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Foreword

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This Special Issue of Molecular Physics is dedicated to the memory of Professor Lutosław (Lutek) Wolniewicz, our friend and teacher, an initiator of rigorous thinking in quantum chemistry. Lutek passed away in December 2020 at the age of 90.[1]

In 1968, very precise and repeatedly confirmed calculations by Włodzimierz Kołos and Lutosław Wolniewicz, carried out at the Laboratory of Molecular Structure and Spectra (LMSS) in Chicago, the most advanced centre of computational quantum chemistry at the time, showed that the variational energy of the hydrogen molecule was lower than the accepted experimental energy, the discrepancy being one order of magnitude larger than the experimental error bar. It was difficult to believe that the experimental data could be wrong – the measurements had been performed by Gerhard Herzberg, the world's most renowned spectroscopist and Nobel laureate. Could it be that quantum mechanics itself, the most fundamental theory of modern physics, was incorrect? But, a few months later, after new measurements by Herzberg, a revised experimental value was found to be in perfect agreement with theory. For most scientists, this was a relief – the foundations of physics remained intact; for some, including three of us (SD, JK, JF), close friends of Lutek, this outcome was a disappointment – a revolutionary scientific discovery had become yet another confirmation that everything is as it should.

At the time, we were unable to understand the true importance of this event, beyond the media attention that it had attracted. In the sixties, the aim of quantum chemistry was to formulate qualitative models to help us understand chemical phenomena – the idea that quantum chemistry could be a precision tool, challenging experiment, was quite simply beyond our imagination. But, armed with a deep knowledge of the mathematical tools of quantum mechanics and quantum field theory, Lutek was able to formulate rigorous models and develop advanced computational algorithms that enabled him to make predictions whose precision exceeded the limits of experimental accuracy. This work paved the way for a new approach to quantum chemistry, where all known effects are accounted for with the highest possible rigour. As a result, not only experimental and theoretical flaws can be detected but, more importantly, discrepancies between theoretical and experimental results can eventually be used to invalidate the basic theory – as formulated by Toichiro Kinoshita in his inspiring statement: *It is important to keep pushing the limits; new physics might reveal itself in the next decimal place in theory and measurement.*

Wolniewicz always considered himself a physicist. His 15-year collaboration (1960–1975) with Włodzimierz Kołos, a world-famous quantum chemist from the University of Warsaw, resulted in 14 joint papers that reshaped the foundations of quantum chemistry. Their collaboration was based on a remarkable synergy – Kołos formulated problems that appeared unsolvable to chemists; Wolniewicz presented solutions, using the mathematical apparatus of physics.

From the very outset of his research, Lutek viewed the hydrogen molecule as a system of four interacting particles, rather than as a system of two hydrogen atoms linked by a chemical bond. Eschewing the approximate models of chemists, Lutek not only achieved the greatest possible numerical precision, but also, for the first time in quantum chemistry, provided explicit error bars. To this day, his results serve as benchmarks, for computational as well as experimental work.

We are proud and delighted to present this Special Issue of Molecular Physics, comprising 31 articles submitted by friends, coworkers, and followers of Lutek Wolniewicz. Many of these papers build, directly or indirectly, on the work of Lutek, reflecting his influence on our field and serving as a testament to his lasting contributions to molecular physics and to quantum chemistry.

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Note

1. His life and work are described by us in an article Lutosław Wolniewicz (1930–2020) published in the same issue of Molecular Physics.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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