

# Professor Lauri Halonen's Curriculum Vitae

Born 29th November 1953 in Helsinki, married, three children

Web page: <http://www.helsinki.fi/kemia/fysikaalinen/research/molspec/index.html>

## Personal data

### Education:

M.Sc. 1976 (Department of Chemistry, University of Helsinki)

Ph.D. 1980 (Department of Chemistry, University of Reading, Reading, England, with Prof. I. M. Mills)

D.Sc. 1994 (University of Reading)

Docent in Physical Chemistry 1983 (University of Helsinki)

### Current positions:

Professor of Physical Chemistry, University of Helsinki 1992 –

Head of the Physical Chemistry Laboratory 1992 –

### Extended visits abroad (altogether about 11 years):

Graduate studies with Prof. I. M. Mills, University of Reading, Reading, England, April 77 – Sept 80

SRC Post-Doctoral Fellow with Prof. M. S. Child, University of Oxford, England, Oct 80 – Sept 82

Academic Visitor, Physical Chemistry Laboratory, ETH, Zürich, April 85 – Dec 86

Visiting Professor, Department of Chemistry, Princeton University, USA, Aug 95 – Aug 96

JILA Visiting Fellow, JILA, University of Colorado, Boulder, Colorado, USA, Aug 99 – Aug 00

University College London, England, Aug 04 – July 05 (altogether about 4 months)

Department of Chemistry, University of Copenhagen, Denmark, Aug 10 – Feb 12 (about 4 months)

Invited visiting Professor, Université Paris Est (Marne-la-Vallée), June 2012 (one month)

### Honours:

Corresponding member in Akademie der Wissenschaften zu Göttingen (<https://adw-goe.de/startseite/>), 2015

Member in the Finnish Academy of Science and Letters (<http://www.acadsci.fi/frontpage.htm>), 1995  
(past chair of the chemistry division)

JILA Visiting Fellow 1999 – 2000 (<https://jila.colorado.edu/>)

Honorary Research Associate at the University College London, Aug 04 – July 05

3-eme Cycle in Switzerland, Basel, Lausanne, Geneva and Bern (series of lectures), Nov 2008

Visiting Professorship, Université Paris Est (Marne-la-Vallée)

## Funding (outside normal university budgets)

University of Helsinki 1990 – 2006: 0.76 M€

EU: 0.57 M€

Academy of Finland (Finnish Science Research Council): 1988 – 2014: 5.01 M€

## International contacts

### Management Committee memberships in European Cooperation in the field of Scientific and Technical Research (COST):

- 1) COST CM0805, The Chemical Cosmos; Understanding Chemistry in Astronomical Environments, 09 –13
- 2) COST CM1002, Convergent Distributed Environment for Computational Spectroscopy, 10 – 14
- 3) COST CM1401, Our Astro-Chemical History, Short term scientific mission officer (STMS), 14 -18 ([http://www.cost.eu/domains\\_actions/cmst/Actions/CM1401](http://www.cost.eu/domains_actions/cmst/Actions/CM1401))
- 4) COST CM1405, MOLIM: MOLEcules In Motion, 14-18 ([http://www.cost.eu/COST\\_Actions/cmst/Actions/CM1405](http://www.cost.eu/COST_Actions/cmst/Actions/CM1405))

## EU activities:

- 1) HCM network *Spectroscopic Investigation of Hydrides in Highly Excited Rovibrational States Allowing the Modelling of Potential Energy Surfaces within and beyond the Experimental Accessible Regions*, 1995-96, 23 750 ECU
- 2) TMR network *Potential Energy Surfaces for Molecular Spectroscopy and Dynamics (THEONET I)*, 1996-00, 90 620 ECU
- 3) Improving Human Potential Network *Spectroscopy of Highly Excited Rovibrational States (SPHERS)*, 2000-03, 125 000 euro
- 4) Improving Human Potential Network *Theoretical Studies of Electronic and Dynamical Processes in Molecules and Clusters (THEONET II)*, 2000-04, 132 200 euro
- 5) Marie Curie Research Training Network *Quantitative Spectroscopy for Atmospheric and Astrophysical Research (QUASAAR)*, 2005-09, 198 378 euro

**Foreign collaborators:** H. Kjaergaard (Copenhagen), R. Hinde (Tennessee), F. Harren (Nijmegen), G. Johanson (Stockholm), K. Buse (Freiburg), K. Vodopyanov (Florida), J. Tennyson (London), B. Gerber (Jerusalem), C. R. Phillips (ETH, Zürich),

## Research surrounding

**Research topics:** Molecular spectroscopy including laser and Fourier transform infrared spectroscopy and applications to human breath, development of new infrared laser systems, computational quantum chemistry including density functional theory of continuous matter and high-precision *ab initio* calculations on molecules and metal clusters, atomic and molecular interactions at long distances and theoretical chemistry

**Scientific achievements:** Development of the local mode model including vibration and rotation, discovery of vibrational Renner-Teller effect, geometric algebra applied to molecular problems, high-order coupled cluster theory applied to ammonia, simulation of spectroscopic and thermodynamic properties of molecular complexes. simple dispersion interaction models between atoms of different metals clusters, energetics and the role of entropy in water clusters, the non-existence of ferroelectricity in ice, deprotonation reactivity of acids on ice surface defects, quasi-liquid layer of ice and wet quartz surfaces, first intracavity photoacoustic experiment with a Titanium:Sapphire ring laser, high-repetition rate laser cavity ring-down experiment, first stimulated emission pumping experiments with continuous wave infrared lasers, development of continuous wave parametric oscillators in the mid-infrared region, frequency-comb-referenced mid-infrared source for high-precision spectroscopy, frequency comb generation in near- and mid-infrared based on cascaded quadratic nonlinearities, first quantitative observation of acetylene in exhaled human breath and a clarification of the high ammonia concentration in exhaled human breath

**Research group:** 3 senior scientists, 2 post-doctoral fellows, 6 graduate students

**Past and present foreign postdoctoral fellows:** 16 (Italian (3), German, Russian, Chinese (2), Austrian (2), Polish (2), Spanish (3), Australian and American)

**Visiting professors:** Qingshi Zhu (Dalian, China, 2-3 months, 90), Robert Hinde (Univ. of Tennessee, 6 months, 07, 12), Marie-Pierre Gageot (Paris, 1 month, 12) and Benny Gerber (Univ. of Jerusalem, currently)

## Major laboratory equipment:

- (1) Home-built continuous wave optical-parametric-oscillator (cw OPO) systems, 2400 – 3700  $\text{cm}^{-1}$ , pumped by Yb-fiber and Titanium:Sapphire ring lasers
- (2) Coherent Titanium:Sapphire/dye ring laser 899-21, 700 – 1100 nm and Titanium:Sapphire ring-laser MBR-110, 700 – 1100 nm
- (3) Coherent Neodymium Vanadate Lasers Verdi 10 W, 532 nm and 18 W, 532 nm
- (4) Diode laser New Focus Velocity 6328, 25 mW, 1520 – 1570 nm
- (5) High-resolution infrared interferometer Bruker IFS 120HR, 400 – 20 000  $\text{cm}^{-1}$ , max res. 0.002  $\text{cm}^{-1}$

- (6) Ytterbium fiber lasers 15 and 20 W, 1064 nm, single mode, linearly polarized, mode hop free scanning range > 40 GHz
- (7) EXFO wavemeters 600 – 4000 nm, resolution 60 MHz
- (8) Picarro G2103 Trace Ammonia Analyzer.

**Supervised doctoral dissertations:** 14. Tuomas Lukka, 20 years old, was the youngest ever in independent Finland. He is one of the founders of Zenrobotics Ltd (<http://www.zenrobotics.com/product/>). Currently, we have 6 graduate students.

**Centre of Excellence, (Academy of Finland):** *Computational Molecular Science* 2006-2011 with 5 groups. Halonen was the vice-director 2006-2008 and the director 2009-2011. (<http://www.chem.helsinki.fi/Research/CMS>).

**Graduate School:** Graduate School of *Computational Chemistry and Molecular Spectroscopy* (<http://www.laskemo.fyke.fi/>), where Halonen was the director 1998-2011.

**FiDiPro Professorship project of the Academy of Finland:** Professor Benny Gerber from Jerusalem is spending about 6 months yearly in Helsinki in 2011-2015

**Major international conferences arranged/to be arranged:**

- 1) *Theoretical Studies of Electronic and Dynamical Processes in Molecules and Clusters*, (THEONET II), in Katajanokka, Helsinki in September 2001, about 60 participants from Europe.
- 2) *30th International Symposium of Free Radicals* in Savonlinna in July 2009 (<http://www.helsinki.fi/kemia/FRS2009/>). More than 160 participants from 20 different countries. **Guest editor** of the conference issue: *J. Phys. Chem. A*, **2010**, *114* (14).
- 3) *Optics Days 2013*, in May 2013 in Helsinki (<http://www.helsinki.fi/kemia/OD2013/>). It has been arranged almost yearly since the foundation of the Finnish Optical Society, FOS, in 1996. Three plenary speakers from abroad and about 30 invited, short presentations of mainly young scientists. About 120 participants.
- 4) *The Twenty-Fifth Colloquium on High Resolution Molecular Spectroscopy* in Helsinki, August 2017. Expected number of participants is 200 -400.

**Reviewer:** *Opt. Express*, *J. Chem. Phys.*, *J. Phys. Chem.*, *Mol. Phys.*, *Appl. Phys. B*, *Chem. Phys. Lett.*, *PCCP*, *Chem. Phys.*, *J. Mol. Spectrosc.*, American, Danish, Dutch and Swiss National Science Foundations etc.

**Publications:** 189 publications. The *h*-index is 38. Citations over 5000 (Web of Science).