

Preface

This volume collects 20 selected papers from the scientific contributions presented at the Seventeenth International Workshop on Quantum Systems in Chemistry and Physics (and Biology), QSCP-XVII, which was organized by Prof. Matti Hotokka at Åbo Akademi University, Turku, Finland, from August 19 to 25, 2012. Over 120 scientists from 27 countries attended this meeting. Participants of the QSCP-XVII workshop discussed the state of the art, new trends, and future evolution of methods in molecular quantum mechanics, as well as their applications to a wide variety of problems in chemistry, physics, and biology.

The large attendance attained in this conference was particularly gratifying. It is the renowned interdisciplinary character and friendly atmosphere of QSCP meetings that makes them so successful discussion forums.

Turku is located in the southwestern part of Finland. It was the capital city of the country as well as its religious and cultural center throughout the Swedish period. Christina, Queen of Sweden, founded the Åbo Akademi University in Turku in 1630. When Finland became a Grand Duchy under Alexander I, Czar of Russia, in 1809, the former University was transferred to the new capital, Helsinki, and eventually became the University of Helsinki.

The present-day Åbo Akademi University was founded in 1918, shortly after Finland became independent from Russia. Some of the buildings of the old Åbo Akademi University, such as the Ceremonial Hall, are still used by the University. Today, Turku is the seat of the Archbishop of Finland and an active cultural and industrial city endowed with numerous museums, art galleries and historical sites, as well as an important seaport.

Details of the Turku meeting, including the scientific program, can be found on the web site: <http://www.qscp17.fi>. Altogether, there were 19 morning and afternoon sessions, where 56 plenary talks were given, and one evening poster session, with 21 flash presentations for a total of 55 posters displayed. We are grateful to all participants for making the QSCP-XVII workshop such a stimulating experience and great success.

QSCP-XVII 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).

The lectures presented at QSCP-XVII 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-XVII 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. Fundamental Theory (4 papers);
- II. Molecular Structure, Properties and Processes (5 papers);
- III. Clusters and Condensed Matter (9 papers);
- IV. Structure and Processes in Biosystems (2 papers).

In addition to the scientific program, the workshop had its usual share of cultural events. There was an entertaining concert by a tuba orchestra on the premises. The City of Turku hosted a reception on the museum sail ship Suomen Joutsen, and one afternoon was devoted to a visit to the archipelago on board of the old-fashioned steamship Ukkopekka. The award ceremony of the CMOA Prize and Medal took place in the historical Ceremonial Hall of the old Åbo Akademi University.

The CMOA Prize was shared between two selected nominees: Marcus Lundberg (Uppsala, Sweden) and Adam Wasserman (Purdue, USA). The CMOA Medal was awarded to Pr. Martin Quack (ETH, Switzerland). Following an established custom at QSCP meetings, the venue of the next (XVIIIth) workshop was disclosed at the end of the banquet: Paraty (Rio de Janeiro), Brazil, in December 2013.

We are pleased to acknowledge the generous support given to the QSCP-XVII conference by the Federation of Finnish Learned Societies, the Svenska Tekniska Vetenskaps-Akademien i Finland, the City of Turku, the Åbo Akademi University, the Walki company, and Turku Science Park. We are most grateful to the members of the Local Organizing Committee (LOC) for their work and dedication, which made the stay and work of the participants both pleasant and fruitful. Finally, we

would like to thank the members of the International Scientific Committee (ISC) and Honorary Committee (HC) 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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