

## Preface

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In this issue of the *Journal of Mathematical Chemistry (JMC)* you may find a suitable selection of papers submitted in connection to the *International Conference on Computational Methods in Sciences and Engineering 2005 (ICCMSE-2005)*, which took place between 21 and 26 October 2005 in the Hotel Poseidon, Loutraki, Korinthos, Greece.

The ICCMSE-2005 was an impressively successful international conference and it attracted around 500 participants from all over the world. The conference had around 40% increase in participation compared to the 2004 event and during its five days duration approximately 460 papers were presented in numerous parallel and special sessions.

A part of this issue has a representative selection of papers on silicon and silicon-based nanocrystals. The 7 carefully selected papers of this section, appearing in

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this issue, are representative of the main computational approaches on the subject, involving *ab initio*, semiempirical, real space and *k*-space methods, examining the key properties of these nanocrystals (structural, electronic, optical and transport properties) and the changes induced by surface conditions and doping. The quality of the papers and their contribution to the field of silicon nanocrystals is admittedly high.

The other 14 selected papers are on the subjects of computational chemistry, numerical methods, symbolic computations and mathematical and computer modelling.

The 21 meticulously selected papers appearing in this issue have been chosen from a very large selection of around 250 submitted full-length conference contributions. The quality of the papers is remarkably high and the contributors collectively achieved to noticeably progress the field of mathematical chemistry.

We would like to warmly thank the many (anonymous) referees, the conference's participants and specially Professor Dr. Paul Mezey, Editor-in-Chief of the Journal of Mathematical Chemistry, for providing us with the opportunity to produce this guest editorial work.