ENERGY LANDSCAPES

The study of energy landscapes holds the key to resolving some of the most important contemporary problems in chemical physics. Many groups are now attempting to understand the properties of clusters, glasses and proteins in terms of the underlying potential energy surface. The aim of this book is to define and unify the field of energy landscapes in a reasonably self-contained exposition. This is the first book to cover this active field. The book begins with an overview of each area in an attempt to make the subject matter accessible to workers in different disciplines. The basic theoretical groundwork for describing and exploring energy landscapes is then introduced, followed by applications to clusters, biomolecules and glasses in the final three chapters. Beautifully illustrated in full colour throughout, the book is aimed at graduate students and workers in the field.

DAVID J. WALES was awarded his B.A. degree and the Norrish Prize for Chemistry by Cambridge University in 1985, and gained his Ph.D. from the same institution in 1988. During 1989 he worked with Professor R. S. Berry at the University of Chicago as a Lindemann Trust Fellow, before returning to a research fellowship at Downing College, Cambridge in 1990. He subsequently held a Lloyd's of London tercentenary fellowship and a Royal Society research fellowship before being appointed to a lectureship in Cambridge in 1998. He was awarded the Meldola Medal of the Royal Society of Chemistry in 1993, and was elected a fellow of the Society in 2001. His research interests are mostly concerned with energy landscapes, incorporating a broad range of topics in chemical physics.

Cambridge Molecular Science

As we enter the twenty-first century, chemistry has positioned itself as the central science. Its subject matter, atoms and the bonds between them, is now central to many of the life sciences on the one hand, as biological chemistry brings the subject to the atomic level, and to condensed matter and molecular physics on the other. Developments in quantum chemistry and in statistical mechanics have also created a fruitful overlap with mathematics and theoretical physics. Consequently, boundaries between chemistry and the other traditional sciences are fading and the term *Molecular Science* now describes this vibrant area of research.

Molecular science has made giant strides in recent years. Bolstered both by instrumental and theoretical developments, it covers the temporal scale down to femtoseconds, a time scale sufficient to define atomic dynamics with precision, and the spatial scale down to a small fraction of an Angstrom. This has led to a very sophisticated level of understanding of the properties of small molecule systems, but there has also been a remarkable series of developments in more complex systems. These include: protein engineering; surfaces and interfaces; polymers; colloids; and biophysical chemistry. This new series will provide a vehicle for the publication of advanced textbooks and monographs introducing and reviewing these exciting developments.

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DAVID J. WALES
University Chemical Laboratories, Lensfield Road,
Cambridge CB2 1EW, UK

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Preface

The motivation for writing this book was to produce a unified and reasonably self-contained account of how potential energy and free energy surfaces are used to study clusters, biomolecules, glasses and supercooled liquids. Making connections between these different fields, where the same ideas frequently resurface in different guises, will hopefully assist future research and interdisciplinary communication.

While this is essentially a theoretical book, I have tried to provide sufficient background information and references to experiments to put the objectives in a proper context. Readers are assumed to be familiar with the basic ideas of quantum mechanics, statistical mechanics and point group symmetry. Most other derivations are treated in sufficient detail to make them accessible to nonspecialists, graduate students and advanced undergraduates. A number of more peripheral topics are covered at an introductory level to provide pointers to further reading.

Some of this material has formed the basis of lecture courses on the subject of energy landscapes delivered to students at Cambridge and Harvard Universities, and at Les Houches Summer Schools, although it has all been rewritten in the current endeavour. I am particularly grateful to all the people who read initial drafts, and helped me to prepare figures.

No molecules were harmed in the writing of this book, although a number underwent significant rearrangements.