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Preface to the Second Edition

Preface to the First Edition

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This second edition has been written since the first edition was published, and many things have moved on.

I have added a new chapter on density functional theory, which I think is the most important area of modern quantum mechanics. I have also added a new chapter on molecular dynamics, and expanded the text as appropriate.

Some topics have been removed after five years. Density functional theory (and especially the DFT-D method) has become the workhorse of modern computational chemistry. I have therefore removed the section on Hartree-Fock calculations, and expanded the text as appropriate. I have also removed the section on Z-matrices, because I have never had to teach it. Thankfully that page of our lives the Z-matrix has been consigned to history, and I will have fond memories of struggling to get cyclic structures to work in Z-matrices.

The remaining chapters have been updated, including the chapters dealing with Monte Carlo and molecular dynamics, the QM/MM chapter, and solvent models. I have also added a completely new chapter on 'Computational Energy', and I hope you will enjoy reading it.

It is hopefully now easier to download and website with any new teaching text, and I have therefore added a link to my website:

<http://www.manchester.ac.uk/~hinchliffe>

where you will find all the code samples and their solutions. Feel free to use them anyway you like, or to contribute your own solutions to teaching. Perhaps you have a corresponding set that you would like to share with the rest of us? Let me know.

I did all the figures in this book using either Gaussian 03 or HyperChem; these were done either on a desktop computer, a laptop, or on the University of Manchester's High Performance Computer, a Sun Sparc Enterprise, a Bull Transilium2 system.

As always, I am happy to receive comments and can be reached at: Alan.Hinchliffe@manchester.ac.uk.

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