



**The Lise Meitner-Minerva Center
for Computational Quantum
Chemistry Announces with Deep
Grief the Passing Away of
Professor Walter Thiel with
Whom We All Shared Decades of
Friendship and Science.**

Starting August 24th, 2019, we slowly received the shocking and unbelievable news that Prof. Walter Thiel (for us, simply Walter) passed away all of a sudden, on August 23, 2019, while he was packing his suitcase to travel to the ACS Meeting in San Diego for the symposium honoring the 75th birthday of H.F. Schaefer III. To the three of us and to many of the scientists, PhD students, postdocs, and visitors who worked in and visited the Lise Meitner-Minerva Center for Computational Quantum Chemistry, Walter was a personal friend, a scientific collaborator, one of the **Central Pillars of The Center**, and a major figure of its Executive Board (the Beirat) from the early 2000s to 2017 when the Center ceased its activity. Because of his involvement in the Beirat we were fortunate to have Walter in Israel almost every year and thus in addition to participate in the annual Lise-Meitner conference, he visited and lectured in all Israeli universities enriching our students and faculty with his profound knowledge in computational chemistry in particular and chemistry in general.

Walter was a Mensch. He carried himself with modesty but with innate dignity that was obvious to anyone who looked at him. His reasoning and advice were always clean of self-interest, respectful, fair and clear-cut. This demeanor, and the little good-natured smile, which accompanied his advice and decisions would always disarm the strongest objections. For us, as the Chair of the Beirat, Director and Co-Director of the Center, Walter's presence was immensely important. I am sure this feeling is shared by many who were associated with The Center.

Our Center was extremely fortunate to have an incredible Advisory Boards (from the early 2000s on, these were Amiram Goldblum, Zeev Gross, David Milstein, Peter Schreiner, Helmut Schwarz, and Walter Thiel, and up to the early 2000s, these were Amiram Goldblum, Sigrid Peyerimhof, Addy Pross, Joachim Sauer, and Helmut Schwarz). Helmut Schwarz, the Chairman of the Beirat, was also the President of the Alexander von Humboldt Foundation. Sigrid Peyerimhoff was the Vice President of the DFG, and Walter was the President of WATOC, which is now the largest organization of theoretical chemists, and at the same time, the Chair of the [Max-Planck-Institut für Kohlenforschung](#).

Walter was a fast and agile programmer in quantum chemistry. He has developed the semiempirical quantum-chemical method MNDO, which gave rise to other semiempirical methods (AM1, PM6, PM7, OMx, etc.). In the 1990s, Walter focused his interest in multi-scale calculations of enzymes, and contributed in major way to the development of QM/MM

methods for calculating enzymes and proteins. After 2010, he devoted programming effort to reactions in excited states using semiempirical methods, which made key contributions to the field of photochemistry. His passion for programming in quantum chemistry ushered him through his retirement days, and he had many plans. But with his untimely death, someone else would have to lead the way.

Here are a few personal reminiscences on Walter:

Sason Shaik: Walter's and my paths intersected scientifically and in a most fruitful way. We knew each other early on, but became friends since the early 1990s. At that time, I was struggling to convince the chemical community that the π -electrons do not have the role that organic chemistry attribute to them, for example, these electrons do not dictate the uniform C-C bond lengths of benzene, etc. This idea met with a lot of objections and I was considered as an iconoclast. But Walter was different than many of the theoreticians I met, he seemed to like the idea and invited me to Zurich, to give a talk on this work. Common scientific interests form the flicker of scientific friendships, and so we became friends.

The second intersection was in August 1999, during the WATOC meeting in London. Walter heard my talk on two-state reactivity of the enzyme cytochrome P450. After the talk he offered me to collaborate with him, since he was developing the QM/MM tools that will enable one to calculate the active species of the enzyme within its natural protein environment. We collaborated on this topic till 2011, and published many papers, among which are two influential chemical review articles. This work has made a great impact on the communities of chemical biologists and bioinorganic chemists, and has paved the way to many other groups in the area. Walter's death is a personal loss for me as a friend and as a long-time scientific partner.

Helmut Schwarz: Being a hard-core experimentalist with an admiration for the insight theoretical and computational chemistry can provide, early on I admired Walter for at least two reasons not to speak of his role as a member of the LMC-Beirat. 1) His undisputed standing as a scientist and the way he interacted with the scientific community, and 2) the unconditional help and support he was always ready to provide to his much less-gifted fellow colleagues. Walter Thiel was rightly seen as the embodiment of a "Vorbild".

Yitzhak Apeloig: I first met Walter around 1983 when I spent a summer with Paul Schleyer in Erlangen. Walter just started his independent career at the University of Wuppertal and came to Erlangen to present a seminar. After the seminar we joined Paul to have a beer, and there was an immediate "click reaction" between us. I loved Walter's open and warm personality and admired his knowledge of computational methods and talent in programming computational programs, which were so useful for experimentalist like me and my students. Although we never collaborated our personal relations deepened through his yearly visits to the Center. I will miss him very much.

We feel Walter's loss with sadness and disbelief. The Israeli computational community owes Walter a lot. We are sure he will rest in peace, much as he has always lived.