Proceedings of the first conference of the "Asian Consortium for Computational Materials Science (ACCMS-1)", Bangalore, 2001

FOREWORD

Computational materials science (CMS) is rapidly emerging as a powerful multidisciplinary branch of science that contributes towards a better understanding of materials. There is a broad spectrum of length scales that describe different systems and phenomena right from nano- to micro- to meso- to macroscopic level. However, it is the interatomic interactions that hold the key for understanding the microscopic properties of materials. For electronic/atomistic simulations of solids, surfaces, interfaces and clusters, first-principles electronic structure and molecular dynamics calculations based on density functional theory (DFT) are being extensively used. It is the accuracy, reliability and most importantly predictive power of these simulation tools that can be exploited in designing novel materials whose properties can be tailored to suit the desired application.

The ACCMS initiative was undertaken to consolidate the rich human resources and expertise available in the Asian region, and to promote collaborative research amongst member countries in the field of CMS. Accordingly the first conference was organized in Bangalore during 29 November–1 December 2001, by the Materials Research Society of India (MRSI) Subject Group on Computer Aided Design of Materials, jointly with the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore and the Indian Institute of Science (IISc), Bangalore. This international meeting brought together active researchers from various Asian countries, viz. Bangladesh, China, India, Iran, Japan, Korea, Singapore, Thailand and Vietnam. Some leading experts from Europe in the field of electronic structure were also invited to this Meeting.

In the conference, there were excellent overviews of materials modeling and predictions of material properties using density functional tools. Several pioneers in the field discussed the state-of-the-art electronic structure methodologies and also the multi-scale modeling which combines the information about atomic-scale processes obtained from DFT with techniques suitable to treat longer length scales. Oxides, perovskites, borides, different alloys, clusters and nanostructured materials were among some of the application areas covered in this meeting.

It gives us pleasure to bring out the proceedings of this conference as a special issue of the Bulletin of Materials Science. We thank all the authors for their contributions and hope that this special issue will serve as an important landmark of the beginning of ACCMS and a useful collection to the practitioners as well as to other researchers interested in getting initiated in this field. We would also

like to take this opportunity to thank all our colleagues in India and abroad who assisted us in making ACCMS-1 conference successful. Financial support from MRSI, JNCASR, IISc, BRNS, CSIR, DRDO, DST, Mr R Aida, Nihon Technos Co Ltd, Japan and Prof. Y Kawazoe, IMR Sendai, Japan are gratefully acknowledged. We also acknowledge the efforts put by the editorial staff of the Bulletin of Materials Science in bringing out this special issue.

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