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Conference Proceedings

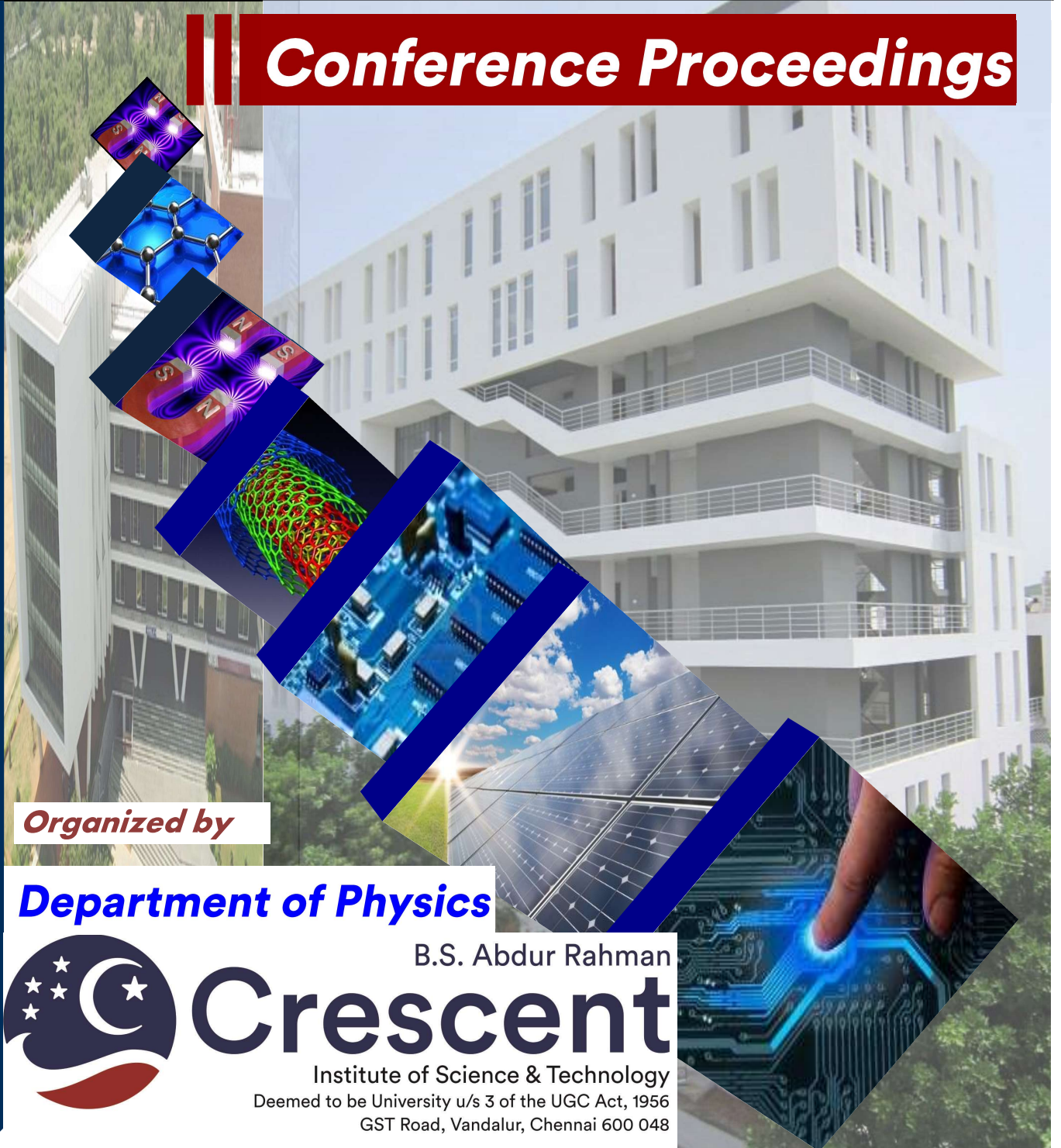
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FP 19 Charge density and crystal structure analysis of $\text{La}_{0.85}\text{Ce}_{0.15}\text{FeO}_3$ ceramic

G.Gowri^{a,*}, R.Saravanan^a, N.Srinivasan^b, O.V.Saravanan^a, S.Sonai^a

^aResearch centre and Post Graduate Department of Physics, The Madura College,
Madurai 625 011, Tamil Nadu, India

^bResearch centre and Post Graduate Department of Physics, Thiagarajar College,
Madurai 625 009, Tamil Nadu, India

*Corresponding author email: gowrikanna01@gmail.com, saragow@gmail.com,
vasan692000@gmail.com, ovsaravanan2258@gmail.com, physonai@gmail.com

ABSTRACT

The cerium substituted LaFeO_3 ($\text{La}_{0.85}\text{Ce}_{0.15}\text{FeO}_3$) has been synthesized by solid state reaction method. The structural analysis has been done on the powder X-ray diffraction data of the sample using Rietveld refinement technique. The XRD pattern and structural refinement results reveal that $\text{La}_{0.85}\text{Ce}_{0.15}\text{FeO}_3$ crystallizes in orthorhombic structure with space group Pnma. The charge density analysis has been done qualitatively and quantitatively using Maximum Entropy Method (MEM). The band gap energy is estimated using UV-Visible absorption spectrum.

1. INTRODUCTION

The perovskite oxide LaFeO_3 is a canted G-type wide-gap antiferromagnetic insulator with high Néel temperature ($T_N \sim 740^\circ\text{C}$) [1] and crystallizes in an orthorhombic phase [2] at room temperature. It is one of the most important multiferroic material due to the coexisting states of coupled magnetic (ferro/antiferro magnetic) and electric (ferro/antiferro electric) ordering in that system. As LaFeO_3 exhibits significant physical and chemical properties, it is used in many branches of modern technologies such as solid oxide fuel cells, non-volatile magnetic memory devices and ultrasensitive magnetic read heads of modern hard disk drives etc. [3-5]. Extensive research work is aimed at both synthesise of LaFeO_3 and cationic substitution in place of $\text{La}^{3+}/\text{Fe}^{2+}$ site and hence its application.

2 EXPERIMENTAL

$\text{La}_{0.85}\text{Ce}_{0.15}\text{FeO}_3$ was synthesized by high temperature solid state reaction route. Stoichiometric amounts of the high purity precursor oxides namely La_2O_3 (99.99 %, Alfa Aesar),

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Editors

Dr. I.B. Shameem Banu
Dr. M. Basheer Ahamed
Dr. S. Sathik Basha
Dr. R. Amiruddin

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