

Foreword

This issue of *Molecular Physics* is dedicated to Trygve Helgaker, professor of chemistry at the University of Oslo (Norway) on the occasion of his 60th birthday.

Professor Trygve Helgaker was born in Porsgrunn (Norway) in 1953. After completing his military service at the Armed Forces Language Course, he spent a year studying Russian at the University of Leningrad before enrolling at the University of Oslo in 1975 to begin his studies in chemistry. During his science studies, he translated two works of Russian fiction to Norwegian.

After completing his Cand.Scient. (Master) degree in experimental gas-phase electron diffraction with Professor Arne Haaland at the University of Oslo in 1980, he switched to the subject that would become his lifelong scientific passion: molecular electronic structure theory.

He received the degree of Dr. Philos. from the University of Oslo in 1986 with a thesis entitled ‘Development of Quantum Chemical Methods for Analytical Calculation of Molecular Properties’, in which the first MCSCF implementation of an analytic Hessian was presented. The thesis covers the three topics that since have become Trygve’s main scientific interests: (1) the understanding of electron correlation, (2) the evaluation of molecular integrals, and (3) the calculation of molecular properties – all topics where he has made a number of significant contributions to the state-of-the-art in these fields.

For his Dr. Philos. thesis, Trygve worked under the supervision of Professor Jan Almlöf. However, his scientific pursuits also led him to collaborations with other leading experts in his chosen field, and his studies brought him to Aarhus where he met and worked with three scientists who would become lifelong collaborators and friends: Poul Jørgensen, Jeppe Olsen and Hans Jørgen Aa. Jensen. As a result of the work they initiated during the years 1981–1986 on molecular integral evaluation, MCSCF wave function optimisation using second-order methods and the analytic calculation of molecular properties, the foundations for the DALTON program package were laid. DALTON was released to the public in 1997 as a stand-alone program package free of charge for academic use, to a large extent due to Trygve’s dedication to the program and its release. Today, DALTON is undergoing continuous development and remains one of the most versatile quantum chemistry programs available.

While Trygve was still working towards his Dr. Philos. degree in Oslo, Jan Almlöf took a position at The University

of Minnesota, where Trygve joined him as a postdoc after receiving his degree in Oslo in 1986. In 1987, he moved on to a postdoc position with Poul Jørgensen at the University of Aarhus. During this period, he also established long-lasting scientific collaborations and friendships with Hans Ågren and Kurt V. Mikkelsen, working together on molecular response theory and dielectric continuum models.

In 1989, Trygve was appointed associate professor at the University of Oslo and he was promoted to full professor already in 1993. He has remained at the University of Oslo ever since, except for two one-year sabbaticals: 1999–2000, at the University of Cambridge, hosted by Nicholas Handy, and 2006–2007, at the University of Durham, hosted by David J. Tozer. One of the first works published after his appointment at the University of Oslo was the first implementation of direct dynamics, published together with Einar Uggerud and Hans Jørgen Aa. Jensen, an approach that is now most commonly referred to as *ab initio* molecular dynamics.

Trygve quickly became a popular teacher at the University of Oslo and was awarded ‘Den gyldne spatel’ (‘The golden spatulum’) for excellence in teaching from the chemistry students at the department. Through his excellent and dedicated teaching, he quickly attracted a number of students and established his own research group at the University of Oslo, which has since become the centre for quantum chemistry in Norway.

During his now almost 25-year career at the University of Oslo, Trygve has been continuously producing excellent research on a very diverse range of problems in electronic structure theory. We would in particular like to highlight his work on recasting non-variational wave functions in a variational form using the Lagrangian approach, greatly simplifying the derivation of energy derivatives and response functions of non-variational wave functions; his work on extending the use of London atomic orbitals (or Gauge-Including Atomic Orbitals as they are more commonly referred to) to a wide range of magnetic properties and electronic-structure methods; and his work on basis-set convergence and energy extrapolation schemes for obtaining highly accurate energies of molecular systems. In recent years, his research activity focuses on the study of molecules in very strong magnetic fields, linear-scaling methodology and understanding the foundations of density

functional theory through the use of the Lieb variational principle.

Trygve is currently Norway's most cited chemist and the recipient of a number of national and international research prizes, of which we would like to highlight the research prize of the University of Oslo in 2006, the award for outstanding research (Arets Møbius) by the Research Council of Norway in 2011, and the Centenary Lectureship and Medal awarded by the Royal Society of Chemistry in 2007–2008, the first Norwegian to receive this honour since nobel laureate Odd Hassel. He is also an elected member of the Norwegian Academy of Science and Letters since 2004, the International Academy of Quantum Molecular Science since 2005 and from the same year also the scientific board of the World Association of Theoretical and Computational Chemists.

In addition to his many scientific achievements, Trygve is among the younger generations of quantum chemists equally well known from his dedicated outreach and teaching activities. He has, since 1990, been spending two weeks every year either organising and teaching at the Sostrup Summer School in Quantum Chemistry together with Poul Jørgensen and Jeppe Olsen, or participating as a lecturer at the European Summer School in Quantum Chemistry (ESQC), initiated by Bjørn Roos and now organised by Trond Saue (Toulouse). In both of these summer schools,

he excels as a teacher and mentor to new generations of quantum chemists. His dedication to teaching also led to the publication of the monograph 'Molecular Electronic Structure Theory', co-authored with Poul Jørgensen and Jeppe Olsen, a reference work in electronic structure theory.

As former student and postdoc of Trygve, it has been a privilege for us to act as guest editors for this special issue of *Molecular Physics* dedicated to Professor Trygve Helgaker on the occasion of his 60th birthday. In soliciting contributions to the special issue, the response has been overwhelming, reflecting Trygve's high scientific standing as well as his kindness and openness in scientific collaborations. We are particularly pleased that in addition to long-term friends and colleagues, also former students of the many summer schools at which Trygve has taught have contributed to this special issue.

We thank all contributors for making this a great special issue, and on behalf of all contributors, friends and colleagues, we thank Trygve for sharing his scientific knowledge and enthusiasm with all those that have met him. We wish him all the best for the future and look forward to many years to come of science and friendship.

Kenneth Ruud
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