Preface

We have entered into a new era where it is possible to synthesize, characterize and model numerous materials that will enhance our capability to understand, design and develop new materials. Computational Materials Science proposes new materials by integrating *ab-initio* methods using a wide variety of computational techniques, such as *ab-initio*, Monte Carlo, phase-field and finite-element methods. Modelling of these materials provide a solid base for performing scientific research by considering broad range from atomic to mesoscale. Due to the advancement in hardware and software over the past one decade, there has been an increase in computational power by an average of a million. Interest of the researchers in Computational Materials Science has led to the development of new tools for computer simulations and models of exceptional fidelity. Motivated by the need of exploring new materials with enhanced computational abilities, Advanced Material Research Group (AMRG) has implemented the idea of providing a platform for discussion on various tools and approaches for Computational Condensed Matter Physics and Materials Science. To realize this concept, the 3rd E-Workshop/Conference on Computational Condensed Matter Physics and Materials Science has been organized from 18 to 22 October 2015.

The Advanced Materials Research Group at Computational Nanoscience and Technology Laboratory (CNTL) started at ABV-IIITM in August 2008, with an aim to provide complete theoretical platform for the young researchers of this region as well as other institutions in India and abroad, is a centre of excellence in the Materials and Device Modelling Research. The five-day workshop/conference had been dreamed up with roots in international relations of AMRG for bringing together the scientific and technical community, to share their knowledge in the recent trends on the advanced materials, its applications and various computational as well as experimental techniques. Success of this workshop/conference can also be visualized with the participation of renowned scientists from Uppsala University Sweden, MPI Germany, CNR-IOM SISSA Italy, UNESP Brazil, Clemson University USA and Michigan Technology University, USA along with senior scientists from Indian scientific laboratories/institutions. The workshop comprised four sessions allocated for familiarizing the participants with Quantum Espresso package organized

by a research group of IISER, Pune. An Industry Session by Quantumwise was also held by Integrated Micro Systems, where they have demonstrated their DFT-based package Atomistix ToolKit-Virtual NanoLab to the participants.

This workshop/conference witnessed 21 invited talks and 90 contributed technical papers, covering almost every aspect of Materials Science, such as preparation, analysis of structure and other properties in the macro to nanoscale and their possible application in the automotive, chemical, electronics and electrical engineering. The announcement of undertaking the publication of selected research work in the reputed *Pramana – Journal of Physics* was made in the first circular itself and the peer-reviewed and finally accepted 16 original research papers are published in this issue, with the intention that these findings will be helpful for scientific community.

The overall response by the young participants and senior scientists was very encouraging, and without their support and input this workshop/conference would have never achieved such success. Finally, it is appropriate that we record our thanks to our fellow members of the technical advisory, organizing committee and Institute authorities for their enormous cooperation and guidance.

We are confident that this workshop/conference has sensitized the young participants in the theme areas of the workshop and open up new avenues for the interdisciplinary research and the finally selected 16 contributions in this special issue will reflect the standard of this workshop/conference.

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