

## Preface

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Welcome to Volume 4 of the ‘Chemical Modelling’ SPR. Naturally, I want to start by thanking my team of authors for the hard work they have put into making this the best and most comprehensive volume so far.

It seems a long time since I wrote the following in my Preface to Volume 1 (1999) . . .

*‘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 2001 + n where n = 0, 2, 4, . . . . This process will continue until equilibrium is reached.’*

I think we have now reached equilibrium; some topics have reached maturity and so don’t need cover every Volume, whilst a casual monthly glance at the content pages of JACS, JCP, JPC, CPL, THEOCHEM, Faraday Transactions (to name my favorites, not given in order of merit) reveals growth areas.

As an example of a ‘mature’ topic, consider Density Functional Theory (DFT). DFT is far from new and can be traced back to the work of John Slater and other solid state physicists in the 1950’s, but it was ignored by chemists despite the famous papers by Hohenberg/Kohn (1964) and Kohn/ Sham (KS) (1965). The HF-LCAO model dominated molecular structure theory from the 1960’s until the early 1990s and I guess the turning point was the release of the rather primitive KS-LCAO version of GAUSSIAN. DFT never looked back after that point, and it quickly became the standard for molecular structure calculations. So this Volume of the SPR doesn’t have a self contained Chapter on DFT because the field is mature.

As an example of a ‘perennial’ topic, consider the theory of liquids. Almost every undergraduate physical chemistry text tells us that gases

and solids are easy to understand because in the first case we have random motion, whilst in the second rigid structures. The gist of this argument is that liquids are really tricky, as indeed they are. The first computer simulation of a liquid was carried out in 1953 at the Los Alamos National Laboratories. The MANIAC mainframe was much less powerful than the PC I am using to write this Preface but the early work by Metropolis et. al. laid the foundations for modern liquid modeling. David Heyes (Volume 2) and Karl Travis (Volume 3) told you how things were in a few years ago, and the story is continued by Billy Todd and Debra Bernhardt in Volume 4.

My final sentence for Volume 1 was

*'I am always willing to listen to convincing ideas for new topics'*

as indeed I am. My colleague J Jerry Spivey is Editor for the Catalysis SPR; he took me at my word and as a result it is a pleasure to welcome our first contribution from David S Sholl on Heterogeneous Catalysis.

I haven't space to give glowing descriptions of the remaining contributions from each colleague. We hope you will derive benefit and perhaps even pleasure from our efforts.

On a rare personal note, I should tell you that UMIST and the Victoria University of Manchester recently decided to merge to become the UK's largest University; I'm still sitting at the same desk in the same office but my employer is now 'The University of Manchester' and my e-mail has changed to [alan.hinchliffe@manchester.ac.uk](mailto:alan.hinchliffe@manchester.ac.uk)

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