

Tom Ziegler 1945-2015



It is with great sadness that we heard of the sudden death of Tom Ziegler on 24 March 2015 during a research stay at the University of Bonn.

Tom was fascinated by density functional theory throughout his entire career. He was a pioneer in the development of DFT-based methods and their application to chemistry. On the methodological side, his contributions include DFT-based energy derivatives, relativistic treatments, methods for calculating magnetic properties such as NMR chemical shifts and g -tensors, TD-DFT implementations for computing chiroptical properties, and most recently constricted variational density functional theory. On the application side, Tom focused on transition metal chemistry. He is most famous for his comprehensive seminal work on olefin polymerization, but he also investigated other industrially relevant processes such as hydrocarbon functionalization and olefin epoxidation. He advanced the understanding of the bonding in transition metal complexes through energy decomposition analysis and other related concepts, on the basis of reliable computations.

Tom has made a lasting impact on chemical research by demonstrating the merits of density functional theory as a practical tool for studying energetics and dynamics, especially in transition metal chemistry and catalysis.

Tom received his Ph.D. degree from University of Calgary in 1978. He joined the faculty of his Alma Mater in 1986 and was Full Professor at the University of Calgary since 1993. His many distinctions include the Canada Research Chair, the Steacie Award of the Canadian Chemical Society, and the Senior Humboldt Research Award. He served on the WATOC Board and received the WATOC Schrödinger Medal in 2004.

Tom's magnificent contributions to the field of theoretical and computational chemistry are known to everyone associated with WATOC. We will miss him dearly.

W. Thiel on behalf of WATOC