PREFACE

The process of researching and writing this handbook was undertaken because of our start-up experience when we began our molecular dynamics studies of phonon–electron interface energy transport. It was very difficult to locate proper potential functions for the particular materials we wanted to work with. The Lennard-Jones (LJ) potential function had served as the standard potential function for many materials, since it was easy to understand, easy to apply, and very well known. Every undergraduate engineering, chemistry, and physics student has seen it in their courses, and of course it has the correct general physics in it. For higher-level research though, the question soon became whether or not the LJ potential function was the best for the molecule system of interest. Thus an extensive literature search was undertaken to identify potential functions and all their empirical constants for the specific systems that were of interest to our study.

To begin our research, we dedicated time to search for and record all potential functions in all the literature we identified where MD simulations were instituted. We soon had a significant collection of potential functions, and we started to work with them in our research with confidence that previous researchers had helped establish an acceptable level of accuracy for a particular potential function for a particular system.

This handbook is a result of our research in identifying potential functions for use in MD simulation. We have listed potential functions by name and cross-listed them by the molecular systems that they have been used to simulate. We hope that this handbook will prove useful to others involved in performing MD simulations. We are continuously looking for more potential functions and information about the systems that they can describe.

This preface would not be complete without recognizing Mr. Tom Pabst, an undergraduate Mechanical Engineering student from Michigan State University, who worked a summer to initiate this collection of potential functions. His contributions to this compilation were invaluable.

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