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PREFACE

Theoretical and computational chemistry in Spain

Mariona Sodupe · Enrique Sánchez Marcos

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1 Preface

The Ninth Congress of the World Association of Theoretical and Computational Chemists, one of the most important scientific meetings focusing on Theoretical Chemistry, will take place in Santiago de Compostela (Spain) in July 2011. The decision to celebrate this Congress in Spain represents an implicit recognition of the increasing role of the Spanish community in this field. Indeed, this phenomenon had already been illustrated in several bibliometric studies that had pointed out the amount and quality of Spanish theoretical chemistry over the last 30 years [1]. With this as background, the Editor of Theoretical Chemistry Accounts, Christopher Cramer, proposed the coordination of a special issue devoted to Theoretical Chemistry in Spain. We, the guest editors, have tried to assemble a collection of papers that surveys a wide landscape of the various research lines that are presently under study by investigatory teams spread all over the nation.

The current state of Spanish Theoretical Chemistry is built upon a historical foundation developed by several generations of professors and researchers, all of whom elevated the level of this discipline so as to occupy a prominent role within both the Spanish Chemistry and the world Theoretical Chemistry communities. The seeds of Quantum Chemistry in Spain were introduced by the late Professors José Ignacio Fernández Alonso and Salvador Senent, in the 1950s. Fernández Alonso was introduced to the discipline first at the *Centre de Chimie Thèorique de France*, working with Sandorfy, and later on at the California Institute of Technology, collaborating with Pauling. Senent was introduced to the field in the English School, at King's College and Oxford University, where he collaborated with Coulson. These two pioneers of Spanish Quantum Chemistry began to develop their research activity in this new discipline at the Universities of Valencia, Valladolid and Autónoma de Madrid. A significant number of young researchers were instructed in these two schools during the 1960s and 1970s. These individuals disseminated Quantum and Theoretical Chemistry to a large number of universities as they took up professorships primarily in Physical Chemistry.

Parallel to this evolution within the academic environment, the first quantum chemistry group in Barcelona was founded under the auspices of the Spanish Research Scientific Council (CSIC) by Santiago Olivella, who had been a collaborator with Dewar at the University of Texas. Similarly, at about the same time, Carmela Valdemoro and the late Yves Smeyers started their activities at the Instituto Rocasolano in Madrid, and Joan Bertrán began his studies at the Centre de Mecánique Ondulatoire in Paris, with Daudel as his Ph.D. supervisor. Bertran's academic mobility over the course of his career contributed significantly to the wide dissemination of Quantum Chemistry in Spain and further contributed to the development of many of the currently working teams in the field, particularly in Catalonia. Finally, Ramón Carbó, first at the Instituto Químico de Sarriá and later at the University of Girona, was also a cornerstone for the development of Theoretical Chemistry in Catalonia.

During the 1980s, a new generation of scientists, many of them the scientific progeny of the pioneers mentioned

M. Sodupe
Departament de Química,
Universitat Autónoma de Barcelona,
08193 Bellaterra, Spain

E. S. Marcos (✉)
Departamento de Química Física,
Universidad de Sevilla, 41012 Sevilla, Spain
e-mail: sanchez@us.es

earlier, consolidated and expanded the field and themselves transferred their passion for Theoretical Chemistry to new generations of young researchers. A broad representation from all of these groups was invited to contribute to this special issue. Concluding this historical overview, we note that an interesting overview of the history of Spanish Theoretical Chemistry has recently been written by one of its still active pioneers, Joan Bertran. We refer interested readers thereto for a more in-depth discussion of the subject [2].

We are confident that the manuscripts collected in this Special Issue illustrate the outstanding level of research that exists in Spain in the field of Theoretical and Computational Chemistry. These studies cover the development and application of theoretical methods to study a wide range of relevant topics including chemical bonding [3–6], molecular structure [7–12], molecular properties [13–15], molecular interactions [16–18], reaction mechanisms [9, 19–26], catalysis [27–29], surface science [29–32], photochemistry [33, 34], dynamics [7, 35–39], solvent effects [40], diffusion processes [41], and rational drug design [42], in some cases in tight collaboration with experimental groups. This diversity in covered topics implies ongoing use of almost all computational methods and tools available in the field and has moreover led to ongoing methodological developments, like those devoted to derive localization/delocalization electronic functions and indices to analyze electron correlation, bond formation and aromaticity [3–6]. The electronic structure methods used in these studies range from DFT to wave-function-based methods, such as post-Hartree–Fock MP2 or CCSD(T) for the study of molecular interactions, or multireference CASSCF/CASPT2 when dealing with photochemistry [33, 34] or magnetic coupling in biradicals [14]. Hybrid QM/MM strategies are used to study computationally demanding large-systems [23, 27]. Reaction mechanisms are explored in several works [19–26], with, in many cases, rate constants being determined using either variational transition state theory [20, 24, 37] or by means of time-dependent wave packet calculations [21]. The dynamical aspects of different kinds of processes [7, 35–39] are also considered in several studies by means of quasi-classical trajectories, ab initio molecular dynamics, and quantum dynamics. In addition, Monte Carlo simulations are used to describe adsorption processes in zeolites [32] or diffusion in macromolecular crowded media [41]. The review by Poblet et al., which is the only review in this issue, surveys current trends in the computational modeling of polyoxometalates [7], particularly with respect to their structures, electronic properties, NMR chemical shifts, and reactivities. In the field of drug design, the present issue also includes a study on the performance of different approximations to score and dock compounds with known activity [42]. Finally, the major features of a new and more efficient implementation of a QM/MM method in the SIESTA code are also described [43].

In addition to the thematic and methodological richness on display in this Special Issue, it should be noted that the Spanish community of theoretical and computational chemists is characterized by strong, friendly, and interpersonal relationships. This has fostered many multigroup collaborations undertaken to tackle particularly complex problems and has been instrumental in promoting progress in the field. In this regard, an inter-university Master Degree program and the international ESPA (Electronic Structure Predictions and Applications) meeting (held biannually in Spain) have proven to be excellent tools for promoting scientific exchange. Of course, many international collaborations also exist between Spanish groups and partner groups located in other countries.

This Issue includes contributions from two scientists who sadly passed away during the editorial period, namely Miguel Alvarez Blanco (University of Oviedo) and Luis Serrano (University of Valencia), both of whom were too young to leave us and were highly esteemed by the whole Spanish scientific community. Miguel's scientific activity was devoted to the study of chemical bonding and molecular and material properties in collaboration with Angel Martin Pendás and Evelio Francisco. Luis was an outstanding scientist in the field of excited-state electronic structure and electron spectroscopy. Several of his works, in collaboration with Manuela Merchán and the late Björn Roos, are now foundational references in the field. In addition, Miguel and Luis were deeply involved in the dissemination of Theoretical Chemistry. Both of them lectured in the former National Master in Theoretical and Computational Chemistry, which later became a European Masters. Luis was a regular instructor in the European Summer Schools in Quantum Chemistry. Both were enthusiastically working until the last days of their lives, as they were convinced that scientific research is fundamental to human progress and that its development is paramount. We offer this Special Issue as an attempt to emulate that spirit, and on behalf of the Spanish community, we dedicate it with affection to the memory of Miguel and Luis.

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