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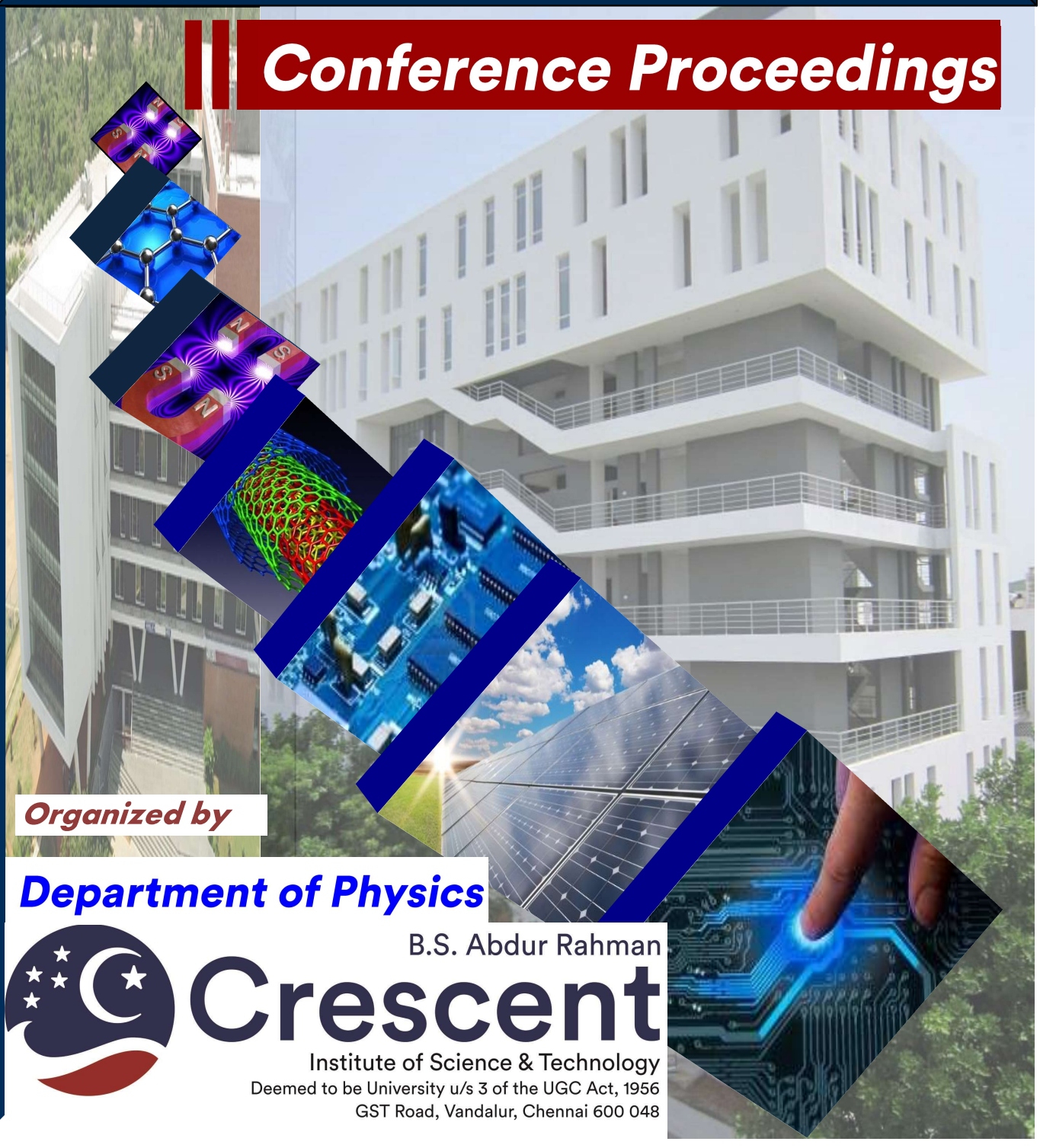

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FP 19 Charge density and crystal structure analysis of $La_{0.85}Ce_{0.15}FeO_3$ ceramic

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ABSTRACT

The cerium substituted $LaFeO_3$ ($La_{0.85}Ce_{0.15}FeO_3$) 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 $La_{0.85}Ce_{0.15}FeO_3$ 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~740°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 synthesize of $LaFeO_3$ and cationic substitution in place of La^{3+} /Fe^{2+} site and hence its application.

2 EXPERIMENTAL

$La_{0.85}Ce_{0.15}FeO_3$ 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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