

# Preface

This volume collects 24 selected papers from the scientific contributions presented at the Twentieth International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XX), organized by Alia Tadjer and Rossen Pavlov in the Golden Sands resort near Varna, Bulgaria, on September 14–20, 2015. Over 90 scientists from 26 countries attended this meeting. The participants discussed the state of the art, new trends, and future evolution of methods in molecular quantum mechanics, and their applications to a broad 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 so successful discussion forums.

The Golden Sands resort is 18 km north of the city of Varna and near the Golden Sands National Park. The name comes from an old legend of pirates burying a huge golden treasure at the waterfront north of Varna. The land took revenge on the rascals and transformed that gold into wonderful sand. It is a magnificent resort, the largest on the northern Black Sea coast, with its richly wooded hills, a white golden beach, and clear blue sea. The old-growth forests between ancient Odessos and Dionysopolis were mentioned by Pliny as the home of mythical dwarfs visited by the Argonauts. There are famous mineral water springs, already known to the Thracians and Roman Caesars. Golden Sands suits both sun seekers and sightseers visiting Varna, the third largest city in Bulgaria and pearl of the Black Sea coast.

Details of the Varna meeting, including the scientific and social programs, can be found on the web site: <http://ntl.inrne.bas.bg/qscp2015>. Altogether, there were 17 morning and afternoon sessions, where 53 plenary talks were given, and two evening poster sessions, with 21 flash presentations for a total of 35 displayed posters. We are grateful to all the participants for making the QSCP-XX workshop a stimulating experience and a great success. QSCP-XX 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 J.-P. 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 G. 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);  
QSCP-XVIII, by M.A.C. Nascimento in 2013 at Paraty (Brazil);  
QSCP-XIX, by Cherri Hsu in 2014 at Taipei (Taiwan).

The lectures presented at QSCP-XX were grouped into seven topics, in the field of *Quantum Systems in Chemistry, Physics, and Biology*, ranging from concepts and methods in Quantum Chemistry, through Relativistic Effects in Quantum Chemistry, Atoms and Molecules in Strong Electric and Magnetic Fields, Reactive Collisions and Chemical Reactions, Molecular Structure, Dynamics, and Spectroscopy, and Molecular and Nano-materials, to Computational Chemistry, Physics, and Biology.

The width and depth of the topics discussed at QSCP-XX are reflected in the contents of this volume of proceedings in *Progress in Theoretical Chemistry and Physics*, which includes five parts:

- I. Quantum Methodology (five chapters);
- II. Structure and Dynamics (six chapters);
- III. Atomic and Molecular Properties (six chapters);
- IV. Biochemistry and Biophysics (four chapters);
- V. Fundamental Theory (three chapters).

In addition to the scientific program, the workshop had its usual share of cultural events. There was a tour of the resort, a visit to the Archaeological Museum and Thracian Treasures in Varna, the Palace and Botanical Garden in Balchik, the Stone forest and Aladja monastery, and the palace and winery of Euxinograd. Foreign participants successfully joined in a show of folk songs and dances. The award ceremony of the CMOA Prize and Medal took place during the banquet in the conference venue: *Berlin Green Park Hotel*.

The CMOA Prize for junior scientists was shared between two selected nominees: Henryk Witek (Taiwan) and Sachar Klaiman (Germany). Two other nominees: Anela Ivanova (Bulgaria) and Olga Khetselius (Ukraine), received a certificate of nomination and a gift. The prestigious CMOA Medal for senior scientists was awarded to Prof. Hardy Gross (Max-Planck Institute of Microstructure

Physics in Halle, Germany). Following a QSCP tradition, the venue of the next workshop was announced: Vancouver, BC, Canada, in July 2016.

We are most grateful to the members of the Local Organizing Committee: Yuliya Mutaфchieva, Zhivko Stoyanov, Martin Ivanov, Chavdar Velchev, and Mitko Gaidarov, as well as to the Sofia University young team, particularly Galia Madjarova and Georgi Stoychev, for their work and dedication, which made the stay and work of the participants both pleasant and fruitful. Last but not least, we thank the members of the International Scientific and Honorary Committees 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.

*The Editors*

Quantum Systems in Physics, Chemistry, and Biology

Advances in Concepts and Applications

Tadger, A.; Pavlov, R.; Maruani, J.; Brändas, E.J.;

Delgado-Barrio, G. (Eds.)

2017, XXXIX, 449 p. 123 illus., 74 illus. in color.,

Hardcover

ISBN: 978-3-319-50254-0