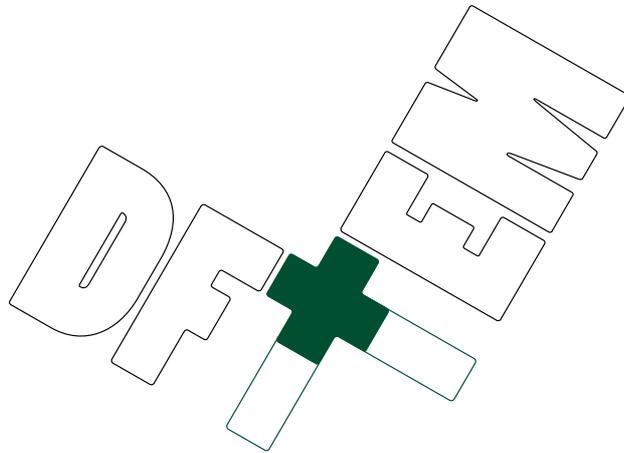


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**DFTEM 2006 – bringing together two communities**

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Density Functional Theory and  
Transmission Electron Microscopy

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## Karlheinz Schwarz

Peter Blaha

During this conference we celebrate the 65th birthday of Karlheinz Schwarz, the father of the WIEN2k program. As one of his scholars, it is my pleasure to write a few lines on this occasion.

Karlheinz was born in Vienna and studied Chemistry at the University of Vienna. During his Dissertation with Prof. A. Neckel (promotion in 1968) he started with theoretical calculations in simple solids using Slaters original Augmented Plane Wave method. It is worth to remind the younger generation what computing during these days meant: Computers had a computing power of less than 1000 Flops (floating point operations per second), not Giga- or Tera-Flops as of today, almost no memory and storage had to be done on punched paper-tapes or cards. There was no keyboard, no mouse and no computer screen, there was only a card-reader and a line-printer. Every calculation was a unique experiment and Karlheinz had to spend several nights in the computing room, since the tapes had to be changed every couple of hours. Karlheinz is truly one of the pioneers of theoretical solid-state calculations.

After the successful completion of his PhD he was looking for a post-doc position, and of course the best place at that time was Gainesville/FL where John Slater was leading the developments in theoretical solid-state physics. Karlheinz was involved in the development of the  $X_\alpha$ -method, a predecessor of density functional theory, and optimized the  $\alpha$ -parameter for all elements. For quite some time this work was one of the most cited publications in this field. After an additional stay at the IBM Research Lab in San Jose/CA, he came back to Vienna and took a position at the TU Vienna, where he soon developed a strong group devoted to calculations of solids. Soon after the introduction of the LAPW method by O. K. Anderson he realized the potential of this method and started to work in this direction. At that time I had the opportunity to join his group and from then on I could benefit from his ideas, expertise and continuous support. It was the time when international competition became strong, because supercomputers like the famous Cray-1 were available, while in Vienna we still had to use old and overloaded mainframes. Due to these constrains and following a suggestion by S. B. Trickey Karlheinz started almost 20 years ago the development of a user-friendly computer code based on the LAPW method, called WIEN, which is now in the latest version WIEN2k one of the most well-known codes available.

Well recognized in the international community, Karlheinz was guest in several famous labs like the MPI Stuttgart, the Quantum Theory Group in Uppsala or the IBM Thomas J. Watson Research Center in Yorktown Heights, NY. He chaired several Gordon-conferences and also organized the DFT97 conference in Vienna.

Besides his everlasting love for science, Karlheinz is happily married with Christine Schwarz, who is supporting him in every respect. He is proud of his daughter Caroline and two sweet grandchildren. In his spare time he very much enjoys classical music – in his youth he even considered a carrier as musician instead of becoming a scientist. He is an expert in alpine skiing, and for quite some time the unofficial requirement for joining his group was to be a good skier.

With these personal comments I would like to conclude, but not before thanking Karlheinz for all his support and encouragement during the last 25 years.