

Introduction

The frontiers of science are expanded thanks to the effort of vast amount of researchers. All of them help in a slightly different way. The goal of this issue of *THEOCHEM* is to celebrate the 65th anniversary of a scientist who, since his young years until present has not only done good science, but has also encouraged others to do good science.

Ramon Carbó-Dorca is an outstanding researcher and an excellent collaborator. This is the reason why so many scientists have been willing to collaborate in this special issue. The number was so large that we have restricted contributions to those who have coauthored papers with Ramon.

We have organized the 26 articles in four sections, which correspond roughly to the four areas where Ramon has focused his research interests. In the first one, dedicated to Mathematical Chemistry and Methodological Developments, papers present topics at the intersection of chemistry and mathematics, and provide clues for methodological developments in state-of-the-art computational algorithms.

In the second section, devoted to another of Ramon's key research areas, namely Molecular Similarity and Molecular Design, his colleagues address a variety of aspects including quantitative structure–property relationships, quantum descriptors for partition coefficients, or toxicity prediction.

Another of Ramon's favourite concerns, Electron

Density and Chemical Bonding, is the subject of the third part of the series of papers. This enlightening part of computational chemistry is tackled by developing new points of view of chemical bond density.

Finally, in the fourth part, Quantum Chemistry links a variety of contributions which address modern aspects of chemistry. Here researchers fully combine the development of methodological and algorithmical improvements with a clever application to actual chemical problems.

The Guest Editors of this special issue highly appreciate Ramon's work. Actually, with this issue they have endeavoured that the contributions herein honour Ramon's past and current research. Hopefully this issue will convince Ramon to continue pushing the frontiers of good science.

Thank you, Ramon, and happy 65th Birthday.

Miquel Duran
Miquel Solá
Emili Besalú

*Departament de Química i
Institut de Química Computacional,
Universitat de Girona,
Campus de Montilivi, 17071 Girona,
Spain*

Available online 27 June 2005