

Preface

The exploration of materials and their properties has for some time evolved beyond the Edisonian paradigm, in which one sets about an experimental investigation of the synthesis and properties of materials. Advances have been experienced by a collaborative process between theory and experiment to create novel materials whose properties have been designed to serve many purposes, structural, chemical, and thermal and electrical transport, to name a few. With the advances of speed and complexity in computational resources, these collaborations have only increased in pace and scope.

Modern computing facilities allow for the modeling of large numbers of entities, whether they be the fundamental constituents of matter, electrons, and nuclei, or the collections of pieces of matter that might comprise a device, like a turbine or integrated circuit, for periods of time that could not have been imagined mere decades ago. These extraordinary capabilities have given rise to a new set of attainable goals for integrated computational materials science. For the realization of this potential, computational materials scientist must create new paradigms for the application of existing and new computational methodologies to problems that cross spatial and temporal scales.

The goal of this volume is to present the student and practicing computational materials scientist with a new framework for thinking about multiscale modeling. Integral to this framework are the concepts of theory, model, and simulation. We propose that a clear understanding of these concepts is vital for the appropriate combining of computational techniques across scales. The goal of any such framework is the faithful transmission of information across interfaces so that the modeling of physical phenomena translates the applicable theory into accurate simulations.

The chapters presented here are self-contained and intended to illustrate the state of the art in computational materials science for the modeling of the address various length and time scales. The reader can feel free to read each of these chapters according to the scales that appeal to their own interests. The final chapter explains how to create a predictive framework for communicating information across scale boundaries.

The work presented here represents not only the contributions of the authors, themselves, but also those from our mentors, collaborators, and students. Space is not sufficient here to appropriate, recognize, and thank them all for their contributions, but we hope that this short acknowledgment will begin to pay the debt we owe them.

Tucson, AZ, USA

Pierre A. Deymier
Keith Runge
Krishna Muralidharan

Multiscale Paradigms in Integrated Computational
Materials Science and Engineering
Materials Theory, Modeling, and Simulation for
Predictive Design

Deymier, P.A.; Runge, K.; Muralidharan, K. (Eds.)

2016, IX, 300 p., Hardcover

ISBN: 978-3-319-24527-0