Preface

Materials design is not a new concept. People are doing this consciously or unconsciously from the beginning of the civilization. As the civilization depends on the materials human being learn to use, as described even in the names of the different ages or stages of civilization, designing or inventing new materials was the prime concern for its development. Design of advanced materials is now a purposive effort, and depends on the knowledge of the composition-microstructure-process-property correlation of the system. The evolution of a large number of methods to model this correlation in a material system at the electronic, atomic and microstructural level made computational designing of new materials possible. Materials theory based physical models are being used for designing new materials, though these models are usually constrained by several boundary conditions and assumptions. There are several methods like density function theory, molecular dynamics, phase field theory, finite element methods among others to model any materials system in different length scale. On the other hand empirical materials models try to capture the inherent correlations among the variables on the basis of available database. Several statistical techniques along with the concept of data mining are now capable of informatics based design, leading to the development of novel materials, which are of academic as well as industrial interest. In addition, modeling based on soft computing techniques enabled the design methodologies to cope up with phenomenological perturbations arising due to non-linearity, imprecision, uncertainty, partial truth and approximation inherent in the system knowledge or in the experimental data. Optimization tools also play important role in designing materials with tailor-made properties or developing easily adoptable processes for manufacturing. Evolutionary optimization algorithms are found to be most effective to search the new solutions to the modern day need of better materials.

All these techniques are drawing interest from theoretical as well as practical application point of view. Researchers are using these approaches for discovering new materials, practitioners at industries are using them to improve the performance of their product or reducing the cost of it. This book provides a comprehensive stock of the different approaches of computationally designing new materials and their probable application, with an emphasis on exploring their relevance in practical/industrial conditions. The objective of the book is to provide a comprehensive collection of all possible computational approaches for designing new improved materials. The book will provide a description of different tools and techniques, and their application in the field of materials design, in separate chapters written by experts of the fields. The first chapter provides an introduction to the computational techniques being widely used for designing new materials. From the second chapter onward authors deal with theories and applications of the different concepts and approaches separately. Ab initio methods of materials design are approached in chapters two and three. The fourth chapter discusses different modeling and simulation techniques applied in the area of microstructure. The finite element method and other micro-

mechanical approaches in the area of modeling are described in chapter five. The issue of integrating different concepts of materials modeling in different length scales is dealt in the sixth chapter with the introduction of the concept of integrated computational materials engineering. The concept applying statistical modeling and data mining in materials engineering is a new domain, being called materials informatics. Computational intelligence techniques like neural network and fuzzy logic are also being used for designing new materials. Chapters seven to ten deal with these concepts. The use of optimization tools occupies an important space for materials design, as the authors of chapter eleven describe. Chapter twelve describes two recent developments in data driven materials modeling using technique hybridization. The final chapter deals with a modeling concept applicable for the complex industrial process of steel making.

The editors convey their gratitude to all the authors for their efforts to make this very important compilation on computational materials design. The effort made by the reviewers to improve the quality of the book is also gratefully acknowledged. Both the editors are extremely thankful to their colleagues, friends and family members who have cooperated for the successful completion of the book. The editors are also grateful to their graduate students. The brilliant effort made by the members of IGI Global to shape this compilation in such a nice way is also acknowledged.

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