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# A Tribute to Walter Thiel

The 60th birthday of a scientist is a reason for celebration—advanced enough for the life's work to shape up, yet so early in time that there is plenty of opportunity for more to come. This is especially true for someone with the activity and creativity of Walter Thiel. It is a pleasure to introduce this Special Issue in his honor.

An important leitmotif throughout his career has been the development and application of semiempirical quantum-chemical methods. In his postdoctoral time with Michael Dewar in the early 1970s, Walter almost single-handedly implemented the godfather of all modern semiempirical methods, MNDO (modified neglect of differential overlap). Enticed by its potential in the application to large systems, he has continued to develop and refine the underlying models and methodologies ever since. These developments are based on a philosophy of designing and fitting parameters with well-defined physical meanings, rather than tweaking results by massive parametrization. By introducing orthogonalization corrections, for instance, fundamental flaws of semiempirical methods in describing molecular conformations can be overcome. Using know-how from sophisticated multireference ab initio techniques, Walter continues to push the development of MNDO-based approaches into terrain that is yet too difficult for other theoretical methods, such as excited states of large molecules.

Theory is at its best when it can enable experimentalists to interpret their results sensibly. In many collaborations with spectroscopists, Walter and his co-workers have provided highly accurate ab initio data for small molecules, which have guided

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the assignment of high-resolution rovibrational spectra in the gas phase and the spectroscopic identification of previously unknown reactive species. Stimulated by the vibrant environment of a Max Planck Institute devoted to catalysis research, he has used state-of-the-art density-functional theory (DFT) methods to shed light on the complicated mechanisms of homogeneous catalytic processes involving transition-metal complexes. In the heyday of fullerene chemistry, when Buckyballs were still frighteningly large for quantum-chemical calculations, Walter's group helped expand the limits of semiempirical and ab initio methods by applying them to ever larger fullerenes, providing new insights into their structures and reactions.

Walter's vision is not one of competition, but of complement. Nothing illustrates this point better than his activities in the area of hybrid quantum-mechanical/molecular-mechanical (QM/MM) methods, which are designed to bring together the best of the two worlds, namely, high accuracy and applicability to large systems. Walter was not the first to invent these methods, but recognizing their potential, seizing the opportunities for their implementation and their further development, and applying them to hot topics has made him one of the world's leading authorities in the QM/MM field. He has always pursued a strategy of flexible integration of the constituent QM and MM parts, so that almost any of them can now be seamlessly wielded together, tailoring the resulting hybrid for specific applications. One particularly fruitful area for such applications is biocatalysis by enzymes, for example, cytochrome P450 chemistry. In collaboration with Sason Shaik, he has used QM/MM methods to characterize the active species of P450 and its electronic structure. By elucidating the reaction mechanisms of P450cam in the wild type as well as in mutants, he is helping to resolve the controversies concerning the catalytic cycles of this important group of enzymes.

Chemistry is not only about the interaction between particles but also about the interaction between people. Respected for his competent, open, and unpretentious way, Walter has long become a renowned scientist, friend, and colleague within the scientific community. He would rather laugh with people than quarrel with them. This also includes the members of his group, whom he tries to motivate by leading instead of pushing.

Walter's big picture of theoretical chemistry is that of a versatile toolbox to complement, precede, and guide experiments in all branches of chemistry. In the concert of theory and experiment, he knows how to play the keys on all the instruments from computational chemistry, including those he himself has helped to shape and design. We hope he will like the multivoiced choir of papers assembled in this issue. Happy birthday, Walter!

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