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## **Foreword to the Special Issue on the “Electronic Structure: Principles and Applications (ESPA 2018)” Conference.**

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### Abstract

The ESPA conference (Electronic Structure, Principles and Applications) is held every two years in Spain. Its purpose is to serve as an international forum for the presentation and discussion of recent advances in the field of Theoretical and Computational Chemistry. Starting in 1998 in Madrid, the following editions were organized in San Sebastián, Sevilla, Valladolid, Santiago de Compostela, Palma de Mallorca, Oviedo, Barcelona, Badajoz and Castellón. The 11<sup>th</sup> edition, ESPA 2018, was jointly organized by the Autonomous University of Madrid and the University of Castilla-la-Mancha, in Toledo, Spain, on the 17<sup>th</sup> - 19<sup>th</sup> July 2018.

The city of Toledo is located 70 km south of Madrid. It has been a World Heritage Site since 1986. Traditionally known as the "city of three cultures", Toledo played a central role in bringing to Europe the wisdom of the ancient Greeks and Arabs through its "School of Translators", a group of scholars who worked together in the 12<sup>th</sup>-13<sup>th</sup> centuries to translate many of the classical philosophical and scientific works. Toledo also houses a unique collection of paintings by El Greco, who settled in the city in 1577 and lived there until his death in 1617. His masterpiece "Burial of the Count of Orgaz" can be seen in the Church of Santo Tomé.

The ESPA conference was hosted on the scientific-technological campus, in the group of buildings known as the Toledo Arms Factory, whose history dates back to the former sword factory of King Carlos III in the 18<sup>th</sup> century. As previous ESPA editions, ESPA 2018 was organized in connection with the Workshop of the European Erasmus Mundus Master and Doctorate programs on "Theoretical Chemistry and Computational Modelling", which was held on the 20<sup>th</sup> July 2018. In addition, ESPA 2018 had a satellite meeting: an international Symposium in Honor of Otilia Mó and Manuel Yáñez (16<sup>th</sup> July 2018) on the occasion of their 70<sup>th</sup> birthdays and retirement. Professors Mó and Yáñez are two prominent figures in the field of Theoretical Chemistry. They have

made key contributions to the understanding of gas phase chemistry, but have also played an immense role in the development of the discipline in Spain, and also in Europe. In particular, they promoted the Theoretical Chemistry and Computational Chemistry program and the European Erasmus Mundus Master's program mentioned above. The Journal of Physical Chemistry has dedicated a special virtual issue to celebrating their career (see J. Phys. Chem. A 2018, **122**, 5671–5672).

ESPA 2018 brought together more than 244 participants from 31 countries, of which 89 were students. The conference included 9 plenary lectures, 13 invited lectures and 16 oral presentations, in addition to several poster sessions. It covered a large variety of problems on theoretical models and methods, spectroscopy, chemical reactivity, materials, biological systems, and environmental effects. Some of the works presented, are gathered in this topical collection, in Theoretical Chemistry Accounts. They offer an excellent idea of the recent theoretical developments and applications in the fields of Quantum Chemistry and Molecular Modeling, while drawing fascinating perspectives for the future.

The guest Editors wish to thank the authors and the reviewers for contributing to this special issue. We also express our gratitude to the Editors-in-Chief of Theoretical Chemistry Accounts, Dr. Ilaria Ciofini and Prof. Carlo Adamo, for their constant support throughout the editing process.

The next ESPA conference will be organized in 2021, and not in 2020 as originally planned, due to the COVID-19 crisis, which is currently affecting many countries. It will be organized in the city of Vigo, Spain, located on the seashore of the Atlantic Ocean. In Jules Verne's *Twenty Thousand Leagues Under the Sea*, the submarine Nautilus came to Vigo to be provided with gold. Undoubtedly, great scientific treasures will be awaiting ESPA 2020 participants in Vigo as well. And with this great hope, we wish the organizers a most successful meeting!



ESPA 2018 Conference group photo.