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Editorial

Dedication: Commemorative Issue in Honor of Professor Karlheinz Schwarz on the Occasion of His 80th Birthday

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Karlheinz Schwarz was born in January 1941 in Vienna (Austria), and he married Christine Schwarz in 1969. They have one child (Caroline), and he is a happy grandfather of four grandchildren. Besides his passion for science, he likes classical music. In fact, when he was young, he was not sure whether he should study chemistry or music, and maybe he would have become a virtuoso pianist instead of a famous scientist. Another passion was skiing; he even became a skiing instructor and impressed (and taught) numerous colleagues at various winter conferences in the mountains with his elegant style.

He studied Chemistry at the University Vienna and obtained his PhD under the supervision of A. Neckel in 1968, where he performed the first theoretical solid-state calculations in Austria using the APW method. I still remember his stories about all the problems he had to solve due to the limited computer resources at that time, including sleeping at the computing center because he had to remount tapes several times during the night, when such a calculation was running.

After his PhD, he worked as a postdoc in John C. Slater's group in Gainesville, FL, and later with Frank Herman at the IBM Research Lab in San Jose, CA. With his programming skills, developed during his PhD in Austria, he could impress the leading solid-state theory groups and speed up their codes by an order of magnitude. He came into contact with the X-alpha method—a predecessor of modern DFT—and optimized the alpha parameter for all atoms in a clever and unique way. The corresponding paper [1] was one of the most cited theory papers at that time.

Coming back from the US, he completed his Habilitation in "Quantum Chemistry" at the Technical University of Vienna, where he became a professor in 1976. His scientific reputation and active scientific life led to many invitations, and he was a guest professor at the Universities of Bochum, Uppsala, Montreal, Duisburg, Gainesville and Paris. He was a research fellow in Tsukuba, Japan, and six times a summer faculty member at the IBM T.J. Watson Research Center, where he worked intensively with Art Williams and Vic Moruzzi. During these times, his interest turned towards magnetism [2] and concepts such as "covalent magnetism" [3] and the "fixed-spin method" (FSM) [4], which laid the foundations to explain the Invar alloy problem [5].

Together with S.B. Trickey, P. Sorantin and myself, he formed the basis for the WIEN code, a full-potential all-electron augmented plane-wave-based computer program. This code, first published in 1990 [6], developed over the years into the WIEN2k code [7,8], a powerful and widely used package able to calculate many different properties of solids. In particular, it is famous for its unprecedented accuracy in solving the Kohn–Sham equations, often referred to as the "DFT limit". This user-friendly program is licensed by more than 3500 groups worldwide in academia and industry and still serves as a benchmark for all newly developed solid-state codes.

Although science was his passion, as a professor, he also served in many management positions. He was department head for 4 years and vice-head/head of the "FG Chemie"

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for more than 8 years. He served as president of the "Chemisch-Physikalische gesellschaft" and of the Austrian Fulbright Alumni Association, paying back the support he received from the Fulbright Association as a young postdoc. Realizing how important a good computer infrastructure for a modern university will be, he became head of the computing center of the Technical University of Vienna (TU Wien) in 1990 and later on head of their advisory board.

Karlheinz Schwarz realized early how important dissemination and discussions with colleagues are, and besides giving excellent invited talks at many conferences, he organized several conferences or served in the corresponding advisory boards. He was chairman of two Gordon conferences ("Phase transitions in non-metallic solids", Volterra, Italy, 1994, and "Electron densities and chemical bonding", Oxford, UK, 1998), and he founded and chaired the famous conference series "Workshop on Novel Materials and Superconductors" at Planneralm and Obertraun for an amazing 32 years (1989–2017). Similarly, to promote our WIEN2k code, he organized 26 WIEN workshops all over the world (Italy, France, Poland, the USA, Canada, Iran, Singapore, Japan and Austria). He was a very good friend of Walter Kohn [9], and his invitation to two conferences organized by Schwarz in Vienna (International Conference on DFT 1997 and Applied DFT2001) helped to settle the relation of Walter Kohn with his country of birth.

Personally, I met Karlheinz Schwarz in 1979 when I was a young chemistry student at the Technical University of Vienna and attending a course on "Solid state theory" given by him. Although most students had problems at the beginning to digest "strange concepts" such as the "reciprocal lattice" or "periodic boundary conditions", our passionate teacher explained this so well and with unique enthusiasm that this topic really started to catch my interest. When I finally realized that K. Schwarz was a scientist with the highest international experience and reputation, I was very happy to accept his offer to start a PhD under his supervision. He introduced me to the LAPW method, and this was the beginning of a deep friendship and, for me, due to his never-ending support, the start of my career. (P.B.)

I met Karlheinz Schwarz for the first time in Montreal, in 1981, where we crossed as postdocs in the Dennis Salahub group. For me, he was the famous author of the optimization of the α statistical exchange parameter [1] I cited and used in all my MS-Xα calculations, e.g., [10,11]. Later, at the beginning of the 1990s, he participated for the first time in the series of DFT congresses we initiated with the passed Alessandro Bencini and Annick Goursot. He organized the meeting in 1997 in Vienna and became more or less the leading member of the scientific committee of the series of these meetings. I am glad that a respectable number of friends (18) accepted to write a paper in this dedicated issue. We can notice the large panel of scientific topics covered by Karlheinz's knowledge. We deeply acknowledge the following contributions related to spectroscopy by Manuel Yañez et al. [12], Juan-Carlos Sancho-García and Emilio San-Fabián [13]; excited states by Ágnes Nagy [14], Kalidas Sen et al. [15] and Fabrizia Negri et al. [16]; DFT developments by Fabio Della Sala et al. [17], Mathias Rapacioli and Nathalie Tarrat [18], Emmanuel Fromager et al. [19], José Manuel García de la Vega et al. [20] and Harry Ramanantoanina [21]; results analysis by Andreas Savin et al. [22] and Manuel Richter et al. [23]; and, of course, the solid state and surfaces by Leila Kalantari and Fabien Tran et al. [24], Denis Salahub et al. [25], Peter Blaha et al. [26], Samuel B. Trickey [27], William Lafargue-Dit-Hauret and Xavier Rocquefelte [28], Tzonka Mineva and Hazar Guesmi et al. [29]. (H.C.)

Conflicts of Interest: The authors declare no conflict of interest.

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