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The novel phenomenon of spin strain coupling in perovskite structures

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1 Abstract

The paper attempts at exploring the novel physical phenomenon yet unexplored. A background on the charge based vs. charge less logic is provided. Later, the computational and other methods are compared as viable techniques to explore the novelty. Finally, the coupling between the electron spin and crystalline lattice is discussed.

2 Introduction

Charge less spin-strain coupling in transition metal oxide perovskites is investigated by employing the first principle computational methods. Oxides of transition metals have ferroic properties which can be utilized for the novel logic design based upon the coupling between spin and elastic strain. Ferroic transition metal oxides exhibit wide range of ferroelectric, ferromagnetic and ferroelastic properties. The naturally occurring ferroic materials are very few. The ferroic properties of naturally occuring materials are weak as it was assumed that a competition exists between the the ferroelectric and ferromagnetic phases until fabrication of multiple composites. Composites of transition metal oxides are fabricated to enhance their weak ferroic properties.

Spin angular momentum is coupled with the elastic properties through atomic orbitals in these materials. However, the quantum mechanical explanation of the elastic coupling in a single and multiple phase ferroics is not fully understood.Attempts are made by scientists understand and enhance the mechanical coupling by fabrication of ferroic compistes. It is observed by testing and charcaterization of these composites that the elastic coupling can

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be strengthened 10-100 times by use of the nanocomposites of these materials. These nanocomposites possess ferroelectric, ferromagnetic and ferroelastic properties inside their respective bulk regions and the ferroic properties are elastically coupled at and across their interface. There has also been some attempts to investigate the causes of weak elastic coupling across the interfaces of these materials. The in-depth research is done in this study into the ferroic materials. An attempt is made to have a thorough understanding of the quantum mechanical origin of the elastic coupling between ferroic properties.

The elastic coupling of ferromagnetic properties in bulk, heterostructure, surfaces and interfaced structures is studied to know its quantum mechanical basis for developing new material designs.Investigation of elastic coupling by $firstprinciplescomputationalmethod$ is attempted with a basic hypothesis that the coupling has a quantum mechanical origin. As a direct consequence, the elastic coupling of the ferroic properties at and around the interface has led us to explore the novel material physics and electronic properties. First principles computations of bulk, composites, surfaces and interfaces of transition metal oxides are carried out. The objective is to understand the quantum mechanical basis of the weak elastic coupling in bulk composites and develop the novel method of material design to utilize the elastic coupling of phases. The computational results are tabulated, observation is done and inferences are based on the computational results.

The computational results substantiate our initial hypothesis about the quantum mechanical nature of elastic coupling. Therefore the elastic coupling between the ferromagnetic and elastic properties of transition metal oxides may be used for a chargeless logic. New ferroelastic properties would enable the novel chargeless spintronic applications. The devices based upon these materials can be operated by the application of electric, magnetic filed and elastic strain. These materials are also expected to increase the data storage capacity and miniaturize the GMR-based sensing devices.

Si microelectronics industry is struggling to maintain its progress. The current pace of miniaturization may eventually stall due to the reduction in the size of the integrated MOSFET which is reaching the critical atomic size. The number of transistors on a Si chip has followed as foreseen by Moor 's [1] law. It has resulted in an extremely small gate lengths of integrated MOSFETs. The trend of miniaturization in Si microfabrication industry is now severely constrained as the reduction in the gate length leads to the quantum mechanical tunneling and high electric field effects appear at the

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gate terminal of the MOSFET channel.

The number of transistors per Si chip as predicted by Gordon Moor 'has become very difficult to maintain due to the everincreasing trend of shrinking feature sizes of MOSFETs. The sub-100 nm gate length is now quantum mechanical and gate size may approach molecular or atomistic levels.

Appearance of high electric field and quantum mechanical tunneling at MOSFET gate results in the degradation of the MOSFET performance. Emergence of these secondary effects in a MOSFET strengthen the case in favor of the computational physics simulations for logic designs. The computational physics methods can assist in the development of new MOSFET and nanologics as these can predict a better understanding of these quantum mechanical effects. The device characteristics at sub-100 nm range do not follow MOSFET scaling laws as these were designed earlier by the Si micro fabrication industry for the bulk MOSFET. So, it is becoming a challenge to design the MOSFET with a sub-100 nm size without using the *ab-initio* computational methods.

As the quantum mechanics resulted in reducing the performance of a sub-100 nm MOSFET. So new logics must be modeled with ab-intio computational physics as a method to predict the new material properties appearing at atomic and molecular scale. A MOSFET transistor with a 35 nm channel size has reached a critical threshold making the first principle computational principles an effective tool for studying not only materials but considerable sections of a nanoscale device. This sets the stage for the first principle computational methods for their entry as tools to study the physically realizable atomistic and molecular level logic designs.

The designs using Si and GaAs materials to build a three terminal spintronic device is not realized. These junctions between Si, GaAs and transition metals has not succeed to materialize at room temperature. Till now, it has remained a challenge to inject, control and detect the electron spin in Si, GaAs, transition metals or combination of these materials. The spin injection in Si and GaAs has failed because of spin relaxation and de-phasing mechanisms due to scattering. Elastic properties of perovskite transition metal oxides can be coupled with the ferrromagnetic properties caused by the spin angular momentum of electron in transition metals. Oxides of transition metals act like magnetic semiconductors. It is observed from the computational results that ferromagnetic properties in transition metal oxides depend upon the position of atoms in a crystal structure. A change in the ferromagnetic and exchange energy is observed in transition metal oxides of Sc to Fe.

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The spin injection, transport and detection realized by coupling with elastic properties is expected to minimize the power power consumption. The philosophy of coupling between ferromagnetism due to electron spin and the elastic properties due to elastic strain in transition metal oxides boldly attempts the theoretical separation of electron charge and spin.

As we know that the magnetoresistance-based spintronics have been successfully implemented for data storage. These early spintronic devices provide a robust solution to existing challenge of high density data storage for the modern microprocessors. Although the spintronics technology based on magnetoresistance logic is relatively free from the challenges associated with the scaling and power consumption in comparison with Si CMOS logic. Magnetoresistance based data storage consumes negligible power as these are primarily based on the spin of an electron. However the flow of electrons parallel or perpendicular to the magnetic field results in the low vs. high resistance in these devices making them partially based upon the electron charge. The nanostructured thin fim of transition metals of Cr, Co and Cu are used in these devices making these highly efficient in spin alignment. Oxides of these materials, however, can also be utilized to separate the electron spin from charge. The efficient coupling of the spin exchange with the elastic properties of these magnetic semiconductors is studied.

Spintronic is also better than charge-based electronics as it is expected to assist Si based logic to maintain the trend as foreseen by Gordon Moore. Ferromagnetism due to electron spin dissociated from its charge may be injected through elastic coupling, transported by spin exchange and detected by elastic coupling. The single crystalline cubic and tetragonal structures of $BaTiO_3$, $BaFeO_3$ and $Ba_xFe_{1-x}TiO3$ are studied as materials of choice. The unit cells of these oxides are simulated by using CRYSTAL09 code.

ab-initio computations are highly adequate as the complex and fascinating new physics of ferroic materials can be explored [**?**] by employing these methods. The major focus of the research is to develop the methods and materials to explore the elastic properties of ferroic nano structures. We have computed elastic constants, bulk modulus and ferromagnetic properties 3-d transition metal oxides. The spin or charge dipole in ferroics are elastically coupled and methods are developed to observe their influence on ferromagnetism.

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3 Methods

The main focus of this research is to design a material for the efficient room-temperature spin injection, transport and detection mechanisms in a spin sensor at room temperature. The major portion of the research is focused on the structural and elastic properties of BaTiO3 and BaFeO3 and other 3-d transition metal oxides. These materials are designed for the coupling between ferromagnetic and elastic properties in a hypothetical spin device. For a hypothetical device,based upon the computational results showing ferroic properties, the electron spin is injected and detected from terminal made of a ferromagnetic $BaFeO_3$ transition metal oxide. The spin is exchange coupled through elastic properties inside a channel of $BaTi_xFe_{1-x}O_3$. A ferromagnetic material is assumed to detect the spins exchange coupled across the ferroic channel. Spin injection and detection in a hypothetical device is possible due to high magnetic moment of $BaFeO_3$. The issues of the resistance mismatch at injection and detection terminals in the hypothetical spin device may be minimized by maintaining the high quality single crystalline interfaces between injector, channel and detector. The spin transport inside the channel of the hypothetical device can be controlled by the application of an electric or magnetic field applied by a gate terminal attached with the channel. The electric field is expected to control the spin exchange inside a ferroic channel of a hypothetical device. The ferromagnetic properties of the injector, channel and detector regions are computed by employing the first principles computational techniques [2].

Our aim is to utilize the materials design for the novel spintronics based on the coupling between the spin and elastic properties. The single-phase ferroic material is a major challenge and the methods are used to analyze the physics and properties of oxides. We address the challenge of a ferroic materials by heterostructure of $BaTiO_3$ with other transition metals and oxides. Transition metals are introduced at particular sites material sites for spin exchange interaction.

An other challenge is the control over ferromagnetic properties spin through electric field. The issue of controlled spin-polarized transport is addressed by selecting a material that is proved to be a ferromagnetic and ferroelectric. The $Ba_{(x)}Fe_{(1-x)}TiO_3$ is computationally proved as a ferromagnetic material. This material has is expected to have its net spins polarized.

The spin-orbit coupling is a relativistic in nature and is basically a weak interaction. A robust spintronic logic based on the control of electron spin

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by electric field has not been possible at room temperature. The ferroic property of $Ba_{(x)}Fe_{(1-x)}TiO_3$ favors the control of spins through electric field. The magnetic as well as electric field can be used to control the electron spin. The main parts of the hypothetical device are source, channel and drain. The mechanical coupling through interfaces at injector-channel, gate-channel and channel-detector interfaces can be improved by the improvement in crystalline quality by the fabrication technology.

The $Ba_{(x)}Fe_{(1-x)}TiO_3$ injects a high number of spins due to spontaneous magnetization. The channel made from $Ba_{(x)}Fe_{(1-x)}TiO_3$ promises an efficient electric field control of spins. The interface properties of a material designed with the fabrication techniques and *ab-initio* modeling [2] is expected to increase the knowledge about the material.

The mechanical coupling of the ferroelectric and ferromagnetic material also necessitates understanding of elastic properties in these materials. The coupling among ferromagnetic and elastic properties is computed with *ab-initio* technique [**?**] to understand the effect of atomic positions at interfaces.

The placement of the channel and the detector, injector and gate contacts is critical for successful working of the device. The lateral injector and detector contacts are suitable, as spins can be injected and transported without any scattering losses. The fabrication technologies like hetero epitaxy, pulsed laser deposition and RF sputtering can fabricate defect-free interfaces between BaFeTiO3 for studying and implementing the device interfaces and device mechanisms. The impedance, magnetization, polarization, IR and Raman vibrations spectra for different compositions of the $Ba_{(x)}Fe_{(1-x)}TiO_3$ must be obtained and results must be compared for the most efficient design.

3.1 $ab-initio$ computational method vs. other models

Often the magnetoelectric bulk, bilayers and multilayers are modeled on the Maxwell's constitutive coupled equations. The electromagnetic and elastic properties are expressed the form of coupled field equations in these models. It is supposed that the ferroic properties are the result of the E and H fields. These fields are applied to a particular layer of the composite. The H and E fields are detected in the adjacent layer of the same composite. In this approach the spontanous spin, dipole and strain effects could not be separated from the external field effects. The ab-initio computational techniques is aimed to model the bulk, composites, bilayer and multilayer and their interfaces emphasizing the quantum mechanical aspects for the first time.

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We have observed that that the ferroic properties arise as a quantum mechanical effect due to the lattice strains in bulk and surface interfaces. The spin exchange arising due to the coulomb interaction between electrons occupying the parent atom and neighboring atoms with the effects arising due to the ionic cores of the parent and neighboring atoms are purely quantum mechanical.

Theoretical model apply the perturbation theory to model the interface between the ferroic bulk. The interfaces are expressed as a perturbative component in the complete Hamiltonian. The perturbative component represents the interactions at the interface between transition metal oxides. We did not apply the perturbation theoretical model. We employed the variational approach in computing the electronic structure and properties of ferroics. We are cautious in using the perturbation theory. The argument in support of the variational approach is based in our computational results of the electronic structure of transition metal oxides. The fact that the ferroic phases appear due to surface effects at an interface. The ferroic effect in composites of different phases, caused by the interfacial properties, make the task of computational modelling the most complex.

In quantum mechanical computations employing the perturbation and Monte Carlo methods, the interface is modeled as a sum of all the coupled quantum harmonic oscillators representing the material interactions on each side of the interface and interacting across it. The external photons injected from an electromagnetic field perturb these harmonic oscillators to vibrate at the frequency of the external field.

The ab-inito Hartree Fock and DFT potential is employed and the model is based on the computational results. CRYSTAL09 code employes the variational approach to compute the structure and property of a pure $BaTiO_3$, $BaFeO_3$ and $Ba_(x)Fe_(1-x)TiO_3$ and other 3-d transition metal oxides. These material structures injector, detector and transport channels consist of spin-spin exchange terms and spin-lattice interaction terms. It should be mentioned that the effect of external field is is important to the nature of interface interactions between the spin injector, detector and channel regions. These small displacements are computed by ab-initio computational techniques done with Crystal06 [2]. The results of the elastic computations are critical to the understanding of the mechanical coupling available at interface.

We have explored a computational physics method to investigate the ferroic properties of batio3. Till now the Maxwell's constitutive coupled equations were widely employed to express the ferroic properties. We have

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employed ab-inito computational techinques to explore the ferromagnetism in ferroic transition metal oxides. Moreover, the computations of electronic structure and properties of nano-structured ferroic materials enable us to express the ferroic structures by the novel *ab-inito* Hartree Fock and DFT models for bulk, surfaces and interfaces.

3.2 *ab-initio* computations

The perovskites are an important class of materials which have potential to find applications in the fields of memory, logic design and switching. However, the theoretical exploration of these materials is not on par with their technological importance. Crystalline $BaTiO_3$ possesses a perovskite geometry which may occur in cubic, tetragonal, rhombohedral and orthorhombic crystalline phase. There is a general lack of the data on the mechanical properties of all phases of $BaTiO_3$. However, there have been attempts [3] to understand the electronic and mechanical properties of this material. The computations of elastic constants and bulk modulus were done by Piskunov *et al* [4] by *ab-inito* computational method for cubic $BaTiO_3$.

At room temperature, $BaTiO_3$ has tetragonal crystalline geometry. In the past, the elastic constants and bulk modulus of tetragonal $BaTiO_3$ could not be computed due to the complexity of these computations. In this paper, the computations of elastic constants and the bulk modulus of tetragonal $BaTiO_3$ are done with *ab-initio* Hartee Fock (HF), density functional theory (DFT) and hybrid potentials. The *ab-initio* computational techniques are employed effectively due to recent advancements in basis sets, geometry optimization, and computational power.

In this work, the computations of the tetragonal phase of $BaTiO_3$ are made with the CRYSTAL09 code using a variety of basis sets. The CRYSTAL09 code has the unique characteristic to employ the Hartree-Fock (HF), exchange correlation potentials and the effective combination of the former with the latter. In addition, the availability of a variety of basis sets and geometry optimization techniques further enhances the efficiency of these computations.

An important factor that affects the efficiency of computation is obtaining the optimized geometry of the crystalline structure. The geometry optimization of the tetragonal phase of $BaTiO_3$ is an essential step during computations of elastic constants and bulk modulus. The total geometry optimization is done to optimize the atomic positions and lattice parameters

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of the unit cell of tetragonal $BaTiO_3$. These special features of the geometry optimization in the CRYSTAL09 code [5] makes it an efficient program to achieve the optimum computational results.

The computations of the bulk modulus are done independently with ELASTCON and EOS programs. These programs employ the geometry optimization techniques available in the CRYSTAL09 code. The ELASTCON algorithm determines the number of crystalline deformations based upon the crystalline geometry of tetragonal $BaTiO_3$. Geometry optimization of the crystalline structure is carried out after each deformation. The analytic first derivative, numerical second derivative and Levenberg Marquardt (LM) curve fitting is done in sequence to compute elastic constants for the tetragonal $BaTiO_3$. A detailed discussion of the ELASTCON program can be seen in ref. [6].

The equation of state algorithm is utilized for computation of bulk modulus from a pressure vs. volume curve. The range of volumes around the optimized equilibrium may be selected by the input parameters available in the EOS program. The computation of total energy is then done for this range of volumes. The geometry optimization is done for each volume while keeping the volume constant. The computation of elastic constants and bulk modulus of tetragonal $BaTiO_3$ is complicated due to its crystalline geometry and the position of the atoms in the perovskite crystalline structure. With the lowering of crystalline symmetry the number of elastic constants increases and geometry optimization steps are increased.

The crystalline geometry of the tetragonal $BaTiO_3$ must be fully optimized during the computation of the elastic constants and bulk modulus. This is possible only if the tetragonal crystalline system is relaxed during each individual computation. The task of crystalline geometry optimization of the perovskite $BaTiO_3$ has remained a challenge as the crystalline system undergoes a sudden decrease in energy when it is deformed. The ELASTCON algorithm has detected this sudden decrease in the strain vs. energy computations as reported earlier [3, 7, 8]. Detailed energy vs. strain computations were carried out to explore the sudden decrease in energy. The ELASTCON algorithm issues a warning message if there is an abrupt and unexpected change in the energy during optimization which helps to understand the optimization process further.

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3.3 ELASTCON and EOS programs in CRYSTAL09 code

The computation of elastic constants and bulk modulus is an automated process in ELASTCON program and is determined from the crystalline symmetry of tetragonal $BaTiO_3$. Deformations are applied depending upon the tetragonal crystalline geometry. The analytic first derivative and the numerical second derivative of total energy are computed for each deformation. The Levenberg Marquardt (LM) curve fitting [9] is used to compute the elastic constants and bulk modulus.

The linear deformation of solids is expressed by Hooke's law as

$$\sigma_{ij} = \sum_{kl} C_{ijkl}\epsilon_{kl} \tag{1}$$

where $i, j, k, l = 1, 2, 3$, $\sigma_{i,j,k,l}$, $\epsilon_{k,l}$ and $C_{i,j,k,l}$ are stress, strain and second-order elastic constant tensors.

The second-order elastic constants may be computed with different techniques. The molecular dynamics and *ab-initio* computational techniques are two prominent methods to compute the elastic constants and bulk modulus. The *ab-initio* computational techniques compute the second-order elastic constant (SOEC) from the total energy. The elastic constants can be computed from the Taylor series expansion of the total energy with respect to the applied strains, as shown in Eq. (2). The Taylor series terms up to the second-order may be utilized for the estimation of the elastic constants and bulk modulus if the strains are very small and the higher order terms have negligible effects on the computational results.

$$E\left(V, \epsilon\right) = E(V_0) + \sum_{\alpha} \sigma_{\alpha}\epsilon_{\alpha} + \frac{V}{2}\sum_{\alpha\beta} C_{\alpha\beta}\epsilon_{\alpha}\epsilon_{\beta} + ... \tag{2}$$

The terms $\alpha, \beta = 1, .., 6$ express the elastic constants in Voigt notation and V_0 is the equilibrium volume. In Eq. (2), the non-zero stress term may be ignored if the crystalline geometry of the system is fully optimized. The third term in Eq. (2) can be rewritten to express the elastic constant as the second derivative of the total energy with respect to the applied strain in a crystalline direction

$$C_{\alpha\beta} = \frac{1}{V}\frac{\partial^2 E}{\partial\epsilon_{\alpha}\partial\epsilon_{\beta}}\bigg|_0. \tag{3}$$

In Eq. (3), the terms $C_{\alpha\beta}$, E, and V express the elastic constant tensor, energy and volume of the crystalline structure, respectively.

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The *ab-initio* computations are done by calculating the analytic first derivative of the total energy and numerical second derivative with respect to the applied strain. The appropriate number of strains are applied in a systematic manner, the elastic constants are calculated, and the compliance coefficients are computed from Eq. (4). The compliance coefficients are then utilized for the computation of the bulk modulus as shown in Eq. (5).

$$[S] = [C]^{-1} \tag{4}$$

$$B = 1/(S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{13} + S_{23})). \tag{5}$$

The terms S_{ij} and B in Eq. (5) express the compliance tensor elements and bulk modulus respectively.

The EOS algorithm in CRYSTAL09 computes the energy for a range of volumes around the optimized equilibrium volume. The Crystal09 code is equipped with a wide variety of equations of state such as Birch Murnaghan, 3rd order Birch Murnaghan, logarithmic, Vinet and polynomial. In this paper, the 3rd order Birch Murnaghan equation of state algorithm was utilized for computing the bulk modulus from the energy vs. volume computations as expressed in Eq. (6):

$$E(V) = B_o V_o \left[\frac{1}{B'(B'-1)} \left(\frac{V_o}{V} \right)^{B'-1} + \frac{V}{B'V_o} - \frac{1}{B'-1} \right] + E_o. \tag{6}$$

In Eq. (6), V_0 represents the volume at the lowest energy, B_0 is the bulk modulus at pressure $P = 0$, $B^{'}$ is the derivative of bulk modulus B at $P = 0$ and E_0 is the minimum energy. The optimization of crystalline geometry at each step is done during energy-volume (E-V) calculations. The bulk modulus results are obtained with Levenberg-Marquardt curve fitting of the E vs. V computations.

4 *ab-initio* computations of spin-strain coupling

The success of giant magnetoresistance (GMR) effect based devices has revived the interest in chargeless spin strain coupling in single and multiple phase of ferroics. Sirinivasan has explored the theoretical and experimental aspects of coupling in the thin films of ferroelectric and ferromagnetic composites. Tsymbal has also carried out the first principles computations and

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fabrication of the interfaces between Fe and $BaTiO_3$. Sirinivasan and Tsymbal have discovered that the coupling between multiple phases is enhanced due to the elastic strain, atomic orbitals, chemical bonds at the boundary between the ferroelectric and ferromagnetic phases.

It has also been reported in $La_xCa_{1-x}MnO_3$ that more than one phase can coexist in manganites due to compression of the lattice structure. Compression or expansion of the octahedral cage due to the change in the cation versus anion radius determines the phase transition from one phase to the other in manganites [**?**].

The studies of transition metals and their oxides by Goodenough and C. N. Rao is mainly focused on highly correlated transition metal orbitals. Tokura has also emphasized the interaction between the electron orbitals, crystalline lattice and pressure in the phase change of transition metal oxides. That work represents a detailed theoretical and experimental study of orbital electronics.

It is important to note that Sirinivasan and Tsymbal have performed the seminal research on the role of elastic strains, atomic orbitals and chemical bond in the field of phase coupling in ferroics. However, the detailed understanding of the interdependence between the elastic strain, atomic orbital, chemical bond and spin exchange has not been explored due to its complexity.

Numerous attempts have been made by Sirinivasan, Tsymbal and other researchers to model and fabricate thin film composites to couple the ferroelectric and ferromagnetic phases. The experiments on the elastic coupling of these thin film composites of separate phases have resulted in the weak coupling.

To the best of our knowledge, there has been no attempt to study the coupling between the ferromagnetic spin exchange and bulk strain in cubic perovskites. There is also a lack of systematized scientific theory and methods to understand the real causes of the weak coupling across ferroics.

The coupling between the electron spin and bulk strain is explored in the cubic crystalline structures of a wide variety of transition metal oxides. First principles computational techniques are employed to compute the spin exchange coupling with the compression or expansion of the periodic crystalline lattice structure. The unrestricted Hartree Fock method is employed for the computation of ferromagnetic and antiferromagnetic spin exchange. The coupling between the ferromagnetic, antiferromagnetic spin exchange and lattice strains is computed for a wide range of 3-d transition metal oxide perovskites.

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Studies of the lattice constant, spin resolved density of states, band gap and other electronic properties have been performed by first principles computational techniques. We have employed the first principles computational techniques to the exchange energy for the ferromagnetic and antiferromagnetic spin exchange in the bulk $BaScO_3$, $BaTiO_3$, $BaVO_3$, $BaCrO_3$, $BaMnO_3$ and $BaFeO_3$.

These materials are chosen carefully to a wide range of transition metals for understanding the role of elastic strains on the exchange energy. The supercell is utilized to compute the change in ferromagnetic and antiferromagnetic exchange energy. The compressive and tensile strains are introduced by decreasing or increasing the experimental lattice constant for each transition metal oxide in steps of .005 Angstrom.

5 Conclusion

The paper explores the novel coupling between the electron spin and lattice in transition metal oxides ocuring in perovskite transition metal oxides. The novelty of the method and the complexity of the materials as well as their complex crystalline structure have been some of the reasons why these materials and their crystalline structures have remained unexplored. Nevertheless an attempt has been made to explore a novel physical phenomenon. A partial success have been achieved as a series of the transition metals have been explored for their coupling between the electron spin and the lattice. The novel pheonomenon and the technique need to be applied further to explore other materials to test the validity of the technique and hence generalize the research technique applied on perovskite crystals of transition metal oxides.

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