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DeSève Theatre – McConnell Building – Concordia University

**Density Functional Theory as A Practical Tool in Transition Metal Chemistry**

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Approximate density functional theory (DFT) [1] has over the past decade emerged as a tangible and versatile computational method in organic as well as inorganic chemistry. DFT affords molecular structures [2], vibrational frequencies [3], bond dissociation energies [4] as well as NMR [5a] and ESR parameters [5b] comparable in accuracy to high level ab initio methods, at a fraction of their cost. The method is further able to trace energy profiles for elementary reaction [6] steps and provide accurate estimates [7] of activation energies. DFT can also be used to simulate reaction dynamics [8] and incorporate solvent effects as well as the steric bulk of large ligands through a combined DFT and Molecular Mechanics approach [9]. A discussion will be given of how DFT can be used to solve problems in transition metal chemistry and catalysis [10].

1. (a) T. Ziegler, *Chem. Rev.* **91**, 651 (1991). (b) T. Ziegler, *Can. J. Chem.* **73**, 743 (1995).
2. L. Fan and T. Ziegler, *J. Chem. Phys.* **95**, 7401 (1991).
3. (a) L. Fan and T. Ziegler, *J. Chem. Phys.* **96**, 9005 (1992). (b) L. Fan and T. Ziegler, *J. Phys. Chem.* **96**, 6937 (1992). (c) A. Berces and T. Ziegler, *Top. Cur. Chem.* **182**, 42 (1996).
4. E. Folga and T. Ziegler, *J. Am. Chem. Soc.* **115**, 5169 (1993).
5. (a) G. Schreckenbach and T. Ziegler, *J. Phys. Chem.* **99**, 606 (1995). (b) G. Schreckenbach and T. Ziegler, *J. Phys. Chem. A* **101**, 3388 (1997).
6. L. Deng and T. Ziegler, *Int. J. Quant. Chem.* **52**, 731 (1994).
7. L. Fan and T. Ziegler, *J. Am. Chem. Soc.* **114**, 10890 (1992).
8. P. Margl, J.C.W. Lohrenz, T. Ziegler and P. Blöchl, *J. Am. Chem. Soc.* **118**, 4434 (1996).
9. T.K. Woo, P.M. Margl, P.M. Blöchl and T. Ziegler, *J. Phys. Chem. B* **101**, 7877 (1997).
10. L. Deng, T.K. Woo, L. Cavallo, P.M. Margl and T. Ziegler, *J. Am. Chem. Soc.* **119**, 6177 (1997).

Tom Ziegler earned an M.Sc. in Theoretical Chemistry from University of Copenhagen in 1972 and a Ph.D. in Inorganic/Theoretical Chemistry in 1978. He was then a Netherlands Organization for the Advancement of Pure Research Postdoctoral Fellow at the Free University of Amsterdam and a Natural Sciences and Engineering Research Council (NSERC) Postdoctoral Fellow at McMaster University, before joining the Department of Chemistry at University of Calgary, where he moved up the ranks at University of Calgary and was promoted to Professor in 1993. Dr. Ziegler has collected a number of prestigious awards such as the Canadian National Committee- International of Union of Pure and Applied Chemistry Award (1988), the Alcan Lecture Award of the Canadian Society of Chemistry (1994), the Award in Pure and Applied Chemistry of the Canadian Society of Chemistry (2000), the Catalysis Award of the Canadian Institute of Chemistry (2000). Dr. Ziegler is a Fellow of the Royal Society of Canada and of the Royal Society of Denmark. Dr. Ziegler was a member of NSERC Grant Selection Committees and of the advisory board of Organometallics, published by the American Chemical Society. He has produced over 270 research articles published in major peer-reviewed journals as well as several review articles and book chapters, and he is one of the three most cited chemists in Canada. Dr. Ziegler was a Canada Council Killam Professor from 1996 to 1998 and was appointed Canada Research Chair in Theoretical Inorganic Chemistry in 2002.

