Prof. Martin Quack
Emeritus Professor for Physical Chemistry

- Dr es sces techn EPF Lausanne 1975
- Max Kade Fellow, University of California, Berkeley 1976/77
- Habilitation Universität Göttingen, 1978 (Priv .Doz. and Prof. C2 until 1982)
- Full Professor (C4), Universität Bonn 1982–1983
- Professor for Physical Chemistry (Head of Group Molecular Kinetics and Spectroscopy) at ETH Zurich 1983–2013
- Member of the Research Council of the Swiss National Science Foundation 2002–2011
- President (1. Vorsitzender) of the Bunsen Society 2011–2012
- Elected Member of the Presidium of the German Academy of Sciences Leopoldina 2014–present
- Chairman of the ETH Zurich Prize Committee 2016 –present

Acknowledgement of main funding sources (past and present)

- European Research Council ERC Advanced Grant
- Swiss National Science Foundation Research Grants
- Alliance for Global Sustainability (Avina Foundation) grant on project 'Spectroscopic Approach Towards Local and Global Management of the Earth's Atmosphere'
- COST project MOLIM (Molecules in Motion)
- ETH Zurich research and equipment grants

Research highlights and future priorities

The group "Molecular Kinetics and Spectroscopy" of Martin Quack has as main research theme "Molecules in Motion", the understanding of fundamental, physical-chemical molecular primary processes (see M. Quack, Chimia 55 (2001), 753–758). The basic research question concerns the fully quantum mechanical molecular motion which is at the origin of all chemical reactions. An essential aspect of the research is the systematic combination of experimental and theoretical studies. The experimental studies concentrate on high resolution infrared spectroscopy, infrared multiphoton excitation and time resolved kinetic spectroscopy. While most of the experiments address fundamental questions, some practical applications relate to atmospheric and astrophysical spectroscopy and to isotope separation. The theory covers full-dimensional quantum dynamics by discrete variable representation techniques, finite basis set representation as well as diffusion quantum Monte Carlo methods. Approximate theories are developed and tested in relation to exact theories (an example is the quasiadiabatic channel reaction path Hamiltonian theory for tunnelling reactions). Another focus of theory is the time dependent quantum dynamics in intramolecular energy flow and vibrational redistribution, coherent infrared multiphoton excitation and laser chemistry as well as time dependent quantum statistical mechanical approaches to these processes. Finally, the group studies fundamental symmetry principles in molecular processes and molecular chirality in relation to parity violation. The theoretical developments in the group have led to large increases in the predicted parity violating energy differences between the enantiomers of chiral molecules D_{pv} (by up to a factor 100), making these now a realistic goal for their current experiments.

The group has been leading high resolution Fourier Transform Infrared Spectroscopy including several prototype spectrometers over several decades and a current (2009) prototype at the Swiss Synchrotron Light Source (SLS) with a proven resolution of better than 0.0006 cm^{-1} and a resolving power approaching 2×10^6 , still unique worldwide.The group has also developed several time resolved and non-time resolved high resolution infrared laser spectroscopic techniques combined with molecular beams. A recent experiment, a laser-molecular beam setup following a special scheme originally proposed by M. Quack in 1986 has been successfully demonstrated to reach a sensitivity sufficient to measure a D_{pv} of about 100 aeV, which can be translated into a resolving power of better than 10^{15} (in the infrared-visible-UV range). With these techniques numerous results on molecular primary processes have been obtained. Using the method of extracting the time dependent molecular quantum dynamics from non-time resolved high resolution molecular spectra developed in this research as an alternative to the common techniques of short time pump probe kinetic spectroscopy, it was discovered, that different functional groups can show very different time scales for intramolecular energy flow ranging from less than 100 fs in the alkyl-CH chromophore to more than 100 ps in the acetylenic CH-chromophore, for example. This has led to the concept of the quantum dynamics of functional groups related to highly mode specific intramolecular energy flow. The femtosecond pump-probe experiments of the group with bichromophoric molecules have corroborated these results also for these exceptional prototype molecules. The results are of importance also for infrared multiphoton excitation, where the group has established for the first time the infrared multiphoton pre-ionization of a polyatomic molecule (C_{60}) as well as nuclear spin hyperfine resolved product state distributions (in Iodine atoms arising from the dissociation of organic iodides). The group has also provided the first fully-6-dimensional vibrational-tunnelling quantum dynamics of stereomutation reactions for transiently chiral molecules with the example of hydrogen peroxide (HOOH). This has recently been extended to fully 9-dimensional results (including all rotational and vibrational degrees of freedom) in the prototype system ammonia (including chiral NHDT). Further results concern the full-dimensional quantum tunneling dynamics derived from high-resolution spectroscopy of the hydrogen bonded dimer $(HF)_2$ as well as larger clusters $(HF)_n$ and their isotopomers (including the first infrared spectroscopic detection of nanoclusters).

A theoretical framework has been established which allows the interpretation of the vastly different time scales for intramolecular primary processes in terms of successive symmetry breakings. This includes the first formulation of

Major honors and awards

- 2017 Foreign Honorary Member, American Academy of Arts and Sciences
- 2014 Corresponding Member, Academy of Sciences, Göttingen
- 2012 August Wilhelm von Hofmann Denkmünze, GDCh
- 2009 Dr honoris causa University of Göttingen
- 2005 Visiting Miller Research Professor, University of California, Berkeley
- 2002 Paracelsus Prize, Swiss Chemical Society
- 1999–present Elected to Berlin Brandenburg Academy of Sciences
- 1998–present Elected to German Academy of Sciences Leopoldina
- 1991 Otto Bayer Prize
- 1990 Fellow of the American Physical Society
- 1984 Otto Klung Prize (Berlin)

Research collaborations

- **Within ETH Zurich:** F. Merkt
- **Within Switzerland:** EPFL, T. Rizzo; SLS/PSI, P. Lerch and others
- **International:** Tomsk University, O. Ulenikov; University of Braunschweig, S. Bauerecker; University of Budapest, A. Császár; University of Strasbourg, R. Marquardt; University of Munich, O. Trapp; Lanzhou University, China, Z. Chen; Kingston University, Canada, T. Carrington; Leader WG2 EU COST project MOLIM (Molecules in Motion)

Memberships

- Ownership Board Physical Chemistry Chemical Physics, Royal Society of Chemistry
- Board of Molecular Physics
- Co-editor Chemistry, Molecular Sciences and CHEMICAL Engineering (Elsevier) and Hot Topic Book
- Board of Division Fundamental Research Swiss Chemical Society
- Numerous previous boards

detailed state to state symmetry selection rules for chemical reactions, based on the approximate conservation of nuclear spin symmetry and parity subsequently tested and confirmed by experiments.

Teaching activities

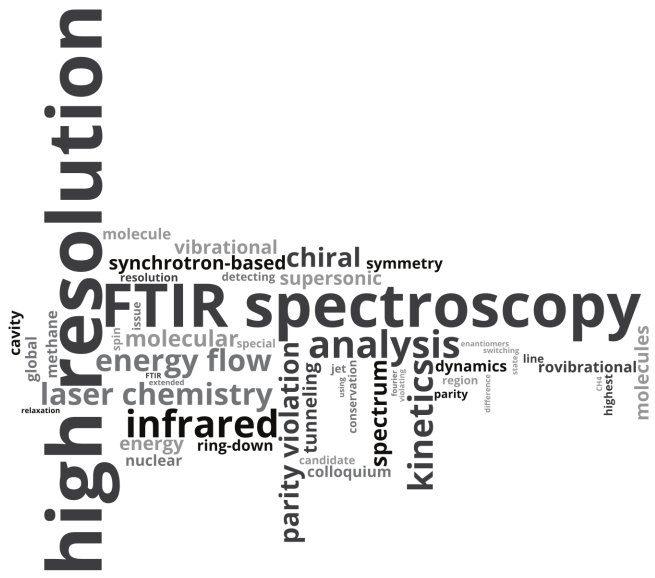
Martin Quack taught continuously various courses in the physical chemistry curriculum, but stopped course teaching in 2013 as Emeritus, continuing to hold research seminars etc.

Promotion of young academics

Martin Quack has for many years been responsible for the curriculum Interdisciplinary Natural Sciences from 1992 in the Department (as 'Delegate for Studies' until 2008 and then still as deputy of F. Merkt in this function until 2013). He has advised the students in this select group personally and individually encouraging them to independent thinking and to developing their own academic personality. Many of his previous Master and doctoral students and postdocs have become professors and major research group leaders all over the world (see Mol. Phys. 11 (2013), 1939–63 for details).

Challenges, opportunities, and outlook

The new orders of magnitude derived from their theory of molecular parity violation combined with their experimental developments make the measurement of parity violating ground state energy differences of enantiomers in the order of 100 aeV to 1 feV a realistic goal for experiments. The current work concentrates on this topic. They have identified by theory and spectroscopy some molecules where this experiment should be feasible and the current challenges arise from the analysis of the very complex vibration-rotation-tunneling spectra of the corresponding molecules which have to be unraveled in order to afterwards apply the existing 'Zurich experimental laser-molecular beam set-up' to a suitable chiral molecule. A successful experiment will be the very



first ever detection of the parity violating energy difference between the enantiomers of chiral molecules in the ground state as well as of the time dependent primary process of parity change in isolated molecules. This has significance for fields as diverse as fundamental symmetries and the Standard Model of high energy physics as well as possibly the evolution of biomolecular homochirality. The methodology has also potential for future quantum technology (as exemplified by the recent demonstration of a molecular quantum switch).

10 key publications

Kushnarenko A et al. (2018). Intramolecular vibrational energy redistribution in $HCCCH_2X$ (X = Cl, Br, I) measured by femtosecond pump-probe experiments in a hollow waveguide. Phys Chem Chem Phys 20: 10949–59 10.1039/c7cp08561c

Fábri C et al. (2018). A molecular quantum switch based on tunneling in meta-D-phenol C_6H_4DOH. Phys Chem Chem Phys. 20: 7387–94 10.1039/c8cp00133b

Albert S et al. (2017). High-resolution FTIR spectroscopy of trisulfane HSSSH: a candidate for detecting parity violation in chiral molecules. Phys Chem Chem Phys. 19: 11738–43 10.1039/C7CP01139C

Quack M (2016). Die Spiegelsymmetrie des Raumes und die Chiralität in Chemie, Physik, und in der biologischen Evolution. Nova Acta Leopoldina NF 412: 119–66 (in „Symmetrie und Asymmetrie in Wissenschaft und Kunst", M. Quack und J. Hacker eds, Book with 275 pages and contributions in English and German by several authors)

Albert S et al. (2016). High resolution GHz and THz (FTIR) spectroscopy and theory of parity violation and tunneling for 1,2-dithiine ($C_4H_4S_2$) as a candidate for measuring the parity violating energy difference between enantiomers of chiral molecules. Phys Chem Chem Phys. 18: 21976–93 10.1039/C6CP01493C

Dietiker P et al. (2015). Infrared laser induced population transfer and parity selection in $^{14}NH_3$: A proof of principle experiment towards detecting parity violation in chiral molecules. J Chem Phys 143: 244305 10.1063/1.4936912

Prentner R et al. (2015). Wavepacket Dynamics of the axially chiral molecule Cl-O-O-Cl under coherent radiative excitation and including electroweak parity violation. J Phys Chem. A 119: 12805–22 10.1021/acs.jpca.5b08958

Quack M (2014). On biomolecular homochirality as a quasi-fossil of the evolution of life. Adv Chem Phys. 157: 249–290 10.1002/9781118959602.ch18

Albert S et al. (2011). Synchrotron-based highest resolution Fourier transform infrared spectroscopy of naphthalene ($C_{10}H_8$) and indole (C_8H_7N) and application to astrophysical problems. Faraday Discuss. 150: 71–99 10.1039/C0FD00013B

Quack M (2011). Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy in Handbook of High Resolution Spectroscopy, M. Quack and F. Merkt editors, Wiley, Chichester, New York, Vol. 1: 659-722, 10.1002/9780470749593.hrs077