

TRIBUTE

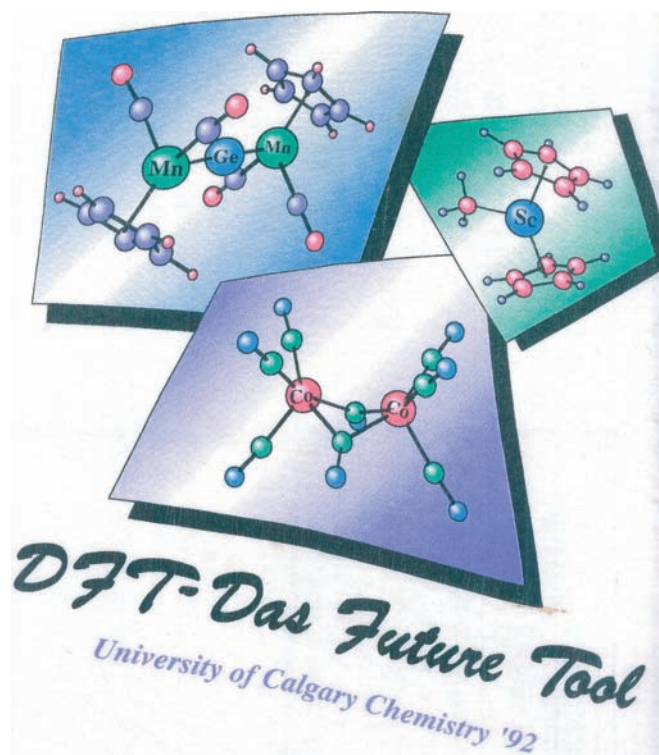
DFT — Das Future Tool

“Das Future Tool” was the title of the group T-shirt¹ that we had made for Tom Ziegler as graduate students in the early nineties. In those days, DFT was only beginning to gain popularity in theoretical chemistry community. Tom had just published his influential review article “Approximate Density Functional Theory as a Practical Tool in Molecular Energetics and Dynamics” in *Chem. Rev.* and had organized one of the first, if not the first, ACS symposium dedicated solely to DFT titled “Chemical Applications of Density Functional Theory” at the spring national meeting in Anaheim. Even the Gaussian suite of programs had finally incorporated DFT into their G92 package (However, not with the original G92 release but as a later interim release they dubbed G92/DFT).

Nonetheless, even at that time, there were a large number of detractors in the theoretical chemistry community who were skeptical of DFT and considered it just another semi-empirical method.² Tom, however, realized that DFT was “Das Future Tool” long before then and in fact had started to develop DFT as a practical tool in chemistry some ten years before beginning in the late 1970s. In those “early days”, there was an even more skeptical attitude towards DFT in the theoretical chemistry community. For example, Tom’s first NSERC operating grant, intended to run his whole research program, was a mere \$5000 per year. Even adjusting 1982 dollars for inflation which brings this grant amount to \$10 585 in today’s dollars, that is a very skeptical level of funding. Things have dramatically changed since the 1980s. Not only is Tom’s research funding level much higher, but DFT is now the quantum chemical method of choice for most researchers.

One impressive aspect of Tom’s body of work is that he is able to communicate both to “hard core” theoretical chemists interested in fundamental theory, as well as non-theoretical chemists who were interested in gaining a deeper understanding of their chemistry from a theoretical point of view. Tom’s work has always focused on two equally important aspects of computational chemistry, namely the development of new methodology and its application to problems of chemical relevance. Owing to this duality, Tom’s work has inspired theoretically as well as experimentally inclined researchers alike. This is evidenced by that fact that Tom is one of Canada’s most highly cited chemists with a towering H-index of 70.

Tom’s kaleidoscopic research interests present many different facets. If five out of Tom’s former graduate students were asked to name their favorites out of all his contributions to science, five different answers would probably be generated – be it his work on molecular structure and properties, or on the nature of the chemical bond, or on relativistic effects which led to the Dutch Revolution in the theory of relativity, be it his work on NMR calculations or his contributions to catalysis or DFT based molecular dynamics. With all the different hats that Tom wears, DFT is the common denominator that amalgamates his many interests, from the early days up to the present time. Based on his work done in fulfillment of a Ph.D.



degree, Tom published a seminal work in which he became aware of and circumvented the problem of calculating reliable bond energies by DFT. The transition state method was at the heart of many research topics that Tom worked on in the beginning of his career. Now, some thirty years later, Tom tackles excited states as well as solid states in search for answers to many relevant chemical problems.

Tom and his Calgary group were certainly pivotal in the meteoric rise of DFT as a powerful tool in chemical research. Tom was not only an early pioneer some 25 years ago, but he has continued to make significant contributions to fundamental DFT theory and its applications to chemical systems since then. In these two special issues of *Can. J. Chem.*, we wish to celebrate Tom Ziegler’s vision and many contributions to chemistry. It was a privilege to be a group member in the early nineties and to witness our then whimsical interpretation of DFT (Das Future Tool) become a reality alongside one of its most influential contributors.²

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¹The T-shirt featured images of “large” organometallic complexes, that were chosen not only for their aesthetic beauty and symmetry, but also to symbolize the fact that DFT could treat these systems accurately and with a practical amount of computing effort, when, at the time, no other quantum chemical methods could do so. There was also an ongoing discussion as to whether we should use “Der” or “Das”. From a German language point of view “Der” may be better but we opted for “Das”.

²We recall a number of heated debates at the ACS meeting in Anaheim involving some of the “unconverted”.