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SPECIAL ISSUE OF MOLECULAR PHYSICS IN HONOUR OF JÜRGEN GAUSS

Foreword: Prof. Gauss Festschrift

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As guest editors, we are excited to present the *Molecular Physics* Festschrift in honour of Jürgen Gauss, professor of theoretical chemistry at the Johannes Gutenberg-Universität Mainz, Germany, on the occasion of his 60th birthday in August 2020. A truly diverse collection in terms of both content and demography, the present special issue brings together a great number of former as well as current students, postdocs, collaborators, and friends of Jürgen's, spanning not only new methodological developments, but also a wide range of applications, thus aligning itself very well with the research interests of the honoree and the general scope of his scientific career. We are grateful to all contributors and reviewers for helping to curate this successful volume of original work.

Born in Konstanz, on the shore of the picturesque Lake Constance, in the summer of 1960, Jürgen studied chemistry at the University of Cologne, where he went on to obtain his diploma degree in chemistry in 1984. Working under the supervision of Dieter Cremer, he received his PhD degree from the same institution in 1988. In April the following year, Jürgen left Germany for a one-year research position in the group of Eric J. Heller at the University of Washington, funded by the German Science Foundation (DFG). His stay in the Emerald City was followed by another postdoc in the US – namely, a seminal one-year stay 1990–1991 in the group of Rodney J. Bartlett at the Quantum Theory Project in Gainesville, Florida. During this prolific time of his career, Jürgen initiated several long-lasting collaborations – in particular, with John F. Stanton, a fellow postdoc in the Bartlett group at that time.

Jürgen next returned to Germany for another formative stay, working as a research assistant with Reinhart Ahlrichs at the Universität Karlsruhe (nowadays part of the Karlsruhe Institute of Technology) for a total of four years. Upon completing his *Habilitation* in theoretical chemistry in January 1994, Jürgen accepted a position as associate professor (C3) at Johannes Gutenberg-Universität Mainz in 1995. In October 2001, he was appointed full professor (C4) of theoretical chemistry at the same university.

In the course of his career, Jürgen has received many awards and honours – most notably the Dozentenstipendium by the Fonds der Chemischen Industrie (1995), the Carl Duisberg Memorial Prize from the German Chemical Society (1996), the annual medal of the International Academy of Quantum Molecular Science (1997), the academy award from the Berlin-Brandenburg Academy of Sciences and Humanities (2003), and the prestigious Leibniz Prize from the German Science Foundation (2005). Jürgen was elected a member of the International Academy of Quantum Molecular Science in 2009 and a foreign member of the Norwegian Academy of Science and Letters in 2018. In addition to his honorary appointments, Jürgen has served on the international editorial advisory boards of a number of respected journals – for example, *WIRES Computational Molecular Science*, *Journal of Chemical Physics*, and *Molecular Physics*. His services to the community further include the organisational involvement in several scientific conferences such as the *Molecular Quantum Mechanics (MQM)* meetings in Lugano, Switzerland (2013) and in Heidelberg, Germany (2019).

To his students, postdocs, collaborators, and colleagues, Jürgen is known as an eloquent science communicator and a scrupulous theoretician with careful attention to detail and a genuine interest in quantum chemistry. He has always chosen to keep his research group small and has, throughout his career, in addition to working with his group, pursued projects with little, if any involvement from co-workers, writing code and running calculations on his own. At the same time, his former

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and current students and postdocs will recognise him as a kind and supportive mentor and a compassionate and considerate human being. His talent for sparking an interest in quantum chemistry in his younger co-workers resonates with all who have worked with him over the years and is reflected in the fact that most of his former PhD students, postdocs, and *Habilitanden* have since pursued independent careers in science – to date, a total of twelve of these have become professors of quantum chemistry in different parts of the world.

Jürgen's enthusiasm for teaching may also be recognised from his involvement in several summer schools, where he has taught various aspects of quantum chemistry. Besides a long bond with the *European Summer School in Quantum Chemistry*, Jürgen has recently – together with Frank Neese – initiated the *MWM Summer School* on modern wave function methods in electronic structure theory. As an aside, Jürgen has the honour of being the only invited surprise lecturer at the *Sostrup Summer School* (in 2010).

The most important leitmotif of Jürgen's scientific career is the accurate treatment of electron correlation effects by means of wave function-based quantum mechanics. His contributions to the *ab initio* prediction of nuclear magnetic resonance parameters – as enabled by the use of gauge-including atomic orbitals – were among his earliest major contributions to the field. These theories and techniques, initially developed within many-body perturbation theory [1], were soon adapted to coupled cluster theory, [2,3] another key concept that has reverberated through the more than three decades of state-of-the-art research that Jürgen has engaged in. Based on either single-determinantal [4–8] or multi-determinantal [9–11] reference functions, Jürgen's developments in coupled cluster theory have further enabled his ventures into computational spectroscopy [12–16], relativistic quantum chemistry [17,18], and computational thermochemistry [19]. Most recently, Jürgen has immersed himself in the study of near-exact approximations to the electronic Schrödinger equation [20] and the finer details of molecular reactivity [21,22].

Jürgen is one of the principal authors of the CFOUR quantum chemical program package, whose origins go back to his and John F. Stanton's stay at the University of Florida with Rod Bartlett in the early 1990s. Today, CFOUR represents one of the most renowned and versatile coupled cluster codes, with many unique capabilities developed by Jürgen and his co-workers over the years [23].

Jürgen has always offered a lot of insight – educationally, scientifically, and culturally – to those who have visited his group in Mainz over the years or acted as his host during sabbaticals, in Europe and the US. Eager to broaden his scientific interests, Jürgen has initiated new collaborations and forged new friendships during these stays. To his friends, Jürgen is known as a connoisseur of the fine arts, with strong interests in literature and classical music. He is particularly enthusiastic about the opera and closely monitors the schedule of the *Oper Frankfurt*, to which he has often invited visitors to his group. As treasured pastimes, he is fond of nature and sports, particularly enjoying hiking and skiing in the mountains and supporting his favourite football team, *Borussia Mönchengladbach*, through good and bad times. Strongly determined not only in science but also sports, Jürgen completed the full *Frankfurt Marathon* in 2011, having run half marathons on an annual basis for several years.

Many scientists have benefited from Jürgen's extensive knowledge of electronic structure theory over the years. The strong support behind the forthcoming symposium in his honour, the *OPERA2020* meeting [24], is a testament to his valued role in the community. Moreover, among those who have contributed to the present Festschrift are not only friends and collaborators, but also a number of up-and-coming peers, some of whom have never worked with the honoree before.

We would like to close this foreword by once again expressing our sincerest gratitude towards everyone involved in its making and extending our warmest congratulations to Jürgen on his 60th birthday. *Herzlichen Glückwunsch und alles Gute!*

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[24] *OPERA2020*, an International Symposium on Theoretical Chemistry in Honour of Professor Jürgen Gauss on the Occasion of his 60th Birthday (postponed until 2021). see < https://www.opera2020.info/ > .