

## Memories on Walter Thiel

I met Walter for the first time at the end of the 1970s, when he had just returned to the Philipps-University Marburg from his postdoctoral stay with Michael Dewar at Austin, Texas. His name had become known in the community and was very familiar to me because of his three publications where the program MNDO was introduced. Semiempirical programs were at that time the most advanced quantum chemical methods for calculating larger molecules. The advent of a program that had atom-specific parameters and which was based on the less severe NDDO approximation rather than the INDO approach leading to a significantly higher accuracy than its predecessor MINDO/3 made a great impact on computational chemistry. MNDO has become the mother of nearly all semiempirical methods that have developed ever since.

I drove with my VW Beetle from Berlin, where I was still working on my doctoral thesis, to Marburg and I vividly remember our first meeting at his office at the Fachbereich Physikalische Chemie. He greeted me with the warmth and kindness, which was one of the hallmarks of his character. After some warm-up small talk I was invited to spend the night at his apartment at Georg-Voigt-Strasse, not knowing that many years later I would end up in a house just a few blocks away. He showed me around the old town of Marburg and I enjoyed the hospitality of Walter. But I made one mistake: I agreed at the evening to play chess with him. I realized already that something was going wrong when he not only brought the chess game but also a chess clock, which was new to a bloody amateur like me. After five minutes Walter kindly smiled, opened a bottle of wine and discretely removed the chess game saying that we should better engage in other activities. He had a wonderful way of coping with the situation that he was superior.

I noticed already during this first encounter that Walter had a maturity which was unusual for someone of this age and that he sticks out from the crowd. Although I was three years elder than him, I had no problem to realize this and to accept it, which was made easy by his unpretentious personality. We stayed in close contact ever since and I was not surprised that he received in 1983 a call for a C3 (Associate) professorship at the University Wuppertal shortly after he finished his habilitation. To the best of my recollection, it was the only opening of a professorship for theoretical chemistry in Germany for a period of five years.

When he invited me a few years later for a seminar at Wuppertal he had a young family with his wife Elisabeth and the two little children Sonja and Thomas. He was living in a wonderful maisonette apartment in an old traditional house. And of course, I stayed in their apartment and enjoyed the warmth and hospitality of the now Thiel family. I remember sitting at the breakfast table, when little Thomas was whipping in his child chair and appeared to fall backwards. I have never seen someone as fast as Walter saving the faltering chair. If necessary, Walter could be very fast. The next moment he was composed again.

I remember a second stay at Wuppertal in his apartment, when he and Elisabeth gave a big farewell party in 1992 after he had accepted an offer for a chair position at the University of Zürich. It was a long cheerful fete with many people celebrating the event and with lots of music, dancing on the floor, much wonderful food including the world-best best Tiramisu made by Elisabeth, endless drinks and a lot of laughing and jokes. There was a joyful atmosphere of excitement and departure as if everyone would now go on a safari. It became the starting point for a world career as a leading scientist in theoretical chemistry.

I was again invited by Walter a few years later to give a seminar at Zürich and I stayed again at his home, a very nice house at a small village close to Zürich. I had moved to Marburg in the meantime and I noticed his progress and his standing in the scientific community, where he had gained a high reputation because of his work. But it had not changed his personality; he remained calm, friendly and unpretentious. There was no need for him to engage in excitement and any ballyhoo. When Walter gave a talk at a conference there was no skepticism afterwards, there was rather the information what could be done at the forefront of computational chemistry. In 1997 I spent two weeks with my family in his house at Zürich while he and Elisabeth went on vacation with their children. Walter was a great scientist but also a family person.

Two years later he left Zürich and accepted an offer as director at the Max Planck Institute at Mülheim/Ruhr, an internationally renowned top address. At Zürich they tried to keep him and offered a joint chair position at the University and ETH, but he declined, partly for personal reasons by his family. The time at Mülheim became the heyday of his career. He received numerous awards and honors and he was a highly respected authority for international offices and duties. I was a close ally when he served as president of the WATOC from 2011 – 2017, because I was the secretary/treasurer of the organization. I remember board meetings when controversial issues came up. When Walter gave his arguments, there was no reason to argue anymore. It was not because of Walter's position but by the sheer power of his arguments. Sometimes I watched him and recalled our first meeting in Marburg in the late 1970. It appeared to me as if Walter had little changed. He was simply a born leader.

The last time I met Walter was in April 2019, when a symposium was held at Beijing in honor of his 70th birthday. There had already been a birthday symposium in Mülheim in March of this year, which I could not attend because of urgent duties. I was very happy that a second chance came up when his numerous former Chinese coworkers wanted to honor Walter, so I flew to Beijing. It was a spectacular event, which culminated in a splendid banquet where nearly everyone was drunk at the end – except Walter, who never lost control. It was at this evening that he told me that he would really retire at the end of this year after finishing some duties. He had already nearly completely scaled down his group and he had declined all offers from universities abroad. He had decided to spend his upcoming time with his wife Elisabeth and to enjoy life as private person.

On August 25 this year I was sitting in a conference room at the ACS Meeting in San Diego where a symposium celebrating the 75th birthday of Fritz Schaefer was going to take place. It was a Sunday morning and Walter was scheduled at 9.00 am as the second speaker. It was a very special event for me and I had a special reason to see Walter again. Seven weeks earlier I suffered a stroke and I had just recovered to make it for the symposium. The experience had an impact on my future plans, and I wanted to talk about it with Walter remembering his saying about retirement when we met at Beijing. When Walter's talk was cancelled without further explanation, I feared that something serious had happened. Monday morning I learned that Walter had died from a heart attack while preparing for the trip to San Diego.

The scientific community has lost one his leading persons. And I have lost a friend.

Gernot Frenking