

## Curriculum vitae

Name: **Karlheinz Schwarz** Title: **Univ.Prof.Dr.phil.**  
Birthdate: 16 Jan. 1941 Place of birth: Vienna, Austria  
Nationality: Austria Sex: Male  
Married with Dr.Christine Schwarz (Schuppich), one daughter Caroline (born 1972) and four grand children.

### Education: *Chemistry*

University of Vienna, Austria	Ph.D.	1968
Institute of Physical Chemistry		
Techn. Univ. Vienna	Venia Docendi (Habil)	1974
Techn. Univ. Vienna	Professor	1976 (retired since Oct.2006)

### Major Research Interests:

Electronic structure calculations (within density functional theory)  
Development of the WIEN2k code (used worldwide by about 3500 groups)  
based on the LAPW (linearized augmented plane wave) method  
Band structure and chemical bonding, Itinerant magnetism  
Relation between electron density, total energy, and properties of materials  
Ab-initio calculations of electric field gradients  
Car-Parrinello type ab-initio molecular dynamics calculations  
Refractory metals, intermetallic compounds, superconductors, minerals,  
zeolites, organometallics, holographic materials, surfaces  
computational physics and chemistry, parallelization

### Publications:

More than 360 publications in major international physics and chemistry journals  
(Nature, Science, Phys.Rev., Phys.Rev.Lett., J.Phys.Cond.Matter, J.Magn.Magn.Mat.,  
PCCP.,Angew.Chem.,Solid St. Commun., J.Amer.Chem.Soc., J.Appl.Phys., PNAS,  
J.Comp.Phys., J.Chem.Phys., Inorg.Chem., Int.J.Quantum Chem., Theoret.chimica Acta,  
Nature, Acta Cryst., Comput.Phys.Commun., Euro Phys. J., Computation, Molecular Physics,  
Chem.Phys.Lett., etc)

### Career, affiliations and scientific activities:

**1967-1968** Institute for Statistics (Univ. Vienna)  
**1968-1969** Institute f. Physical Chemistry (Univ. Vienna)  
**1969-1971** Post Doctoral Scientist with Prof. J.C.**Slater** at the Quantum Theory Project,  
University of Florida, Gainesville, Florida, USA.  
**May-Aug.1971** and **July-Sept.1972** Post Doctoral Scientist am Department of Large Scale  
Scientific Computations, **IBM** Research Laboratory, San Jose, California, USA.  
**1971-1998** Institute f. Technical Electrochemistry (Vienna Univ.Techn.)  
**since 1999** Institute f. Physical and Theoretical Chemistry (Vienna Univ.Techn.)  
**June-July 1974** Guest scientist at Max-Planck-Institute for Solid State Research, **Stuttgart**.  
**1975** Venia docendi (**Habil.**) for Quantum chemistry (Vienna Univ.Techn.)  
**Dec.1976** **Professor** at Vienna Univ.Techn. and head of *Theoretical Solid State Chemistry*  
**April 1977** Guest prof. Ruhr-Universität **Bochum**, Germany  
**Feb.-July 1978** Guest prof. at Univ. **Uppsala**, Schweden; Quantum Chemistry Group.  
**July-Sept.1981** Guest prof. at Université de **Montreal**, Canada.

**Aug.1981** Consultant at **IBM T.J.Watson Research Center, Yorktown Heights, NY, USA**  
**April 1983** Guest prof. in **Japan**.  
**July-Sept.1983, 1984, 1985, 1986, 1989** Summer Faculty Member at  
**IBM T.J. Watson Research Center, Yorktown Heights, New York, USA.**  
**Sept. 1987** Guest prof. at Ruhr-Univ. **Bochum/Duisburg, BRD**  
**Sept.-Oct. 1988** Guest prof. at Quantum Theory Project, University of Florida,  
**Gainesville, Florida, USA**  
**1992** Joint Project with **IBM Zürich Research Laboratory, Rüschlikon, Switzerland**  
**March-April 1994** STA (Science and Technology Agency) Fellow at NIRIM (National  
Institute for Research in Inorganic Materials), **Tsukuba, JAPAN**  
**May 1994** Chairman of **Gordon** Research Conference on  
"Phase Transitions in non metallic solids", **Volterra (Italy)**, 8-13 May, 1994  
**Sept. 1997** Chairman of the **DFT97** conference, "7<sup>th</sup> Intern.Conference on the application of  
the density functional theory in chemistry and physics", Vienna 1997  
**Sept 1998** Chairman of **Gordon** Research Conference on "Electron Distribution &  
Chemical Bonding", **Oxford, UK**, 30.Aug.-4.Sept, 1998  
**May 2000** Université Pierre et Marie Curie, **Paris, France**  
**Oct. 2006** retired, but still active

#### Organisational Activities:

**1979-1983** **Head** of Institute for Technical Electrochemistry, Techn. Univ. Vienna  
**1980-1988** Member **Advisory Editorial Board:** Intern. J. of Quantum Chemistry  
**1990-1994** **Head** of **Computing Center**, Techn. Univ. Vienna  
**1993-1999** Vice-chairman of **Department of Chemistry**  
**1993-1995** **Co-ordinator** of the Inter-University Cooperation Programme (**ICP**)  
ICP-93-A-3008/13 (**Erasmus**) *Computational Physics and Chemistry*  
**1988-1994:** **Co-ordinator** of the Austrian activity on "*High-temperature superconductivity*"  
**1991-1995** Member of **Beirat** Fritz-Haber Institute, Max-Planck-Society, Berlin  
**1991-1995** Member of the International Committee on Nuclear Quadrupole Interaction  
**1996-1999** Chairman of IUCr Commission on "Charge, Spin and Momentum Densities"  
**1998/99** President of **Chemical Physical Society**  
**1999-2018** President of the Austrian **Fulbright alumni**  
**1999-2001** Chairman of **Department of Chemistry**  
**2000-2004** Editorial board of *Zeitschrift für Kristallographie*  
**1999-2003** Member of **Senat** Vienna Univ.Terchn. (**Vice-Chair 2001-2003**)  
**Since 2013** **Editor in chief** of *Computation* (MDPI)

#### Organiser of conferences and workshops

**1997** **DFT Conference** in Vienna (with Walter Kohn as invited speaker)  
**1988-2016** Workshop: **High Tc superconductors** and Novel Materials (skying conference)  
Friedberg, Velm, Wien, (1988) Mallnitz (1989), Obergurgl (1990)  
Panneralm (1991-1993), Sekarhaus (1994, 1995), Planneralm (1996-2013),  
Obertraun (2014-2016)  
**1995-2000** **Wien workshops** (Vienna, Triest 1998)  
**2001-2019** **Wien2k workshops**  
Vienna (2001,2003, 2006, 2008, 2017, 2019), Esfahan, Iran (2002),  
Kyoto (2005), Tokyo (2012), Boston USA (2018), McMaster, Canada (2016),  
Penn State, USA (2002, 2004, 2007, 2009, 2011), Singapore (2007, 2015),  
Nantes, France (2010, 2014), Warsaw; Poland (2014)

**Awards:**

1972 IBM World Trade Fellowship

1972 SANDOZ-Award

1975 Cardinal Innitzer Award for Natural Sciences

1994 Science and Technology Agency (STA) Fellowship Award, Japan

1995 Rudolf Wegscheider-Award of the Austrian Academy of Sciences

2001 Corresponding member of the Austrian Academy of Sciences

2006 Foreign Member of The Royal Society of Sciences at Uppsala (founded 1710)

2007 Award from the City of Vienna

2012 Viennese Engineering Award (Wiener Ingenieurpreis)

2016 Zsigmondy-Medaille (TU Vienna, Chemistry Faculty)