Preface

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Introduction to the Special Issue of “The International Year of Quantum”

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On June 7, 2024, the United Nations proclaimed 2025 as the International Year of Quantum Science and Technology (IYQ) following extensive discussions by the United Nations Educational, Scientific and Cultural Organization (UNESCO). The resolution was co-sponsored by over 70 countries, representing over 5 billion people. According to the proclamation, this year-long, worldwide initiative will “be observed through activities at all levels aimed at increasing public awareness of the importance of quantum science and applications.” As the world authority on chemical nomenclature and terminology, standardized methods for measurement, atomic weights and many other critically evaluated data, the International Union of Pure and Applied Chemistry (IUPAC) is naturally a supporter of all UNESCO initiatives relevant to chemistry and allied fields. For example, IUPAC coordinated many events to celebrate the International Year of Chemistry in 2011 (IYC 2011).

In September 2024, Dr. Fabienne Meyers, Executive Director of IUPAC, encouraged Russell Boyd (RJB) to consider editing a special issue of *Pure and Applied Chemistry* (PAC) dedicated to the celebration of IYQ. RJB subsequently invited Manuel Yáñez (MY) to join him as a guest editor of a special issue of PAC dedicated to the celebration of IYQ. The proposal was accepted by A. Ganesan, Editor in Chief, and the PAC Board in October 2024. Invitations were extended to more than 50 leading researchers in quantum chemistry in late-2024 with the goal of obtaining about 20 or more articles that celebrate the impact of quantum science and technology in many branches of chemistry, materials science and related disciplines. We did not anticipate high acceptance of our invitations and were pleasantly surprised when our vision of one excellent issue dedicated to the celebration of IYQ rapidly expanded to three impressive issues.

We will not attempt to summarize the contents of about 40 articles, but we note that the coverage is very broad. Some papers describe state-of-the-art research, while others provide authoritative reviews. A few provide fascinating insight into the contributions of leading researchers and the evolution of the early days of quantum and theoretical chemistry into what we may call more broadly computational chemistry.

Naturally, there is a heavy emphasis on quantum chemistry, the component of computational and theoretical chemistry that uses the principles of quantum mechanics to understand and predict the behavior of molecules and chemical reactions. Quantum mechanics provides the framework for understanding how atoms and molecules interact with each other. Furthermore, the application of quantum mechanics is crucial for understanding chemical properties, predicting molecular behavior, and developing new technologies in areas like materials science and drug design.

Article note: A collection of invited papers to celebrate the UN’s proclamation of 2025 as the International Year of Quantum Science and Technology.

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While curating this celebration of IYQ, it was natural that we ourselves would reflect upon our careers and experiences as quantum chemists. We received our educations to the PhD level in our respective countries and then pursued postdoctoral research abroad with two legendary figures in quantum chemistry, MY with John A. Pople at Carnegie Mellon University in the USA and RJB with Charles A. Coulson at Oxford University in the UK. Our postdoctoral years were very satisfying and had inestimable effects on our careers. In due course we returned to the countries of our births, and we began our independent careers, MY at the Autonomous University of Madrid in Spain and RJB at Dalhousie University in Halifax, Canada, about 50 years after the introduction of quantum mechanics. At the time, it was possible to carry out modest *ab initio* calculations with small basis sets on small molecules. All calculations were done on a mainframe computer on our respective campuses. There is no way that we could have foreseen the dramatic advances of the next 50 years. It is interesting to note that we both spent our entire careers at the universities that offered us positions a half century ago and to this day we maintain our associations as Professors Emeriti.

We will conclude this brief introduction by highlighting some of the remarkable advances we have observed during our lifetimes. If we take 1970 as a reference year – perhaps simply because the most widely used code in quantum chemistry at the time was Gaussian 70 – we find that the number of published papers employing quantum chemistry methods to analyze chemical systems was somewhere between 600 and 800 per year. Of these, fewer than 400 utilized ab initio self-consistent field (SCF) calculations, with a similar number relying on semi-empirical methods. Who could have imagined that, 54 years later, over 177 000 articles would be published in a single year in which computational modeling techniques were applied to an ever-expanding range of topics? A similar trend is observed in molecular dynamics (MD). In 1970, fewer than 50 papers reported MD simulations. By 2024, that number had grown to over 75 000 per year.

The progress in accessible timescales for simulation has also been remarkable. A major breakthrough occurred in the middle eighties when, for the first time, it became possible to couple quantum electronic structure calculations with atomic motion, enabling the simulation of reaction mechanisms at the atomic level. This innovation laid the foundation for femtochemistry, allowing realistic simulations of bond-breaking/forming processes and photo-induced dynamics on the femtosecond (fs) timescale. Today, simulations can even reach the timescale of electronic motion itself, giving rise to the new and revolutionary field of attochemistry.

In the early years, most computational studies focused on molecular ground states, as the theoretical treatment of excited states was far more demanding. In 1970, fewer than 100 papers addressed molecular excited states. By 2024, that number had increased to over 4000 per year.

Equally impressive is the evolution in the size of systems that can be modeled. In 1970, ab initio calculations (without electron correlation) on molecules with 4–6 “heavy” atoms were a real challenge and it was not until the late eighties that quantum-chemical calculations (including electron correlation) applied to molecules with more than three heavy atoms became routine.

Today, thanks to linear-scaling density-functional theory (DFT), systems with more than 10 000 atoms can be treated computationally. Even the most accurate methods can now be applied to systems with 500 atoms or more – an unimaginable feat just a few decades ago.

A direct outcome of this rapid expansion of quantum chemistry, from the late 20th into the early 21st centuries, was the development of extensive databases containing detailed information on 3D molecular geometries, bonding arrangements, and quantum chemical properties, typically computed using DFT, for hundreds of thousands of small molecules, datasets that are widely used in both computational chemistry and molecular machine learning.

According to the IYQ website (quantum2025.org), the mission of the International Year of Quantum Science & Technology is to use the occasion of 100 years of quantum mechanics in 2025 to help raise public awareness of the importance and impact of quantum science and applications on all aspects of life. We trust that this issue of PAC will provide a lasting legacy of the state of quantum chemistry in 2025.