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Volume 1

senior reporter A. HINCHLIFFE

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Applications and Theory

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Volume 1

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Preface

Richard Dixon and Colin Thomson were the Senior Reporters for the Specialist Periodical Reports 'Theoretical Chemistry', which ran for four Volumes. Richard summarized the state of the art, 1974, in his Foreword to Volume 1 when he wrote:

'This is the first volume of the biennial series of Specialist Periodical Reports devoted to *Theoretical Chemistry*. Theoretical Chemistry is an extremely wide subject, since it provided the background for the interpretation of so many chemical phenomena, and it is therefore necessary to define the scope of these volumes. Quantum theory plays an important role in theoretical chemistry, both through the application of valence theory to the interpretation of molecular structure, and also in the development of spectroscopic models based on quantum mechanics, which are used in the determination of structural information from experimental spectroscopy. Indeed, to many chemists theoretical chemistry is synonymous with quantum chemistry. Quantum chemistry will thus constitute a major part of this series. There is, in addition, a second important aspect of theoretical chemistry, particularly concerning chemical reactions, where the dynamics of molecular motion and their statistical behaviour is more important than specific quantum effects. This aspect will be included in the general coverage of the series. The intended coverage of the series may thus be summarised as: the quantum theory of valence, with application to the calculation of the structure and properties of molecules, and to the calculation of potential energy surfaces for chemical reactions; theoretical aspects of spectroscopy; the dynamics of chemical reactions; intermolecular forces; and developments in fundamental theory and in computational methods.'

Many of the topics treated in Volumes 1–4 are still of interest to a small band of professional theoretical chemists. Twenty years ago, Molecular Mechanics was in its infancy. A number of calculations had been reported for hydrocarbons, but force fields were rather primitive, as was the graphical user interface. In my opinion, it was the GUI that was responsible for the exponential growth of Molecular Mechanics and Molecular Dynamics. Many

people now associate the acronyms MM and MD with theoretical chemistry, despite the classical nature of the techniques. It is now fashionable to speak about Modelling, which is the generic term for anything to do with the structure, properties and reactions of atoms, molecules and materials. The term does *not* imply quantum mechanics.

Again, we have seen the action of market forces and the rise in the number of consumers of Theoretical Chemistry. These are our colleagues who believe that Theoretical Chemistry has something to offer them, and the market has responded with sophisticated black boxes such as Gaussian98, Hyperchem 5.1 and so on. We should be pleased at the success of our marketing.

There was always going to be an overlap between this new SPR and the original Theoretical Chemistry volumes, but things have moved on from the 1970s and so it seemed appropriate to start again with a new name. After much heart-searching, we decided on 'Chemical Modelling: Applications and Theory' to capture the spirit of the new Millennium, and to emphasize that Theoretical Chemistry is no longer dominated by quantum mechanics.

The atom plays a key role in chemistry, and it seemed appropriate to ask Theodore Simos to start off our new SPR with a review of the status of atomic structure calculations.

Stephen Wilson contributed a chapter to Volume 4 of Theoretical Chemistry entitled 'Many-body Perturbation Theory of Molecules', in which he described the beginnings of diagram techniques. Again, it seemed appropriate to ask Stephen to tell us how things now stand. He has done just this, with key references through May 1999.

John Slater preached the message of Density Functional Theory (DFT) in his book 'The Calculation of Molecular Orbitals', published in 1979. In fact DFT had been widely used by solid state physicists for many years before that. Norman March's chapter in Volume 4 of the Theoretical Chemistry SPR showed that chemists were beginning to come to grips with DFT by that time. The 1990s have seen the growth and growth of density functional theory. In comparison to the computer-resource-bound MPn methodology, DFT gave us the first genuine tool for treating electron correlation in the electronic ground states of large molecules. Michael Springborg's article will bring you completely up to the minute in this growth area.

The idea of Molecular Atoms can be traced back to Richard Bader's work in the 1960s. It didn't get a mention in the original Theoretical Chemistry SPR, but is now a widely used technique. It is now an option in packages such as Gaussian98. Consumers will have to get used to the atomic charges, which seem to make much more sense than those of conventional Population Analysis. I therefore asked Paul Popelier, Fiona Aicken and Sean O'Brien to bring us up to speed.

I didn't think our new series would have credibility without a mention of Relativistic Pseudopotentials, and I have to thank Pekka Pyykkö and Hermann Stoll for providing a concise summary of the state of the art.

Janos Ladik contributed a chapter entitled 'The Electronic Structure of Polymers' to the 1981 Volume 4 of the Theoretical Chemistry SPR. This again

is a growth area, and Janos has very kindly written a masterly article for our new SPR summarizing the latest trends.

David Pugh remarked that there seemed to be very much more to write about electric and magnetic properties than when David Bounds and I wrote our own Theoretical Chemistry SPR contribution all those years ago. New techniques in non-linear optics and non-linear spectroscopy have given a new impetus to the accurate calculation of quantities such as the dipole hyperpolarizability.

A visitor to the discovery labs of any pharmaceuticals company will note the importance attached to biology and biochemistry. Richard Maurer and Chris Reynolds show us how seriously modelling is taken in the world of biology.

Starting a new SPR is never easy, and there was the problem of where the contributors should start their accounts; since time began? five years ago? An SPR should be the first port of call for an up-to-the-minute account of trends in a specialist subject rather than a dull collection of references. My solution was to ask contributors to include enough historical perspective to bring a non-specialist up to speed, but to include all pertinent references through May 1999. Volume 2 will cover the literature from June 1999 to May 2001 and so on. In subsequent volumes, I shall ask those Contributors dealing with the topics from Volume 1 to start from there. New topics will be given the same generous historical perspective opportunity as Volume 1 but will have to cover the literature to May 2001 + n , where $n = 0, 2, 4 \dots$. This process will continue until equilibrium is reached.

You may have noticed that there are holes in the coverage of the topics. Perhaps you are wondering about ONIOM, QSAR, theories of liquids, scattering and so on. One can only do so much in the first volume. Perhaps you would like to become a 'Reporter' yourself?

I am always willing to listen to convincing ideas for topics and presentations, and you can reach me at Alan.Hinchliffe@umist.ac.uk

Alan Hinchliffe
Manchester, 1999

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