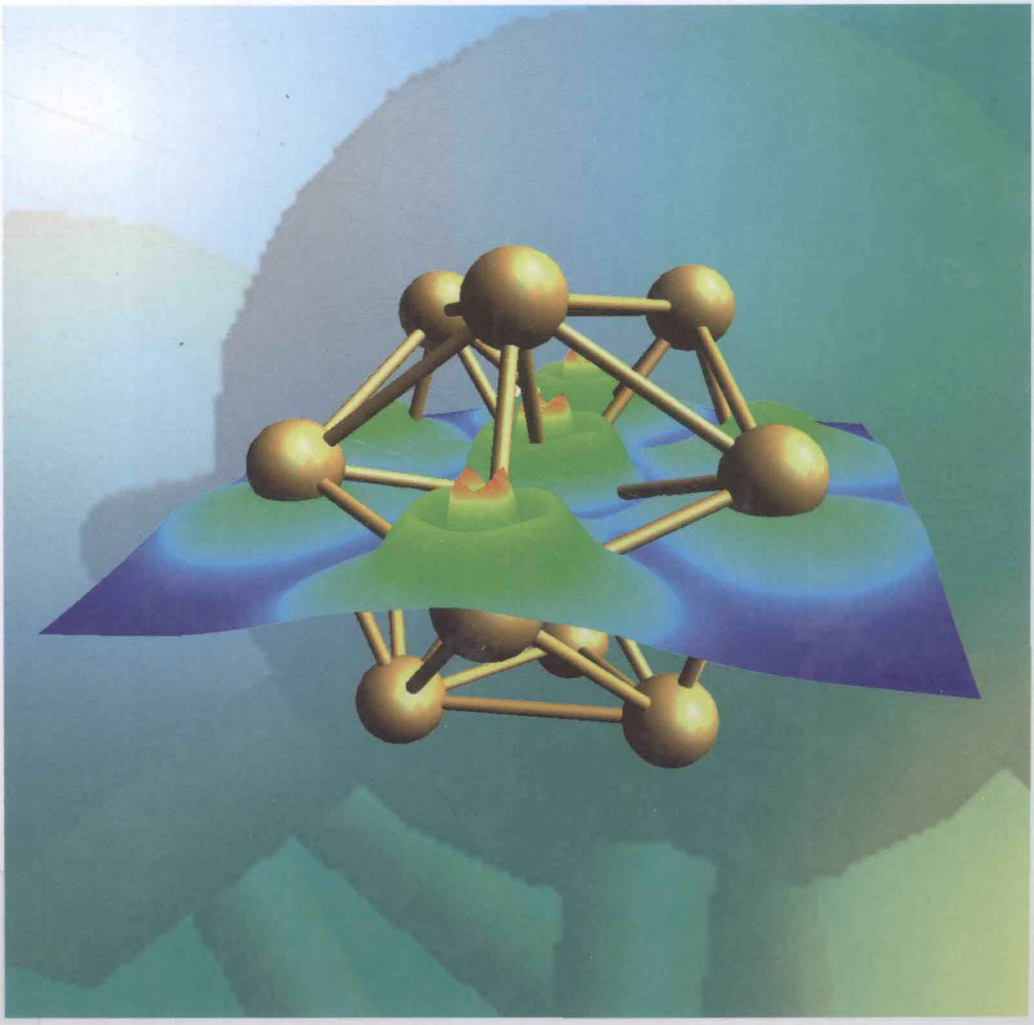
Specialist Periodical Reports

Editor M Springborg

Chemical Modelling: Applications and Theory

Volume 6



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Chemical Modelling

Applications and Theory

Volume 6

A Specialist Periodical Report

Chemical Modelling Applications and Theory

Volume 6

A Review of the Literature Published between June 2007 and May 2008

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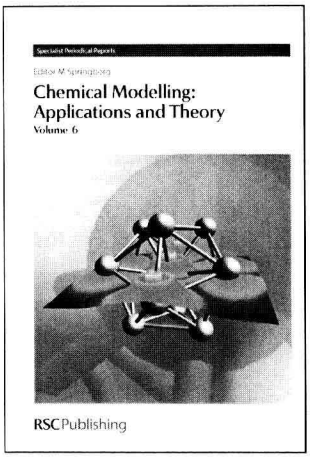

Cover

The icosahedral 'golden fullerene' WAu_{12} reproduced by permission of Pekka Pyykkö, Chemistry Department, University of Helsinki, Finland.

Editorial announcement

Alan Hinchliffe
DOI: 10.1039/b908463k

I'm sure you will have noticed that this SPR (Specialist Periodical Report) has a new Editor, my old friend and collaborator Michael Springborg.

Let me explain.

I recently retired from academic life after some 40 years service at UMIST and latterly The University of Manchester. The question arose as to whether to continue as Editor of the Modelling SPR, and to decide the matter I simulated the tossing of a trillion coins (a trillion being a 2009 buzz word as in the context of 'the number of pounds sterling necessary to bail out a UK bank').

I either won or lost, depending on your viewpoint, and the next problem was the choice of successor. It had to be a sound and respected scientist with a knowledge of, and interest in, the world of publishing.

Over the last 20 years, Michael and I have worked together on a number of significant projects with major publishing houses such as the RSC and John Wiley & Sons Ltd. It is the speculative nature of publishing that some projects will fail and others will succeed. This SPR is one of our best successes and so Michael got my vote.

Naturally, a new Editor will have new ideas, and you will learn about these in his Preface.

I would like to take this opportunity to say a big 'Thank You' to all our contributors over volumes 1 through 5. Next come the hard-working RSC staff who rarely get mentioned in despatches. Jeremy Lucas was adamant all those years ago that the Modelling SPR was going to succeed, as indeed it has. In recent years we have been kept on the straight and narrow by Rob Eagling.

I hope you will continue to give Michael the same level of support you gave me for all those years.

The University of Manchester, Manchester, UK

Preface

Michael Springborg
DOI: 10.1039/b908461b

After ten years and five volumes of the *Specialist Periodical Reports* on *Chemical Modelling: Applications and Theory* edited by Alan Hinchliffe, this sixth volume introduces some changes.

At first, the series has a new editor. I, Michael Springborg, am a professor of physical and theoretical chemistry at the University of Saarland in Saarbrücken, Germany, and have research interests on the border between chemistry and physics. The major parts of the research activities of my group concentrate on development and application of theoretical methods and accompanying computer codes for the calculation of properties of materials. Of particular interest to us are structural and electronic properties of systems that are larger than small molecules, but smaller than macroscopic solids. These systems include clusters and colloids, polymers and chain compounds, and surfaces without and with adsorbants. Also fundamental issues like the theoretical treatment of extended systems exposed to electromagnetic fields as well as foundations of density-functional theory are of interest to us.

Second, it is the plan to increase the frequency of these *Specialist Periodical Reports*. In the future the volumes shall appear annually.

Third, since the internet, including advances in search engines for scientific purposes, has made long lists of recent scientific studies within a well-defined smaller area obsolete, it is my plan to make a smaller change in the format of the reports. Each of these shall contain a short but self-contained introduction to the subject as well as a critical presentation of recent publications within the area of interest. Specialists with expertise in the given area will be asked not only to present their own results but also those of colleagues, thereby covering a broader area.

It is my hope that I can identify exciting and relevant subjects in all areas of chemical modelling, but I will, of course, be grateful for any suggestion, both with respect to authors and with respect to subjects.

Due to these changes, you may not be surprised to discover that many of the topics and authors of the present volume are new compared to the previous volumes. Nevertheless, I hope that the reports will stimulate your interest and that the volume keeps the high standards set by Alan Hinchliffe.

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