

## Preface to the ESPA-2014 special issue

Manuel F. Ruiz-López<sup>1</sup> · Francisco J. Olivares del Valle<sup>2</sup>

Published online: 11 July 2015  
© Springer-Verlag Berlin Heidelberg 2015

This issue of Theoretical Chemistry Accounts collects a compilation of research works presented at the 9th edition of the *Electronic Structure: Principles and Applications* conference (ESPA-2014) held in Badajoz, Spain, on the July 2–4, 2014.

The ESPA conferences were initiated in 1998, and since then, they have been organized every 2 years. The previous editions were organized in Madrid (1998), San Sebastián (2000), Sevilla (2002), Valladolid (2004), Santiago de Compostela (2006), Palma de Mallorca (2008), Oviedo (2010) and Barcelona (2012). The ESPA conferences were initially intended to bring together the Spanish community in the field of Theoretical and Computational Chemistry. However, ESPA has grown over time in terms of national and international participation, and in the last years, it has become a key scientific event of international reputation.

ESPA-2014 was organized by the Quantum Chemistry and Molecular Modelling (QCAMM) group of the University of Badajoz (see Fig. 1). Four main topics were covered in the conference: “Theory, Methods and Foundations,” “Materials Science,” “Structure and Chemical Reactivity” and “Environmental Effects and Modelling.” They were properly represented by means of nine invited Plenary Talks, twenty-four Oral Communications and about 120

Poster Presentations. The meeting was attended by a total number of 178 participants coming from different universities around the world. The official picture of the meeting is shown in Fig. 2. Most of the participants came from Spain, but delegates from 14 other countries were present, which include (in alphabetic order) Austria, Brazil, Czech Republic, Denmark, France, Germany, Italy, Japan, the Netherlands, Portugal, Russia, Sweden, UK and the USA.

Together with a high-quality scientific program, the organizers tried to provide delegates with the opportunity to experience the Extremadura region as part of the congress. To this aim, an engaging social program was designed starting on the evening of July 2 with a welcome reception at the Archeological Museum of Badajoz. Besides, the delegates enjoyed a mid-conference excursion to the old town of Cáceres, a UNESCO World Heritage Site since 1986. Finally, the congress was closed with a banquet at the Ethnographic Museum gardens of the magnificent city of Olivenza.

As an important satellite event of the ESPA-2014 conference, the *Third Annual Workshop of the Joint Doctorate Program on Theoretical Chemistry and Computational Modelling* (TCCM) took place on July 1 at the Faculty of Sciences of the University of Extremadura. Such a workshop event is regularly organized for Ph.D. students, as a complementary training of the TCCM doctorate program, and offers them the opportunity to present their research work via oral communications at the end of the first year of the doctorate studies.

During the conference, the members of the organizing committee brought to the attention of the delegates the extremely difficult situation that is presently facing the Spanish research system as a consequence of the drastic R + D funding reduction decided by the Spanish government. A document describing this situation, known as the “Badajoz Manifesto,” was sent to the media. It stated, in

---

Published as part of the special collection of articles derived from the 9th Congress on Electronic Structure: Principles and Applications (ESPA 2014).

- ✉ Manuel F. Ruiz-López  
[Manuel.Ruiz@univ-lorraine.fr](mailto:Manuel.Ruiz@univ-lorraine.fr)
- ✉ Francisco J. Olivares del Valle  
[fjov@unex.es](mailto:fjov@unex.es)

<sup>1</sup> University of Lorraine, Nancy, France

<sup>2</sup> University of Badajoz, Badajoz, Spain



**Fig. 1** The ESPA 2014 Organizing Committee, from *left to right*: Dr. José Carlos Corchado Martín-Romo, Glauco Garrido Almeida (guest Ph.D. student), Dr. María de la Luz Sánchez Mendoza, Dr. Aurora Muñoz Losa, Dr. María Elena Martín Navarro (Secretary),

Rute Barata Morgado (Ph.D. student), Prof. Francisco J. Olivares del Valle (Chairman) and Dr. Manuel Angel Aguilar Espinosa. Dr. Ignacio Fernández Galván (not in the picture) was also a member of the Organizing Committee



**Fig. 2** The ESPA 2014 official picture with the 178 delegates coming from 15 different countries

particular, that such an unprecedented budget reduction has marked a turning point for the Spanish scientific growth, while it is creating a great discouragement of the Spanish young talents, who do not see any perspectives to develop a scientific carrier in their country.

The next ESPA conference will be organized in 2016 in the city of Castellón, Spain, close to the Mediterranean Sea. All our best wishes to the organizers for a successful conference, and we hope to see you there!