

Preface

This is a second volume of the book on molecular modeling and multiscale problems with attention to electronic materials. The first volume was published in 2012 and even then it was decided to publish a second edition that would cover the new emerging problems in that area. There is no doubt that molecular modeling will draw more and more attention in the future especially due to the growing integration of electronic components and thus the problem of down scaling while at the same time maintaining or even enhancing the performance of the electronic components.

Performance modeling in electronic materials is not a simple application of one scale. It has been recognized by many reliability experts that failure may start at an atomistic level that cannot be easily measured, which propagates upward to scales that can be measured. As many macroscale modeling techniques depend upon the measured property to perform the calculation, what is still largely missing is the connection between the actual molecular structure and how it contributes to the propagation of the failure. Molecular models are significant where properties can be determined only by knowledge of the composition and molecular structure, and measurements are not needed to perform the calculation, although benchmark calibration measurements are required to ensure proper techniques are used. However, even for molecular modelers, there is a scale issue ranging from quantum scale electronic effects to longer range molecular effects. Often these issues are coupled, but the molecular modeler has an opportunity to separate root issues from the perspective of the actual chemical structure in order to help the experimentalist narrow down the types of materials to develop or test and the types of measurements that must be made. From this aspect, molecular modeling is very flexible in that it can be used for both materials development as well as diagnostics, thereby accelerating the development cycle.

The chapters of both the books were compiled from extended papers delivered at the IEEE EuroSimE conference (also known as the International Conference on

Thermal, Mechanical and Multiphysics Simulation and Experiments in Microelectronics and Microsystems), at the Molecular Dynamics. The first volume of the book was based on the conference session between 2007 and 2010 while the current book volume is based on the conference session between 2010 and 2013. Nevertheless both volumes contain illustration and learning tools for the application of molecular modeling in the electronics community.

The annual international EuroSimE is the only IEEE conference devoted to modeling in the electronics community. EuroSimE was initiated in 2000 by the COMPETE network, with sponsorship from the European Commission, to meet research and development needs in the fields of Microelectronics and Microsystems. Since then, EuroSimE has gained worldwide appeal with participants from more than 30 countries, spanning all continents, and has become a fully technically sponsored IEEE CPMT event. EuroSimE conference organizers were also the first IEEE community to recognize the usefulness of molecular modeling for electronic material performance by devoting a session just for molecular modeling in their conference (beginning at the April 16–18, 2007 conference held in London, England). The conference proceedings are part of the IEEE conference publication program and can be found in both the IEL and IEEE Xplore[®] systems. Thanks to IEEE it was possible to collect the adequate manuscripts and extend them into a form of separate book chapters.

We thought it fitting to start a collection of papers from this conference as the community learns how to apply the tools specific to electronic issues. Although molecular modeling has been historically a well-accepted discipline in the pharmaceutical, petroleum, and catalyst industries concerned with chemical performance issues, it has not gained wide acceptance in the materials industry. That is why the acceptance of the discipline by this large modeling community is significant. This book is separated into five sections, each dealing with different scales and performance issues. We have tried to separate the issues based upon the fundamental model size and the performance features being represented and give you examples ranging from the fundamental quantum mechanics calculations all the way to mesoscale examples which is the initial scaling point deviating from explicit atomistic accounting; however the root interactions in mesoscale models can be attributed directly back to the atomistic scale whether by experimental techniques or by explicit parameterization from atomistic models so is included in the book. As you will see, the EuroSimE community has been active in exploring all the possible scales available to the molecular modeler and the ways in which molecular modeling may be used to help materials understanding. As in any modeling endeavor because the specific modeling method may change depending upon the material and the device application, the most value out of this collection may be gained by attention to the techniques and philosophies used to gain the performance understanding sought by the author. By no means are these the only

modeling methods that can be used, but are the ones that were found to be successful for the author and so are instructive for those both starting out in molecular modeling as well as those experienced in the art.

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