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MQM 2019 Introduction

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The 9th Molecular Quantum Mechanics Conference (MQM 2019) took place in the lovely city of Heidelberg, Germany from 30 June to 5 July 2019. The venue ('Kongresshaus Stadthalle') was located in the centre of Heidelberg and provided a beautiful, yet stimulating environment for the intense scientific presentations and discussions that took place over the course of the week. The venue was ideally located to allow the more than 350 participants from 35 countries to enjoy the beautiful summer evenings after long conference days.

The series of 'Molecular Quantum Mechanics' conferences are held as a triannual event and traditionally honour the scientific achievements of leading scientists in the field of molecular quantum mechanics. MQM 2019 was held in Germany to honour German contributions to modern quantum chemistry, and specifically in honour of Prof. Werner Kutzelnigg (Bochum), Prof. Wilfried Meyer (Kaiserslautern) and Prof. Sigrid Peyerimhoff (Bonn) and in memory of Prof. Reinhart Ahlrichs (Karlsruhe).

The conference covered a broad range of subjects in theoretical chemistry but with an emphasis on wave function theory. There were almost 70 oral presentations, including four historical lectures and two poster sessions. Special attention was devoted to ensure that diversity was met in the selection of lecturers and topics.

MQM 2019 demonstrated that the field of molecular quantum mechanics is in an excellent state. The participants witnessed a great deal of enthusiasm and a vibrant atmosphere. New discoveries are being made in the field and new research directions are being explored that extend the realm of molecular quantum mechanics far beyond what was deemed possible even, perhaps, only a decade ago. This great deal of enthusiasm and pioneer spirit was particularly apparent in the excellent contributions by the younger generation of molecular quantum



chemists which will surely lead the field to new heights in the years to come.

Yet, the field firmly rests on the shoulders of the giants who have paved the way for the following generations and provided a solid foundation on which all modern work is built. This became particularly apparent in the historic lectures that were highlighting the life and scientific achievements of the four honoured German theoreticians: Werner Kutzelnigg (historic lecture by Volker Staemmler, Bochum), Wilfried Meyer (historic lecture by Peter Pulay, Arkansas), Sigrid Peyerimhoff (historic lecture by Christel Marian, Düsseldorf) and Reinhart Ahlrichs (historic lecture by Joachim Sauer, Berlin). A particular touching moment was following Volker Staemmler's lecture, where the audience spontaneously provided several minutes of standing ovation honouring Werner Kutzelnigg, who unfortunately passed away only a year later.

Another highlight were the very stimulating poster sessions that demonstrated the very high level at which the young and upcoming master and Ph.D. students as well as postdocs are working. Among the many excellent and highly debated posters, an international committee selected four poster prize winners: Gila Kopper (Mainz), Priyanka Aggarwal (Delhi), Fabian Berger (Berlin), Maximilian Scheurer (Heidelberg).

We are greatly looking forward to MQM 2022 that will be organised by Prof. Daniel Crawford (Blacksburg), who gave an excellent presentation on the closing day of MQM 2019. It is sincerely hoped that by 2022, the global pandemic will have faded and will allow us to continue an exciting and stimulating scientific exchange in person, just as it took place during MQM 2019. The MQM 2022 conference website is at www.mqm2022.org

It was my honour and pleasure to act as organiser of the MQM 2019 together with my colleagues

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Hans-Joachim Werner (Stuttgart), Jürgen Gauss (Mainz), Wim Klopper (Karlsruhe) and Andreas Dreuw (Heidelberg) all of whom took a highly active role and made essential contributions to the success of the conference. We are indebted to the excellent assistance of Ms. Christin Ernst, Ms. Esther Schlamann and Ms. Isabell Schiffhorst (all Mülheim) who meticulously took care of the myriad of issues and details that accompany a large international conference like MQM19. We are furthermore indebted to the numerous sponsors of the MQM 2019 who greatly helped to make this conference financially viable.

I sincerely hope that the papers authored by the conference participants that are contained in this issue will provide an impression of the excitement and excellent scientific atmosphere that we were all privileged to enjoy during the MQM 2019 conference.

Frank Neese, Mülheim an der Ruhr, 9 October 2020



Werner Kutzelnigg receiving a standing ovation. Next to him is session chair and co-organizer Wim Klopper.



The poster prize winners together with organiser Frank Neese. From left to right: Frank Neese, Maximilian Scheurer, Gila Kopper, Fabian Berger, Priyanka Aggarwal.

Disclosure statement

No potential conflict of interest was reported by the authors.

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