

Preface

I laid the foundations for this Series in Volume 1.

The ground rules are very simple: colleagues reporting on new topics are asked to give the rest of us an easily understandable historical perspective together with their own critical comments on the literature for the period under review. Colleagues reporting on continuing topics are simply expected to give a critical review of the literature for the period. The period under consideration for this volume is June 1999 to May 2001, and subsequent volumes will give biennial coverage of the literature to May 2003 + n , where $n = 0, 2, 4, 6, \dots$

Note my repeated use of the word 'critical'. When the RSC and I market researched this new SPR title, it quickly became apparent that colleagues were not interested in a dull and uncritical compilation of literature references. Several of them remarked (rather unkindly, I thought) that they could ask their PhD students to sit at a networked PC, dial up Web of Science, and produce such a comprehensive list by the end of a single afternoon. What they wanted was critical insight into the recent literature.

That is what we are trying to give. There are still many gaps in coverage, and I'm sure you will have your own ideas as to what is good and bad with this very new title. Rather than grumbling to your colleagues and writing acidic book reviews, why not volunteer your own expertise? I am always willing to listen to constructive suggestions, and can be reached at

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Volume 2 consists of eight contributions. Several are continuations from the topics treated in Volume 1, some are new. A couple of existing Reporters in Volume 1 asked to be excused for Volume 2, but will reappear in Volume 3. The contributions are not in any particular order, other than the 'new' topics are towards the start of the volume.

The molecular simulation of liquids is now a vast field of human endeavour, and we open with a contribution on 'Simulation of the Liquid State' by David Heyes. David captures the spirit of the SPR exactly when he writes '...The ready availability of fast computers has meant that there are many more researchers working in this ever expanding field ...[and] ...I have restricted my discussion to ... areas that have interested me'.

Several people pointed out a gap in the coverage of Volume 1, namely the field of enumeration. Nenad Trinajstić and his co-workers have written our first chapter

in this field, which strikes a nice balance between historical perspective and up-to-the-minute literature.

Michael Springborg continues to report on the growth of density functional theory.

Theodore Simos reported on the current status of atomic structure calculations in Volume 1. He has broadened the scope a little for Volume 2, and reports on progress in the solution of 1D, 2D and 3D differential equations in chemistry.

It was always my intention to include industrial applications. Much of this kind of work never reaches the primary journals because of confidentiality restrictions and commercial forces. I am very pleased to tell you that Richard Lewis has been able to give us a fascinating glimpse into the world of commercial computer-aided drug design, without apparently breaching a single one of his employer's trade secrets.

David Pugh continues his coverage of electric and magnetic properties. David also gives us a historical insight into those rare beasts magnetizability and hypermagnetizability.

Steven Wilson continues his coverage of many body perturbation theory, whilst Paul Popelier and Paul Smith continue the story of recent advances in the theory of quantum topological atoms.

Alan Hinchliffe
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