accommodated by the Mn sublattice leading to a novel strain-assisted multiferroic behavior in agreement with many theoretical predictions. Our neutron diffraction results demonstrate the large and tunable suppression of the ferroelectric order at the onset of AFM ordering and confirm the coexistence and strong coupling of the two ferroic orders below T[sub N]. The refined magnetic moments confirm the strong covalent bonding between Mn and the oxygen anions which is necessary for stabilizing the ferroelectric phase. This volume presents advanced synthesis techniques for fabricating Perovskite materials with enhanced properties for applications such as energy storage devices, photovoltaics, electrocatalysis, electronic devices, photocatalysts, sensing, and biomedical instruments. The book attempts to fill a gap in the published literature and provide a detailed reference on Perovskite materials. This book will be of use to graduate students and academic and industrial researchers in the fields of solid-state chemistry, physics, materials science, and chemical engineering. The book summarizes the current state of the know-how in the field of perovskite materials: synthesis, characterization, properties, and applications. Most chapters include a review on the actual knowledge and cutting-edge research results. Thus, this book is an essential source of reference for scientists with research fields in energy, physics, chemistry and materials. It is also a suitable reading material for graduate students. Structure, Properties and Preparation of Perovskite-Type Compounds, Volume 5 presents the various methods of preparing powders, single crystals, and thin films of perovskite-type compounds. This book discusses the structure of perovskite-type compounds and their properties. Organized into 11 chapters, this volume begins with an overview of the structure, properties, and preparation of perovskite-type compounds. This text then examines how X-ray diffraction can be used to determine unit cell data and to orient single crystals. Other chapters consider the effect of nuclear radiation on the properties of ferroelectric materials. This book discusses as well the phase transitions in perovskite-type compounds, which are often associated with a change in ferroelectric properties. The final chapter explores the two techniques in the preparation of the ternary carbides with the perovskite structure, which involves melting the appropriate proportions of the two metals and carbon under argon. This book is a valuable resource for solid-state chemists. PEROVSKITE MATERIALS FOR ENERGY AND ENVIRONMENTAL APPLICATIONS The book provides a state-of-the-art summary and discussion about the recent progress in the development and engineering of perovskite solar cells materials along with the future directions it might take. Among all 3rd generation solar cells, perovskite solar cells have recently been attracting much attention and have also emerged as a hot research area of competing materials for silicon PV due to their easy fabrication, long charge-carrier lifetime, low binding energy, low defect density, and low cost. This book focuses primarily on the perovskite structures and utilizes them in modern technologies of photovoltaics and environmental applications. It will be unique in terms of the use of perovskite structures in solar cell applications. This book also discusses the type of perovskites, their synthetic approach, and environmental and solar cell applications. The book also covers how perovskite solar cells

originated and the recent advances in perovskite solar cells. The reader will find in this book a lucid account that: Introduces the history of perovskite materials. Explores perovskite materials for energy conversion and environmental-related applications. Covers perovskite light absorber materials for the fabrication of high-performance perovskite solar cells. Describes the device architectures and physics of perovskite solar cells. Discusses the role of perovskite absorber, electron transport, and hole transport materials layers. Audience The book is essential reading for all those in the photovoltaic community, including materials scientists, surface physicists, surface chemists, solid-state physicists, solid-state chemists, and electrical engineers. Fuel cell technology is quite promising for conversion of chemical energy of hydrocarbon fuels into electricity without forming air pollutants. There are several types of fuel cells: polymer electrolyte fuel cell (PEFC), phosphoric acid fuel cell (PAFC), molten carbonate fuel cell (MCFC), solid oxide fuel cell (SOFC), and alkaline fuel cell (AFC). Among these, SOFCs are the most efficient and have various advantages such as flexibility in fuel, high reliability, simple balance of plant (BOP), and a long history. Therefore, SOFC technology is attracting much attention as a power plant and is now close to marketing as a combined heat and power generation system. From the beginning of SOFC development, many perovskite oxides have been used for SOFC components; for example, LaMnO -based oxide for the cathode and 3 LaCrO for the interconnect are the most well known materials for SOFCs. The 3 current SOFCs operate at temperatures higher than 1073 K. However, lowering the operating temperature of SOFCs is an important goal for further SOFC development. Reliability, durability, and stability of the SOFCs could be greatly improved by decreasing their operating temperature. In addition, a lower operating temperature is also beneficial for shortening the startup time and decreasing energy loss from heat radiation. For this purpose, faster oxide ion conductors are required to replace the conventional Y O -stabilized ZrO 2 3 2 electrolyte. A new class of electrolytes such as LaGaO is considered to be 3 highly useful for intermediate-temperature SOFCs. Advanced mixed ionic electronic conducting (MIEC) perovskites play an important role in many electrochemical systems for advanced energy technologies. They are major components in such devices as solid oxide fuel cells (SOFCs), oxygen separation membranes, chemical sensors and catalysts. In addition to energy technology, the development of these multifunctional materials is of crucial importance for transportation, aerospace engineering, and electronics. The use of these materials as chemical sensors is also important for anti-terrorism initiatives. The present book discusses progress and problems in the development of ionic, electronic, and MIEC materials as active materials in advanced energy systems; the development and design of solid-oxide fuel cells (SOFCs) for next-generation vehicles, chemical sensors and oxygen separation membranes; and identifies directions for future research, such as conducting mechanisms, stability and reliability of devices, degradation problems, crystal structure, classification of phase transitions exhibited by the materials. This comprehensive handbook and ready reference details all the main achievements in the field of perovskite-based and related mixed-oxide materials. The authors discuss, in an unbiased manner, the potentials as well as the challenges related to their use, thus offering new perspectives for research and development on both an academic and industrial level. The first volume begins by summarizing the different synthesis routes from molten salts at high temperatures to colloidal crystal template methods, before going on to focus on the physical properties of the resulting materials and their related applications in the fields of electronics, energy harvesting, and storage as well as electromechanics and superconductivity. The second volume is dedicated to the catalytic applications of perovskites and related mixed oxides, including, but not limited to total oxidation of hydrocarbons, dry reforming of methane and denitrogenation. The concluding section deals with the development of chemical reactors and novel perovskite-based applications, such as fuel cells and high-performance ceramic membranes. Throughout, the contributions clearly point out the intimate links between structure, properties and applications of these materials, making this

an invaluable tool for materials scientists and for catalytic and physical chemists. This reference offers an overview of the bulk and surface properties of perovskite-like structures, and provides the latest discussions on the applications of these materials and processes. It also introduces ceramic methods for the processing of perovskite-derived high Tc cuprates.;Examining every available procedure for synthesizing high-surface-area perovskite oxides, this book: delineates processing techniques for preparing perovskite-derived high-critical-temperature superconductors; illustrates the relevance of physiochemical methods to investigate bulk and surface structures of perovskite compounds; explicates the importance of surface composition in the context of catalytic behaviour; summarizes methods of changing stoichiometry; shows how to design perovskite oxides for a given purpose; reviews key solid-state properties; and presents the major applications. In this thesis a number of novel perovskite-type oxynitrides (LaxCa1-xTiO3-xNx (x = 0 6 0.7), LaNbON2, SrMo(O, N)3, CaMo(O, N)3, BaMo(O, N)3) were synthesized and their structure, microstructure, physical properties and thermal stability were investigated. Simultaneous substitution of Ca2+ with La3+ and O2- with N3- in CaTiO3 leads to the oxynitride solid solutions of general formula LaxCa1-xTiO3-xNx. All these materials crystallize in a distorted perovskite unit cell. Their optical band gap varies linearly with Ca/N-content. The crystal structure, thermal stability, optical and photocatalytic properties of perovskite type oxynitride LaNbON2 were investigated. The material crystallizes in the distorted GdFeO3 structure type (space group: Pnma). It shows the smallest optical band gap among the early transition metal oxynitride-perovskites and high photocatalytic activity for hydrogen reforming from methanol among the reported oxynitride-perovskites. A number of novel conductive oxynitrides were synthesized. Oxynitrides of the general composition SrMoO3-xNx (x> 1) were synthesized by thermal ammonolysis of crystalline SrMoO4. According to the neutron and x-ray diffraction experiments the materials crystallize in the cubic perovskite structure (space group Pm-3m). X-ray absorption spectroscopy shows evidence of local distortions of the Mo(O, N)6 octahedra. The oxidation states of Mo determined by x-ray absorption near edge structure spectroscopy are lower than calculated from the oxygen/nitrogen (O/N) content. The disagreement arises from the higher covalence of the Mo-N bonding when compared to the Mo-O bonding ("chemical shift"). The electrical transport properties of SrMoO3-xNx (x> 1) are different from SrMoO3. It was found that the conductivity of the samples decreases with the increase of nitrogen content. The Seebeck coefficient values are up to 3 times higher than those of SrMoO3. Reactions of AMoO4 and AMoO3 (A = Ca2+, Ba2+) with ammonia were investigated at T = In this thesis a number of novel perovskite-type oxynitrides (LaxCa1-xTiO3-xNx (x = 0 6 0.7), LaNbON2, SrMo(O, N)3, CaMo(O, N)3, BaMo(O, N)3) were synthesized and their structure, microstructure, physical properties and thermal stability were investigated. Simultaneous substitution of Ca2+ with La3+ and O2- with N3- in CaTiO3 leads to the oxynitride solid solutions of general formula LaxCa1-xTiO3-xNx. All these materials crystallize in a distorted perovskite unit cell. Their optical band gap varies linearly with Ca/N-content. The crystal structure, thermal stability, optical and photocatalytic properties of perovskite type oxynitride LaNbON2 were investigated. The material crystallizes in the distorted GdFeO3 structure type (space group: Pnma). It shows the smallest optical band gap among the early transition metal oxynitride-perovskites and high photocatalytic activity for hydrogen reforming from methanol among the reported oxynitride-perovskites. A number of novel conductive oxynitrides were synthesized. Oxynitrides of the general composition SrMoO3-xNx (x> 1) were synthesized by thermal ammonolysis of crystalline SrMoO4. According to the neutron and x-ray diffraction experiments the materials crystallize in the cubic perovskite structure (space group Pm-3m). X-ray absorption spectroscopy shows evidence of local distortions of the Mo(O, N)6 octahedra. The oxidation states of Mo determined by x-ray absorption near edge structure spectroscopy are lower than calculated from the oxygen/nitrogen (O/N) content. The disagreement arises from the higher covalence of the Mo-N bonding when compared to the Mo-O bonding ("chemical shift"). The electrical

transport properties of SrMoO3-xNx (x> 1) are different from SrMoO3. It was found that the conductivity of the samples decreases with the increase of nitrogen content. The Seebeck coefficient values are up to 3 times higher than those of SrMoO3. Reactions of AMoO4 and AMoO3 (A = Ca2+, Ba2+) with ammonia were investigated at T = Hybrid Composite Perovskite Materials: Design to Applications discusses the manufacturing, design and characterization of organic-inorganic perovskite composite materials. The book goes beyond the basics of characterization and discusses physical properties, surface morphology and environmental stability. Users will find extensive examples of real-world products that are suitable for the needs of the market. Following a logical order, the book begins with mathematical background and then covers innovative approaches to physical modeling, analysis and design techniques. Numerous examples illustrate the proposed methods and results, making this book a sound resource on the modern research application of perovskite composites with real commercial value. Discusses the composition of perovskite materials and their properties, manufacturing and environmental stability Includes both fundamentals and state-of-the-art developments Features the main types of applications, including solar cells, photovoltaics, sensors and optoelectronic devices This textbook entitled Fundamentals of Perovskite Oxides: Synthesis, Structure, Properties and Applications summarizes the structure, synthesis routes, and potential applications of perovskite oxide materials. Since these perovskite-type ceramic materials offer opportunities in a wide range of fields of science and engineering, the chapters are broadly organized into four sections of perovskite-type oxide materials and technology. Covers recent developments in perovskite oxides Serves as a quick reference of perovskite oxides information Describes novel synthesis routes for nanostructured perovskites Discusses comprehensive details for various crystal structures, synthesis methods, properties, and applications Applies to academic education, scientific research, and industrial R&D for materials research in real-world applications like bioengineering, catalysis, energy conversion, energy storage, environmental engineering, and data storage and sensing This book serves as a handy and practical guideline suitable for students, engineers, and researchers working with advanced ceramic materials.

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