

Preface

This volume collects 15 selected papers from the scientific contributions presented at the Eighteenth International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XVIII), which was organized by Prof. M.A.C. Nascimento at the *Casa da Cultura* in Paraty (Rio de Janeiro), Brazil, from December 1 to 7, 2013. Over 100 scientists from 25 countries attended this meeting. Participants of the QSCP-XVIII workshop discussed the state of the art, new trends, and future evolution of methods in molecular quantum mechanics, and their applications to a wide variety of problems in chemistry, physics, and biology.

The high-level attendance attained in this conference was particularly gratifying. It is the renowned interdisciplinary nature and friendly feeling of QSCP meetings that make them such successful discussion forums.

Paraty is located on the south coast of Brazil, 250 km from Rio de Janeiro, the state capital. This historical town, nestled on the *Costa Verde*, is a living memory of the Gold Cycle: gold extracted from the mines of the state of Minas Gerais was transported by mule along the Estrada Real down to Paraty and from there shipped to Rio de Janeiro. The area of Paraty is probably the only place on the planet that brings together a native forest about 80 % preserved, a bay protected from the open sea by over a hundred islands, and a seventeenth-century town which is regarded by UNESCO as the most harmonious baroque location in the world. From this past originate the relics and traditions that so enchant the visitors: a wonderful wealth of cultural and ecological attractions, as well as a tourist infrastructure consisting of cosy inns and picturesque restaurants.

Details of the Paraty meeting, including the scientific program, can be found on the web site: <http://www.qscp2013.iq.ufrj.br>. Altogether, there were 18 morning and afternoon sessions, where 55 plenary talks were given, and two evening poster sessions, with 18 flash presentations for a total of 38 displayed posters. We are grateful to all participants for making the QSCP-XVIII workshop a stimulating experience and a great success. QSCP-XVIII followed the traditions established at previous workshops:

QSCP-I, organized by Roy McWeeny in 1996 at San Miniato (Pisa, Italy);
QSCP-II, by Stephen Wilson in 1997 at Oxford (England);
QSCP-III, by Alfonso Hernandez-Laguna in 1998 at Granada (Spain);
QSCP-IV, by Jean Maruani in 1999 at Marly-le-Roi (Paris, France);
QSCP-V, by Erkki Brändas in 2000 at Uppsala (Sweden);
QSCP-VI, by Alia Tadjer in 2001 at Sofia (Bulgaria);
QSCP-VII, by Ivan Hubac in 2002 near Bratislava (Slovakia);
QSCP-VIII, by Aristides Mavridis in 2003 at Spetses (Athens, Greece);
QSCP-IX, by Jean-Pierre Julien in 2004 at Les Houches (Grenoble, France);
QSCP-X, by Souad Lahmar in 2005 at Carthage (Tunisia);
QSCP-XI, by Oleg Vasyutinskii in 2006 at Pushkin (St Petersburg, Russia);
QSCP-XII, by Stephen Wilson in 2007 near Windsor (London, England);
QSCP-XIII, by Piotr Piecuch in 2008 at East Lansing (Michigan, USA);
QSCP-XIV, by Gerardo Delgado-Barrio in 2009 at El Escorial (Madrid, Spain);
QSCP-XV, by Philip Hoggan in 2010 at Cambridge (England);
QSCP-XVI, by Kiyoshi Nishikawa in 2011 at Kanazawa (Japan);
QSCP-XVII, by Matti Hotokka in 2012 at Turku (Finland).

The lectures presented at QSCP-XVIII were grouped into nine areas in the field of *Quantum Systems in Chemistry, Physics, and Biology*, ranging from Concepts and Methods in Quantum Chemistry and Physics through Molecular Structure and Dynamics, Reactive Collisions and Chemical Reactions, to Computational Chemistry, Physics, and Biology.

The width and depth of the topics discussed at QSCP-XVIII are reflected in the contents of this volume of proceedings in the book series *Progress in Theoretical Chemistry and Physics*, which includes four sections:

- I. Quantum Methodology (3 papers);
- II. Structure and Properties (4 papers);
- III. Molecular Dynamics (4 papers);
- IV. Fundamental Theory (3 papers).

In addition to the scientific program, the workshop had its usual share of cultural events. There was a boat cruise in the Paraty bay and a show by the internationally known group *Contador de Estórias*. The award ceremony of the CMOA Prize and Medal took place during the congress banquet in the most traditional restaurant of Paraty, *Margarida Café*.

The CMOA Prize was shared between two selected nominees: Jer-Lai Kuo and Yuan-Chung Cheng, both from Taiwan. Two other nominees, Jhih-Wei Chu (from Taiwan) and Andriy Loboda (from Ukraine) received a certificate of nomination and a gift. The prestigious CMOA Medal for senior scientists was awarded to Prof. Lorentz Cederbaum (University of Heidelberg, Germany). According to a custom of QSCP meetings, the venue of the next yearly workshop was announced to be in Odessa, Ukraine, in 2015, followed by one in Taipei, Taiwan, in 2016. However, due to the political events, the dates of the two meetings were later reversed.

We are pleased to acknowledge the generous support given to the QSCP-XVIII conference by *Coordenação de Aperfeiçoamento de Pessoal de Nível Superior* (CAPES), the City of Paraty Convention Bureau and *Casa da Cultura* of Paraty. We are most grateful to all members of the Local Organizing Committee for their work and dedication, which made the stay and work of participants both pleasant and fruitful. We also thank the members of the International Scientific Committee and the Honorary Committee for their invaluable expertise and advice.

We hope the readers will find as much interest in consulting these proceedings as the participants in attending the meeting.

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Frontiers in Quantum Methods and Applications in
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