TRIBUTE

A tribute to Tom Ziegler

Biographical sketch — From Copenhagen to Calgary

Tom Ziegler was born in Copenhagen in 1945. He received his M.Sc. degree from the University of Copenhagen in 1972 in the field of Theoretical Chemistry, and his Ph.D. from the University of Calgary, in 1978 in the area of Inorganic/Theoretical Chemistry. After postdoctoral studies at the Free University in Amsterdam and McMaster University, he returned to Calgary in 1981, first as an NSERC University Research Fellow, and then Assistant Professor in 1986. He moved quickly through the ranks to Full Professor in 1993. Between 1996 and 1999, he held a Canada Council Killam Professorship, and two years later, in 2001, became a Tier 1 Canada Research Chair in Theoretical Inorganic Chemistry in recognition of his world-class achievements.

Tom is one of the earliest proponents of density functional theory (DFT), an electronic structure scheme that today is widely accepted as the method of choice in the description of large molecules. He began his life-long development work on a DFT-based computer code during his graduate years (1972–1978) as a Ph.D. student in Calgary under my supervision. This project has since been carried out in collaboration with the group of E. J. Baerends at the Free University in Amsterdam. It has resulted in the powerful Amsterdam density functional (ADF) program package that is widely used and still under development. The applications of this program have in particular been in the area of transition-metal chemistry, a field Tom became acquainted with as an M.Sc. student in Copenhagen under the supervision of J. P. Dahl and C. J. Ballhausen.

During the period 1978–1992, Tom's group (together with a few other sites, including that of D. Salahub in Montréal) demonstrated that DFT in the formulation by their Canadian compatriot A. Becke from Queens University was able to predict molecular energetics and structures with higher accuracy than the traditional electronic structure methods, and at a much lower computational cost. The work on structure and energetics culminated in an influential review paper (*Chem. Rev.* 1991), as well as the general acceptance of DFT in the Becke formulation, as the electronic structure theory of choice for large molecules.

Since 1992, Tom has demonstrated the power of DFT in applications to homogeneous catalysis in a number of highly cited papers mainly concentrating on olefin polymerization. Several petrochemical companies in Europe, Japan, and North America have supported this work. His polymerization research has considerably enhanced our understanding of the different role played by early and late transition metals as polymerization catalysts. More recently, Tom has turned towards heterogeneous catalysis in connection with research on solid oxide fuel cells (SOFC) and Fischer–Tropsch synthesis, again with substantial support from industry and government.

The Ziegler group has at the same time extended the number of molecular properties that can be modelled by DFT. In the period 1992–2000, the group introduced one of the first DFT codes for calculations of NMR chemical shifts and spin–spin coupling parameters as well as the ESR g- and A-tensors. These codes were based on methods that included relativistic effects and could as a result treat catalytic transition-metal systems with heavy metals. The NMR and ESR work is currently being extended to metal surfaces. Another ongoing development of use in homogenous and bioinorganic catalysis has been methods that can calculate electronic (ECD) and magnetic (MCD) circular dichroism. The group is currently applying their ECD and MCD codes to a number of metallo-enzymes. Other developments worth mentioning are their bonding analysis scheme with more than 1000 citations as well as their molecular dynamics method that makes it possible to optimize transition-state structures on the free energy surface.

Most recently, Tom has embarked on a critical assessment of the way in which we describe excited states. He has shown that the currently used method based on time-dependent DFT can be reformulated into a more simple static and time-independent method based on variation theory. The new formulation promises to extend the capability of DFT in studies of excited states.

Tom has been a Visiting Professor at a number of famous universities, the Institute of Molecular Sciences in Okazaki, Japan, the Free University in Amsterdam, and the University of Fribourg in Switzerland. Most recently, in 2008, he was the Lise–Meitner Lecturer at the Lise–Meitner–Minerva Center for Computational Quantum Chemistry in Israel.

Over the course of his career, he has won numerous awards, including a CNC-IUPAC Award (1988), the CSC's Alcan Award (1994), the Award in Pure and Applied Inorganic Chemistry (2000), and Steacie Award (2005). He was elected Fellow of the Royal Society of Canada in 1997, Fellow of the Royal Danish Academy of Sciences and Letters in 2000, and Fellow of the International Academy of Quantum Molecular Science in 2007. In 2004, Tom was awarded the prestigious Schrödinger Medal, the highest award of the World Association for Theoretically Oriented Chemists (WATOC).

Tom has also made significant contributions to the chemical community, serving on the Advisory Boards of *Organometallics* (1998–2001), and *Journal of Computational Chemistry* (2005–2009), and as a member of the NSERC Grant Selection Committee for Analytical and Physical Chemistry (1998–2001), the Fellowship Selection Committee for the Royal Society of Canada (2001–2004), and as Secretary, Academy of Science, Royal Society of Canada (2000–2004). Many of his students and co-workers have gone on to hold academic positions at various Canadian and International Universities, or have accepted industrial positions.

Tom is one of the two most cited chemists in Canada with over 7000 citations, and ranks in the top 100 most cited in the World with an H-index of 70. The number and quality of the papers submitted to this dedicated issue of the *Canadian Journal of Chemistry* attests to the breadth and reach of his influence in the chemical, theoretical, and computational community.

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