COMPUTATIONAL STUDIES OF NEW MATERIALS

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PREFACE

When World Scientific Publishers first approached us three years ago about editing a book on the overall topic of computational materials science, we were flattered but rather awed by the task. Since the project seemed interesting and timely, we agreed to do it. It soon became clear that we would have to narrow down the topic a bit. One possibility, for example, was a book titled *Computational Methods in Materials Science*. However, this would look different from the current volume: it would bristle with computer code, discuss the appropriateness of various basis sets, and be much more of a how-to manual for the computer set. We decided not to edit such a book, partly because we thought it would reach a rather narrow audience.

The title we have chosen, *Computational Studies of New Materials*, puts more emphasis on the materials and somewhat less on the computation. And that is indeed the way this book has evolved. The focus is on the materials, be they fullerenes, fractals or polymers. Of course, computational methods are not far below the surface, and in particular, the volume contains an excellent description of tight-binding methods. But it is our hope that this volume will adorn the shelves of scientists who are not explicitly computationalists.

We have found our contributors to be very good writers, interesting people, and above all, imaginative and talented scientists. Working with them has been a rewarding scientific adventure, and we thank every one of them for the hard work and effort they have devoted to this volume. We also thank Dr. Chi-Wai (Rick) Lee, Scientific Editor at World Scientific, for his guidance and encouragement throughout the course of this project. Finally, we gratefully acknowledge the staff and students in the Office of the Chancellor at UW-Stevens Point for assistance in assembling the index.

The Editors
January 1999