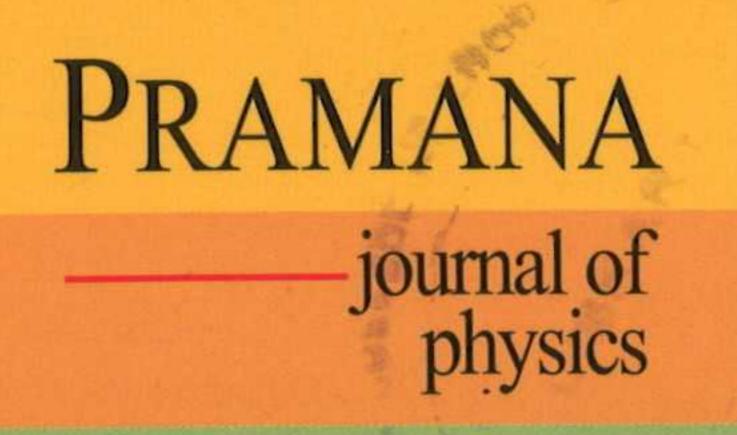
(Continued on inside back cover)



Proceedings of the 3rd E-Workshop/Conference on Computational Condensed Matter Physics and Materials Science	
Preface (1850)	rticle ID
The effects of different possible modes of uniaxial strain on the tunability of electronic and band structures in MoS ₂ monolayer nanosheet via first-principles density functional theory	2
Structural characterization of Mg substituted on A/B sites in NiFe ₂ O ₄ nanoparticles using autocombustion method	
Structural and optical characteristics of Ce, Nd, Gd, and Dy-doped Al ₂ O ₃ thin films	4
Electronic structure and optical properties of prominent phases of TiO ₂ : First-principles study	
Magnetic interactions and electronic structure of $Pt_2Mn_{1-x}Y_xGa$ (Y = Cr and Fe) system: An <i>ab-initio</i> calculation	
Computational studies of third-order nonlinear optical properties of pyridine derivative 2-aminopyridinium p-toluenesulphonate crystal	7
A fragment-based approach towards ab-initio treatment of polymeric materials	
Electronic and structural investigation of buckled antimonene using density functional theory calculation	
Design and analysis of MEMS MWCNT/epoxy strain sensor using COMSOL	
Density functional study of AgScO ₂ : Electronic and optical properties	
Spectroscopic and chemical reactivity analysis of D-Myo-Inositol using quantum chemical approach	

Indexed in CURRENT CONTENTS ISSN 0304-4289 Edited and published by Amitabh Joshi for the Indian Academy of Sciences, Bengaluru 560 080 Printed at Tholasi Prints India Pvt. Ltd., Bengaluru

Registered with Registrar of Newspapers in India, Vide Regn No. 24935/73 Regn. No. KRNA/BGE/337/2015–2017, published on 10/07/2017 Licensed to Post without prepayment No. 49 Posted at Bengaluru PSO, Mysore Road, Bengaluru 560026 16/07/2017

and its experimental verification................ Devendra P Mishra, Anchal Srivastava and R K Shukla

(Continued from back cover)

A theoretical study on the B3 phases of ZnSe: Structural and electronic properties	13
Optical properties of boron-group (V) hexagonal nanowires: DFT investigation	14
Structural and morphological characterization of CdSe:Mn thin films	15
Microscopic theory of substrate-induced gap effect on real AFM susceptibility in graphene	16
Dielectric constant of graphene-on-polarized substrate: A tight-binding model study	17
Quantum chemical computation by DFT application of NLO molecule 2-aminopyridinium <i>p</i> -toluenesulphonate	18
List of Participants	