

Tom Ziegler 1945-2015



Professor Tom Ziegler passed away suddenly on 24 March 2015 during a research stay at the University of Bonn. Tom was a pioneer in the development of density functional theory based methods and their application to chemistry. His contributions include DFT-based energy derivatives, relativistic treatments, methods for calculating magnetic properties such as NMR chemical shifts, g tensors, and magnetic circular dichroism, and most recently constrained variational density functional theory. In applications, 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 bonding in transition metal complexes through energy decomposition analysis and other related concepts. He 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 the University of Calgary in 1978. He joined the faculty of his Alma Mater in 1986 and became Full Professor at the University of Calgary in 1993. His many distinctions include the Canada Research Chair, the Steacie Award of the Canadian Chemical Society, the Senior Humboldt Research Award, and the Schrödinger Medal. He was elected to the International Academy of Quantum Molecular Sciences in 2007.

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