

## Jozef Noga - C U R R I C U L U M V I T A E

**Born:** January 16, 1955 in Bratislava, Slovakia

**Citizenship:** Slovak

**Family status:** married (since 1981 with Monika Kirschhofer, 5 children)

**Mailing address:**

Department of Inorganic Chemistry  
Faculty of Natural Sciences, Comenius University  
SK-84215 Bratislava, Slovakia

**Tel:** +421-2-60296349  
**Fax:** +421-2-60296273  
**E-mail:** jozef.noga@fns.uniba.sk

**Education and academic qualification:**

- 1979 RNDr. - Physical Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava
- 1985 CSc. degree (equivalent to Ph.D.) in Chemical Physics  
Chemical Research Centre, Slovak Academy of Sciences (SAS), Bratislava
- 1995 DrSc. (Research Professor in Chemical Physics)
- 2003 Habilitation, Comenius University, Bratislava
- 2005 Inauguration, Comenius University, Bratislava

**Research and academic positions/appointments:**

- 1980 - 1983 Study stay, Faculty of Natural Sciences, Comenius University  
(1981, 1 year military service)
- 1983 - 1984 Lab. of Microanalysis, Geological Institute of Dionýz Štúr, Bratislava
- 1984 - Institute of Inorganic Chemistry (IIC), SAS, Bratislava
- 1985 - 1988 Research Scientist, IIC SAS
- 1986, 1988 Postdoctoral Research Associate, Quantum Theory Project,  
University of Florida, Gainesville, Florida, USA
- 1988 - 1993 Senior Research Scientist, IIC SAS
- 1993 - Leading Research Scientist, IIC SAS
- 1995 - 1999 Director of the Institute
- 1998 - 2005 Assoc. Guest Professor, Comenius University, Bratislava
- 1998 - 2003 Guest Professor, Laboratory of Astrophysics,  
University J. Fourier, Grenoble, France
- 2002 - dual position; also at Faculty of Natural Sciences, Comenius University
- 2005 - Professor of Chemical Physics, Comenius University
- 2008 - Head, Dept. of Inorganic Chemistry, Fac. Nat. Sci., Comenius University

**Awards and honors:**

- 1986 - Slovak Academy of Sciences Plaque for the Best Work of Young Scientists
- 1987 - The State Prize for Contributions in Quantum Chemistry (team of 7)
- 1990 - 1992 Alexander von Humboldt Fellowship (Ruhr-Universität Bochum, Germany)
- 2000 - elected, Fellow of the Slovak Academic Society
- 2001 - Werner von Siemens Excellence Award for Research (team of 4)
- 2001, 2006, 2010 - Slovak Literature Fund Premium for the Scientific Echo.
- 2002 - Slovak Academy of Sciences Prize for Research
- 2005 - Golden Medal of the Slovak Academy of Sciences
- 2005 - elected, Fellow of the Learned Society of the Slovak Academy of Sciences
- 2010 - Reinvitation by Alexander von Humboldt Foundation
- 2014 - elected, Member of the International Academy of Quantum Molecular Sciences

**Other relevant activities:**

- 1993-1995, 1999-2002 head - Scientific Board, Inst. of Inorg. Chem. SAS (elected)
- 1995-2001 member, Board of Scientists, SAS (elected)
- 1996- member, 2005-2009 chair, Collegium for the Chemical Sciences, SAS
- 1999-2000 vice-chairman, 2001-2002 chairman, Grant Agency of SAS and Ministry of Education of the Slovak Republic (elected)
- 2000-2007 president, Humboldt Club of the Slovak Republic

- 2007 - 2009 member, Accreditation Committee of SAS
- 2013 - chair, The Learned Society of SAS

**Research interests:** quantum chemistry, molecular electronic structure, electron correlation, *ab initio* many-body methods, explicitly correlated methods, electrical properties of molecules, electronic theory of extended systems, intermolecular interactions

**Summary of the scientific outputs:**

**Invited speaker:** > 45 invited talks on international conferences and lectures delivered at over 20 diverse international universities and research institutions

**Refereed publications:** 119, quoted > 5300 times (WOS), H-index 36

Thereof: **Invited book chapters and reviews:** 9                      **Textbooks:** 2 (in Slovak)

**Major projects supported (PI, last ten years):**

- Centre of Excellence: Integrated Center for Advanced Materials and Molecular Research of IIC SAS (FP5 IIC-MATMOL, 2003-05 EC: EUR 250000)
- COST D26/WG-12: Towards a new level of accuracy in computations of molecular structure, molecular properties, spectroscopy and thermo-chemistry. (2002-07, EC, coordinator)
- Centre of Excellence SAS: Centre for Advanced Computational Chemistry (2007-10 SAS: EUR 150000)
- Multireference explicitly correlated coupled cluster theory within the R12 approach (2009-12 RDA SR: EUR 50000)
- Explicitly correlated wave functions: Alternative approaches and their applications in calculations of spectroscopic parameters of small molecules (2008-12 RDA SR: EUR 83300)
- Novel coupled cluster based methods to treat systems with high degree of non-dynamical electron correlation. (2013-17 RDA SR: EUR 115950)

**Selected recent publications relevant to COST Action CM1401**

- O. Demel, S. Kedžuch, J. Noga, J. Pittner: Perturbative triples correction for explicitly correlated Mukherjee's state-specific coupled cluster method, *Molec. Phys.* **111**, 2477-2488 (2013)
- J. Šimunek, J. Noga: Optimised Thouless expansion second-order Møller-Plesset theory, *Molec. Phys.* **111**, 1119-1128 (2013)
- O. Demel, S. Kedžuch, M. Švaňa, J. Pittner, and J. Noga: Explicitly correlated Mukherjees state specific coupled cluster method: Development and pilot applications, *Phys. Chem. Chem. Phys.* **14**, 4753-4762, (2012)
- Kalju Kahn, Bernard Kirtman, Alexander Hagen and Jozef Noga: Convergence of Anharmonic Infrared Intensities of Hydrogen Fluoride in Traditional and Explicitly Correlated Coupled Cluster Calculations, *J. Chem. Phys.* **135**, 131103 (2011)
- S. Kedžuch, O. Demel, J. Pittner, S. Ten-no and J. Noga: Multireference F12 Coupled Cluster Theory: The Brillouin-Wigner Approach with Single and Double Excitations, *Chem. Phys. Letters*, **511**, 418 (2011)
- K. Kahn, B. Kirtman, J. Noga, S. Tenno: Anharmonic vibrational analysis of water with traditional and explicitly correlated coupled cluster methods, *J. Chem. Phys.* **133**, 074106 (2010)
- J. Noga and J. Šimunek: Solving the Independent-Particle Model via Nonunitary Transformation Based on Variational Coupled Cluster Singles, *J. Chem. Theory Comput.* **6**, 2706-2713 (2010)
- G. Czakó, B. Nagy, Gy. Tasi, A. Somogyi, J. Šimunek, J. Noga, B. J. Braams, J. M. Bowman, and A. G. Csaszar: Proton Affinity and Enthalpy of Formation of Formaldehyde. *Int. J. Quantum Chem.* **109**, 2393-2409 (2009)
- J. Noga, J. Šimunek: On the one-particle basis set relaxation in R12 based theories. *Chem. Phys.* **356**, 1-6 (2009)
- P. Valiron, Michael Wernli, A. Faure, L. Wiesenfeld, C. Rist, S. Kedžuch, and J. Noga: R12-calibrated H<sub>2</sub>O-H<sub>2</sub> interactions: Full dimensional and vibrationally averaged potential energy surfaces. *J. Chem. Phys.* **129** 134306 (2008)