Experimental and theoretical study of electronic, magnetic and mechanical properties of Cubic LaMnO$_3$ under extreme stress

Nisar Ahmed$^1$, Ayaz Arif$^2$, Sikandar Khan$^1$, Surayya Mukhtar$^3$, M H Nasim$^1$, Fida Rehman$^4$, M Shafiq$^4$, A Laref$^5$ and Y Saeed$^4$

$^1$ Department of Physics and Applied Mathematics (DPAM), Pakistan Institute of Engineering and Applied Sciences (PIEAS), Nilore, Islamabad, Pakistan
$^2$ Department of Physics, University of Azad Jammu and Kashmir, Muzaffarabad, Pakistan
$^3$ Department of Physics, Allama Iqbal Open University, Islamabad, Pakistan
$^4$ Department of Physics, Abbottabad University of Science and Technology, Havelian, Abbottabad, KPK, Pakistan
$^5$ Department of Physics and Astronomy, College of Science, King Saud University, Riyadh 11451, Saudi Arabia

E-mail: yasir.saeed@kaust.edu.sa

Keywords: ab initio, magnetic materials, LDA + U, DMFT

Abstract

Stable LaMnO$_3$ (LMO) is successfully synthesized in cubic phase by hydrothermal process. The x-ray diffraction (XRD) results obtained are Rietveld refined which gives the best fit for cubic symmetry with space group Pm$ar{3}$m. Experimentally obtained lattice parameters were used to further investigate electronic, magnetic and elastic properties under extreme stress using Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method within density functional theory (DFT). The experimentally observed lattice parameter is optimized by different exchange and correlation functional including LSDA, LSDA + U, GGA, and GGA + U. Also, the dynamic mean field theory (DMFT + DFT) is also employed to optimize the lattice parameter at room temperature which is in good agreement with experimental results. The electronic structure of the system depicts a half-metal to metal transition at 40 GPa. Elastic constants result shows that the cubic LMO is stable under hydrostatic pressure up to 50 GPa. This study provides important contribution in understanding the nature of cubic LMO which is a potential candidate for spintronic devices.

Introduction

Perovskite type oxide crystals, generally represented by notation ABO$_3$ ($A = \text{La, Sr, Ca}; \ B = \text{Mn, Co}$) exhibit very interesting properties such as ferroelectricity, piezoelectricity and conductivity. LaMnO$_3$ (LMO) is an example of this group which is mainly used as cathode material for fuel cells, colossal magnetoresistance and in spintronics domains. The perfect perovskite has cubic symmetry with space group $pm\bar{3}m$. Above 750 K LMO has cubic structure and below 750 K, the structure is orthorhombic [1].

LMO shows complex physical properties due to interplay between charge, magnetic order, and structural stability. Several theoretical studies have been done regarding LMO by adopting different methods to understand various properties of this novel material. Electronic structure and magnetism of cubic phase of LMO was calculated by using the FP-LMTO method [2]. It was found that there are some states at Fermi level for both spin channels, showing metallic character of the compound. Theoretical study based on density functional theory (DFT) was done to investigate electronic and atomic structures of surfaces of the LMO crystal, for both cubic and orthorhombic phases using generalized gradient approximation (GGA) plane wave approach [1]. First principle calculations of electronic structure the bulk LMO were performed using several methods, including GGA [3], the APW+lo method [4], HF LCAO [5, 6] and the relativistic full potential- GGA LAPW method [7]. The PAW method was employed to investigate the magnetic properties of LMO [8]. It was found that the ferromagnetic (FM) state is more stable than the antiferromagnetic (AFM) state, establishing that the ground state of the cubic perovskite LMO structure as FM.

© 2020 IOP Publishing Ltd
Elastic properties demonstrate structural and phase stability of the compound. A small change in chemical composition by either change in ratio of divalent and trivalent atoms at A site or change in ionic radii in ABO₃ compounds can bring change in their physical properties. Therefore, understanding of elastic properties is key point for investigating more complex physical properties [9]. From the literature, extensive theoretical study has been done to investigate the electronic and magnetic properties, but still little attention is paid to explore the elastic properties of LMO. Temperature dependent behavior of elastic constants led to conclude anharmonicity in the RMnO₃ perovskite (R = La, Sr) [10]. It was found that elastic modulus of these perovskite decreases with increasing temperature. Structural stability and elastic constants for cubic LMO were calculated and it was found that the bulk modulus for FM phase was relatively higher than the AFM phase indicating that the FM phase is less hard than the nonmagnetic (NM) phase [2]. Doped LaMnO₃ and SmCoO₃ are important for solid oxide fuel cell cathode materials [11].

In this work we present pressure dependent elastic and electronic properties which are not studied yet. The behavior of LMO under extreme pressure is studied through not only DFT with GGA and GGA+U approximations but also using DMFT optimization of lattice parameter at 300 K and a comparison of spectral function are made at ambient pressure and 50 GPa. The experimental values of lattice parameter are further used to explore band structure, magnetic and elastic properties of LMO at high pressures under density functional theory premises.

Experimental methods

In a typical preparation, an aqueous solution was prepared by dissolving the manganese nitrate (21.58 gram) and potassium manganese oxide (1.2 gram) in 100 ml double distilled water (ddH₂O). Then lanthanum oxide (26.93 gram) was dissolved in 100 ml nitric acid. The prepared solution was mixed in evaporator flask and stirred for two hours. Finally, 1.5 gram of Cetyltrimethyl ammonium bromide (CTAB) was added and further stirred for 30 min. During this process the pH between of the solution is maintained 10 and 11 and 10M sodium hydroxide (NaOH) is added dropwise. After mixing of solutes, the resulting solution was kept at 180 °C for 10 h in PTFE-lined stainless steel high-pressure auto-clave. After hydrothermal process (reaction) the solution the autoclave was cooled naturally to 25 °C. Hence a black product was obtained which then dried and calcined at 1200 °C.

The XRD data were collected in 2θ range from 10° < 2θ < 80° by a small step size of 0.05° with a slow rate (5° min⁻¹). Micro structural features of both samples were observed by SEM 'Jeol JSM-6510 LV'.

Computational methodology

After synthesis and characterizations of LMO in cubic phase we performed DFT calculations for the electronic structure, magnetism and elastic properties under extreme pressure (upto 60 GPa). FP-LAPW technique is the most accurate method employed to solve Kohn–Sham auxiliary system of many electrons within self-consistent field. Generalized Gradient Exchange and Correlation approximation functional PBE-GGA along with onsite coulomb repulsion U has proved to be the best method to treat strongly correlated electrons [12]. These methods have been implemented in WIEN2k codes [13]. The FP-LAPW DFT has been extensively employed to investigate the electronic and magnetic properties of different systems under pressure [14–19]. The radii of muffin tin (MT) spheres were considered as 2.5 for La, 1.99 for Mn and 1.71 a.u. for O. The self-consistent filed cycle (SCF) converged when the total energy was converged within 10⁻⁵ Ry for three consecutive iterations and charge was within 10⁻⁶ e for two consecutive iterations. A fine grid of 21 × 21 × 21 k-points with 286 k-points in irreducible wedge of the Brillouin zone.

It is well known that DFT usually fails to identify electronic structure (e.g. bandgap) of transition metal oxides. Normal exchange correlation functionals such as LDA or GGA are unable to correct the problem of electron self-interaction, resulting in a metallic characterization of perovskites [20–22]. To overcome this problem, we used on-site Coulombic interaction (DFT + U) for 3d-electrons in Mn, to correct this problem. We used Dudarev’s method [23] in this work, where empirically an efficient Hubbard parameter (Ueff) is equipped. For LaMnO₃, according to the previous literature, Ueff = U − J = 3.9 eV was applied to Mn d-orbitals [24]. Pressure dependent Elastic constants (EC) can be calculated using energy method, for details see our previously work in references [25, 26].

Standard DFT treat a system at 0 K, while the phase we stabilized is room temperature allotrope of LMO. Dynamical mean field theory (DMFT) coupled with DFT as implemented in EDMFT. EDMFT is the combination of DFT and DMFT, which is derived from the stationary Luttinger–Ward functional, the method is quite effective and gave good results. The single-particle Green’s function is expanded in the FP-LAPW basis and determined self-consistently (including self-consistent electronic charge). This implementation is designed in a
more precise way that keeps the stationarity of the original functional along with the locality of the correlations in real space [27–31]. The algorithm also implements the exact double-counting of DFT and DMFT. A CTQMC impurity solver was used to simulate the auxiliary problem relating to green functions in EDMFT approach. This EDMFT has been employed to estimate the lattice parameter at finite temperature (300 K) along with GGA and GGA+U methods. 3d electrons of Mn are treated dynamically in DMFT calculation because these show strongly correlated behavior in manganite. The calculations are performed with a strict criteria of charge and energy precision. The charge is accurate within \(5 \times 10^{-6}\) e and the energy is accurate within \(5 \times 10^{-6}\) Ryd. The value of the on-site Coulomb repulsion (Slater F0) is taken as 10. Note that in the charge self-consistent DMFT, one needs larger value of U than it is required for down-folded DMFT calculations, because part of the on-site screening (hybridization screening many itinerant states) is explicitly taken into account in such DMFT calculations. The Hund’s coupling parameter J is taken as 1.14. We expand the Green’s function in the basis of
the SVD of the analytic-continuation Kernel. We have used 25 functions, which are enough for most cases, and used the direct sampling in the Matsubara frequency.

Results and discussion

Crystal structure

Figure 1 show the XRD pattern for LMO sample calcined at 1200 °C. The Rietveld method as implemented in the Rietica code was used for the refinement of the powder XRD data of sample. The experimentally observed diffraction intensities (black dots) along with the calculated intensities (i.e. refinement red lines), their difference (blue line), and the Bragg positions are presented in figure 1. The crystal structure of sample was refined as cubic perovskite with cell parameters \( a = 3.89025 \text{ Å} \), unit cell volume \( = 58.875 \text{ Å}\(^3\)\), and space group \( \bar{pm}3m \) per standard JCPDS-750440. Reliability factors along with goodness of fit are listed in table 1 (in parentheses). No other phase of LMO is detected in the XRD pattern.

The average crystallite size was estimated from broadening of single line index of 110 plane positioned at \( 2\theta = 32.65^\circ \) in the x-ray pattern according to Scherrer’s formula \[33\]. The average size of crystallites was estimated as 27.40 nm.

The morphological features of the prepared sample were investigated by scanning electron microscopy (SEM). From the SEM images (figure 2), it is disclosed that the grains in LMO are mostly well intermixed and connected. Some grains have well defined geometrical shapes and sharp grain boundaries. The pore size is different at different positions, but average pore size is less than 0.5 μm.

For comprehensive exploration of physical properties of LMO, we have optimized this experimental lattice parameter using DFT, employing various exchange and correlation functional like GGA, LSDA, GGA+U, and

![Figure 3. Theoretical optimization of lattice parameter of LMO using different Exchange and Correlation approximation.](image-url)
The EDMFT has also been employed for optimizing lattice parameter. DMFT has been successful in predicting correct phases of strongly correlated systems, especially for manganites [32]. These values along with other results of lattice parameters are presented in table 1.

**Electronic and magnetic structure**

Electronic structure calculations are important to know the fundamental phenomena and properties of solids. We can understand macroscopic behavior of materials via knowledge of electronic structure and magnetic properties at micro scale. The behavior of LMO under stress has been studied using DFT, DFT + U and EDMFT, and it is observed that it sustains half metallicity up to 40 GPa, then a half-metal to metal transition takes place at 40 GPa. This is depicted in total density of states (TDOS) and electronic Band structures at different pressures (figures 4, 5 and 7). Such transitions have already been reported in Cd$_{1-x}$Cr$_x$Z ($Z = S, Se$ and $Te$) systems [34]. The spin polarization is 100% up to transition pressure and then becomes negative which shows that materials response has been suddenly changed at this point, similar behavior can also be seen in elastic properties discussed in next section. Pressure induced charge disproportionation in LMO is discussed in [35] without considering the Jahn-Teller distortion. The electronic band structure shows that valence band is made up of mainly Mn $d$ states, the VBM and CBM both lie on $\Gamma$ point that is there is a direct band gap in minority spin channel. Fermi level shifts when stress is applied this shift can be seen in figures 4, 5 and 7 and in table 2. Due to this shift $d - t_{2g}$ states start crossing Fermi level at 40 GPa. We have fixed the Fermi level at 0 eV by subtracting $E_F$ from the total energy for comparison of density of states at different pressures.

The Fermi surfaces have been drawn and analyzed using Supercell k-space Area Finder (SKSAF) program shown in figure 7. There are mainly two bands which cross the Fermi level we name them band 22 and band 23 in majority spin channel. The band 22 reduces its like character from 100% to 92% gradually under pressure. Band 23 is 97% electron like and it becomes 100% electron like. The Fermi surface for band 22 is multiply connected surface consisting of various cusps which represents hole-pockets at the corners and edges of the Brillouin zone. Band 23 is multiplying connected surface which contains tubular links at the Brillion zone faces. These links which give rise to open orbits gradually vanish with increasing pressure, hence forming a closed electron pocket centered around $\Gamma$ at 40 GPa.

The qualitative picture of the electronic band structures of LMO at different pressures can be portrayed by the fact that in full cubic symmetry, $t_{2g}$ and $e_g$ orbitals are triply and doubly degenerate, accordingly. These degenerate states are shown in figure 7, where we can see that the $t_{2g}$ states are narrow and away from $E_F$. The electronic band structure is given under pressure in the figure 7, the energy eigen values are plotted against wave vector. The path of the k-mesh along high symmetry points and directions is shown in figure 6 $\Gamma$-X-M-$\Gamma$-R. the valence band is built up of Mn 3$d$ states which are hybridizing with O-p states. The gap increases with increasing pressure with a shift of Fermi level. This shift is continued until at 40 GPa the $d-t_{2g}$ states start crossing the Fermi level.
We have also studied magnetic properties of LMO under pressure. The ground state remains ferromagnetic half-metal (FHM) up to 40 GPa where it transforms to ferromagnetic metal (FM). The difference between AFM and FM states is given in table 2. This difference is also responsible for high Curie temperature $T_C$. The total spin magnetic moment decreases from 4.0 to 3.86 on the onset of phase transition. The integer total magnetic moment of Mn is a consequence of half metallicity, and when material transforms from half-metal to metal, the magnetic moment decreases from whole number to a fraction $^{36}$. 

**Figure 5.** Partial DOS of La, Mn and O at different pressures using FPLAPW method with GGA+U functional.

**Figure 6.** Construction of high symmetry wedge within Brillouin zone of $pm3m$ space group for LMO.

**Table 2.** $\Delta E = E_{AFM} - E_{FM}$, Fermi Energy $E_f$, spin polarized DOS, Spin Polarization $P$, Energy band gap $E_g$ in majority spin channel and spin magnetic moment.

| Pressure | $\Delta E$ (meV) | $E_f$ (eV) | $D^z(E_f)$ States/eV | $D^z(E_g)$ States/eV | $P$ | $E_g$ eV | Spin magnetic moment ($\mu_B$) |
|----------|-----------------|------------|---------------------|---------------------|-----|--------|-----------------------------|
| 0        | 299.86          | 9.82       | 0.5434              | 0                   | 1   | 3.18   | 4.00                        |
| 10       | 292.02          | 11.07      | 0.5147              | 0                   | 1   | 3.32   | 4.00                        |
| 20       | 283.08          | 11.95      | 0.4948              | 0                   | 1   | 3.40   | 4.00                        |
| 30       | 271.63          | 12.81      | 0.47059             | 0                   | 1   | 3.46   | 4.00                        |
| 40       | 258.25          | 13.60      | 0.44191             | 0                   | 1   | 0.00   | 4.00                        |
| 50       | 240.66          | 14.30      | 0.3897              | 0.55441             | −0.174 | 0.00   | 3.869                      |
| 60       | 223.96          | 14.86      | 0.36029             | 0.57647             | −0.231 | 0.00   | 3.672                      |
The momentum resolved total spectral functions at 0 and 50 GPa, are presented in figure 8. EDMFT has been employed at 300 K for the calculations of spectral functions. As the EDMFT calculations are computationally very expensive and converge very slowly, so calculations are performed only at two pressures just to confirm the GGA+U behavior to be realistic. The features already presented in figure 7 can be seen in spectral function. The $t_{2g}$ states are present there at Fermi level at 0 GPa and then at 50 GPa the Fermi level has $e_g$ states. The conduction band has states which move away from Fermi level previously residing at 4.5 eV, this means that CBM in majority spin channels shifts upward, while at the same time Fermi level starts crossing $e_g$ states in minority spin channel. The pressure affects the electronic structure of the materials in very interesting manner.

**Elastic properties under pressure**
Elastic constants $C_{ij}$ of a solid give information about the behavior of solids under different stresses and deformations. Second order elastic constants for LMO under stress have been calculated using GGA and

![Figure 7. Electronic Band Structure and Fermi surfaces of LMO under different pressures.](image)
GGA + U method and presented in figure 9. Our calculated second order elastic stiffness constants under pressure (0 GPa to 50 GPa) of LMO satisfy the generalized stability criteria initiated by Born \[37\] for cubic crystal structures, i.e., \(C_{11} - C_{12} > 0\); \(C_{44} > 0\); \(C_{11} + 2C_{12} > 0\). The fulfillment of these criteria shows that LMO is elastically stable under pressure. It is observed that \(C_{ij}\) increase monotonically with increasing pressure in both of GGA and GGA + U studies except \(C_{12}\) which first increase up to 40 GPa and then decreases, the reason for this is the transition from half-metallic state to fully metallic state.

The trend of the mechanical properties of a material could be estimated from its elastic constants. The main mechanical parameters i.e. shear modulus \((G)\), Young’s modulus \((Y)\), Pugh’s ratio \((B/G)\), Cauchy’s pressure \((C^\prime)\), Poisson’s ratio \((\nu)\) and anisotropic ratio \((A)\), which are important for industrial applications are calculated and presented in table 3. All the parameters are calculated under pressure ranging from 0 to 50 GPa. These important parameters are used to characterize the mechanical behavior of a material.

Shear Modulus \(G\) show the rigidity of the materials. It is clear from the table 3 that rigidity of LMO compound increases with increase in pressure. The larger the value of Young’s modulus \((E)\), the stiffer the material will be. One can see from table 3, that stiffness of LMO enhance as the pressure increases. The bulk modulus values in table 3 indicate that the materials under study show lower compressibility as the pressure increases.

The Pugh’s criterion \((B/G\) ratio\), describes a material’s ductility/brittleness behavior. The critical value for ductile/brittle character is 1.75. Our calculated \(B/G\) values for all pressure are greater than 1.75, so LMO behaves in a ductile manner under stress. The Cauchy pressure \((CP)\) defined as \((C_{12} - C_{44})\) is also a criterion for a
material’s ductility. A positive value of CP reveals damage tolerance and ductility of a solid, and material is brittle otherwise. The calculated values of CP for LMO being positive with GGA+U (which in our opinion are more accurate than GGA), strongly suggest the ductile behavior, and indicates angular type of atomic bonding in LMO at ambient and elevated pressure [32].

The Poisson’s ratio ($\nu$) usually quantifies the stability of a crystal against shear strain. The lower and upper limits for force among atoms to be central forces are 0.25 and 0.5 respectively. For LMO at all pressure (0–50 GPa), Poisson ratio remains between the limits 0.29–0.23, and decreases with increasing pressure, this shows that the interatomic forces are central and remain central up to 50 GPa. For brittle materials $\nu > 0.35$ [34]. The Poisson ratio for LMO is less than 0.35 at all pressure, which further confirm the ductile behavior of this material.

Anisotropic ratio ($A$) measures the elastic anisotropy of a material is a very important property and is related to the induced micro cracks in a crystal. For isotropic materials $A$ must be 1. From table 3 it is evident that values of anisotropic ratio are deviated from unity. Therefore, LMO compound is elastically anisotropic at all pressure and its properties are directions dependent.

### Conclusions

This study is an endeavor to explore electronic structure, magnetic, elastic and mechanical properties of LaMnO$_3$ under pressure. The cubic phase of LMO is synthesized by the hydrothermal method. Crystal lattice and morphology of the sample has been analyzed by XRD (Rietveld fitting) and SEM, respectively. Then state of the art FP-LAPW method within DFT using GGA, GGA+U and DFT + DMFT ($T = 300K$) approximations are employed for the investigation of electronic, magnetic, and mechanical properties under pressure using GGA+U. The study reveals the half metallic ferromagnetism is sustained up to 40 GPa and the at 40 GPa a half metal to metal transition occurs. The elastic constants show that cubic LMO is stable upto 50 GPa using GGA and GGA+U. At high pressures the difference in $C_{11}$ values for both approximations become more significant. This is a consequence of strong correlations of 3$d$ electrons of Mn, which are treated in more correct way with GGA+U approximation. The study is important and significant contribution in understanding the nature of cubic LMO which is a potential candidate for spintronic devices.

### Acknowledgments

The authors would like to thank IT department of National Centre for Physics (NCP), Islamabad for supplying computational resources. The author Nisar Ahmed gratefully acknowledges the financial support of the Higher Education Commission (HEC), Pakistan for PhD (Indigenous) Fellowship under scholarship No. 112-25387-2PS1-477/HEC/Ind-Sch-Phase-II/2012. The author A Laref acknowledges support from the ‘Research Center of the Female Scientific and Medical Colleges’, Deanship of Scientific Research, King Saud University.

### ORCID iDs

Ayaz Arif © https://orcid.org/0000-0001-5104-5741
Surayya Mukhtar © https://orcid.org/0000-0003-2066-2565
Y Saeed © https://orcid.org/0000-0003-3080-7385

### Table 3. Elastic Constants, Bulk and Shear Moduli, Poisson’s ratio and anisotropy of LMO at different pressures using FP-LAPW method with GGA+U functional.

| $P$ (GPa) | 0   | 10  | 20  | 30  | 40  | 50  | 60  |
|-----------|-----|-----|-----|-----|-----|-----|-----|
| $C_{11} - C_{12}$ | 165.53 | 204.89 | 232.09 | 311.72 | 334.64 | 381.28 | 430.55 |
| $G_{(110)}$ | 82.77 | 102.45 | 116.05 | 155.86 | 167.32 | 190.64 | 215.28 |
| $C_{44}$ | 80.68 | 109.04 | 124.76 | 145.92 | 155.82 | 156.21 | 162.42 |
| $E_{(100)}$ | 213.11 | 264.44 | 298.11 | 394.4 | 425.75 | 478.1 | 529.59 |
| $B$ | 167.08 | 210.5 | 230.48 | 280 | 311.56 | 323.85 | 326.92 |
| $G$ | 80.68 | 109.04 | 124.76 | 145.92 | 155.82 | 156.21 | 162.42 |
| $B/G$ | 2.07 | 1.93 | 1.85 | 1.92 | 2.00 | 2.07 | 2.03 |
| $E$ | 213.11 | 264.45 | 298.11 | 394.4 | 425.75 | 478.1 | 529.58 |
| $\nu$ | 0.29 | 0.29 | 0.28 | 0.26 | 0.27 | 0.25 | 0.23 |
| $A$ | 0.98 | 1.06 | 1.08 | 0.94 | 0.93 | 0.82 | 0.75 |
References

[1] Mästrikov Y A, Heifets E, Kotonim E A and Maier J 2009 Atomic, electronic and thermodynamic properties of cubic and orthorhombic LaMnO₃ surfaces Surf. Sci. 603 326–35
[2] Hannani M D E, Rached D, Rabah M, Khentata R, Benyad M, Hichou M and Bouhemadou A 2008 First-principles investigations of structural, electronic and magnetic properties of cubic LaMnO₃ Mater. Sci. Semicond. Process. 11 81–6
[3] Geng T, Han Z and Zhuang S 2010 Effective Coulomb interaction in LaMnO₃ Physica B Condens. Matter 405 3714–6
[4] Fuks D, Dorfman S, Felsteiner J, Bakaïnkov I, Gordon A and Kotonim E A 2004 Ab initio calculations of atomic an electronic structure of LaMnO₃ and SmMnO₃ Solid State Ionics 173 107–11
[5] Su Y S, Kaplan T A, Mahant H S and Harrison J F 2000 Electronic structure of LaMnO₃: ab initio crystal Hartree–Fock approximation Phys. Rev. B 61 1324–9
[6] Nicastro M and Patterson C H 2002 Exchange coupling in CaMnO₃ and LaMnO₃ Configuration interaction and the coupling mechanism Phys. Rev. B 65 205111
[7] Ravindran P, Kjekshus A, Pjelløvåg H, Delin A and Eriksson O 2002 Ground-state and excited-state properties of LaMnO₃ from full-potential calculations Phys. Rev. B 65 064445
[8] Choi Y, Mebane D S, Liu M C and Liu M 2007 Oxygen reduction on LaMnO₃-based cathode materials in solid oxide fuel cells Chem. Mater. 19 690–1699
[9] Gaur N, Choiithrani R and Srivastava A 2008 Elastic moduli and thermal properties of La₀.₈₅ Sr₀.₁₇ MnO₃ Solid State Commun. 145 308–11
[10] Varshney D and Choudhary D 2011 Study of elastic moduli and thermal properties of RnMnO₃ (R = La, Nd) compounds Int. J. Comp. Mat. Sci. Eng. 3 1450011
[11] Olsson E, Aparicio-Anglès X and de-Leeuw N H 2016 Cullity B 1978 Elements of X-ray Diffraction Diffusion 2nd Edn (USA: Adisson–Wesley Publishing)
[12] Coticchio H, Khenata R, Bouhemadou A, Haddou A, Rached D and Soudini B 2009 FP-APW calculations of atomic and electronic structure of alkali metal sulides under pressure effects Phys. Rev. Lett. 101 195107
[13] Shaik H, Yee C H and Kim K 2010 Exact double counting in combining the dynamical mean-field theory Phys. Rev. B 81 195107
[14] Banach G and Temmerman W 2004 Pressure induced charge disproportionation in LaMnO₃ J. Phys. Condens. Matter 16 S5633
[15] Sandratski I M and Bruno P 2003 Density functional theory of high-Tc ferromagnetism of (ZnCr)₇Te J. Phys.: Condens. Matter 15 L585
[16] Born M and Huang K 1954 Dynamical Theory of Crystal Lattices (Oxford: Clarendon)