



Foreword to the special issue on the “Electronic structure: principles and applications (ESPA 2022)” conference

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Abstract

The ESPA (Electronic Structure, Principles and Applications) conference is organized every two years in Spain. It brings together international specialists in theoretical and computational chemistry to present and discuss the latest advances in this field. The first edition was held in Madrid in 1998, and then, subsequently, in San Sebastián, Sevilla, Valladolid, Santiago de Compostela, Palma de Mallorca, Oviedo, Barcelona, Badajoz, Castellón, and Toledo. The 12th edition of the conference could not be held in 2020 due to the covid epidemic, and it was held in Vigo from June 21 to 24, 2022. This special issue assembles a collection of articles from presentations given at the conference.

The ESPA conferences cover all major fields of Theoretical and Computational Chemistry, from method development to state-of-the-art applications across computational molecular science. These conferences were initially intended to bring together the Spanish community of theoretical and computational chemists but have grown over time (both in terms of national and international participation) to become a key event with an international reputation in the field.

The 12th ESPA edition (June 21–24, 2022) was organized by the University of Vigo, with Marcos Mandado and Angeles Peña as chairpersons, at the headquarters of the Afundación Management building, which was designed in 1879 by the architect Jenaro de la Fuente Domínguez (Fig. 1). In eclectic style, this beautiful building shows a virtuoso masonry work, with two facades joined by a chamfer and enhanced with cast iron miradors. Tradition and avant-garde have been combined in the renovation of this building for a new multifunctional use.

The conference was originally scheduled for 2020, but was delayed until 2022 due to the covid crisis. As a satellite

activity of the conference, the 9th Young Scientists Workshop on Theoretical Chemistry & Computational Modeling, a meeting that allows young researchers to present their scientific work at an international congress, was organized on June 20. Moreover, during the conference, the second edition of the Biannual Meeting of the Group of Chemistry and Computers of the Spanish Royal Society of Chemistry (RSEQ) took also place.

The following list of plenary lectures reflects the outstanding level of excellence of the congress: Julia Contreras-García (Sorbonne Université, France), Fernando P. Cossio (Euskal Herriko Unibertsitatea, Spain), Laura Gagliardi (University of Chicago, USA), Peter Gill (University of Sydney, Australia), Nuria López (Institut Català d'Investigació Química, Spain), Donald G. Truhlar (University of Minnesota, USA), Maria J. Ramos (Universidade do Porto, Portugal), Krishnan Raghavachari (Indiana University, USA), and Jesús M. Ugalde (Euskal Herriko Unibertsitatea, Spain). There were, in addition, 19 invited lectures, 17 oral communications and two poster sessions. The social program included an excursion to the Cíes Islands, an archipelago located off the coast of Pontevedra, at the mouth of the Ria de Vigo, and a Conference Dinner.

There were more than 250 participants at ESPA 2022. Most of them were Spanish, but others came from many other different countries (from USA to Australia). Numerous discussions were held during the congress in a friendly atmosphere, and we are sure that new collaborations and new friendships emerged from it all. The next ESPA conference will be held in Tarragona from June 3–7, 2024 at the

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Fig. 1 Group photograph and opening ceremony of the ESPA-2022 conference

“Palau de Congressos”, within walking distance from the beach! We are sure you will enjoy the meeting if you decide to attend, and we wish the organizers every success as in previous editions.

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