C u r r i c u l u m V i t a e : Miroslav Urban

Born: June 6, 1942 in Martin (Slovakia).
Marital status: Married, two children

Education:

1959-1964	Faculty of Science Comenius University, Bratislava.
1964	Master degree in chemistry, Comenius University, Bratislava.
1968-1972	PhD. studies at Charles University and Czechoslovak Academy of Sciences, Prague (Supervisors: J.Koutecký, J.Paldus, later on R. Polák, R. Zahradník)
1972	Ph.D. in Chemistry, Charles University, Prague.
1989	Dr.Sc. in Physical Chemistry, Slovak Technical University, Bratislava

Appointments:

1964-1980	Assistant Professor at the Department of Physical Chemistry, Comenius University, Bratislava
1980-1990	Associate Professor at the Department of Physical Chemistry, Comenius University, Bratislava
1990-	Full Professor of Chemical Physics at the Department of Physical Chemistry, Comenius University, Bratislava
1990-1996; 2000-2007	Head of the Department of Physical Chemistry, Head of the Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava
2008	Professor of Theoretical and Computational Chemistry

Research activities:

1984 &1992	6-months, visiting scientist at the Quantum Theory Project, University of Florida, Gainesville, USA
1987-1996	several 1-2-months stays as a visiting scientist at the Max-Planck Institute for Astrophysics, Garching, Germany and at the Dept. of Theoretical Chemistry, University of Lund, Sweden
2001	1-months visit, Distinguished Senior Visiting Professor, Center for Computational Quantum Chemistry, University of Georgia, Athens, USA
2005	Visiting professor, University of Waterloo, Canada
1980,1985	2 books with P. Čársky: "Ab initio calculations. Methods and Applications in Chemistry", Lecture Notes in Chemistry, Vol. 16. Springer Verlag, Berlin, 1980. The book has received about 300 citations. Czech revised edition, 1985
1987	Review "Correlation effects in molecules" (with I Cernušák, V. Kellö and J. Noga) in Methods in Computational Chemistry, Vol. 1, Electron Correlation in Atoms and Molecules, ed. S.Wilson, Plenum Press, New York, 1987, pp 117-250.
1997	Review "Spin adaptations in the open shell coupled cluster theory with a single determinant restricted Hartree-Fock reference. (with P. Neogrády and I. Hubač) in Recent advances in

coupled cluster methods ed. R. J. Bartlett, World Scientific, Singapore, 1997, pp 275-306.

1967-2007 100 research papers in recognized international journals

Other professional activities:

Member of the Board of Directors of International Society for Theoretical Chemical Physics.

Member of the WATOC Scientific Board.

Chairman and a member of the Accreditation Commission, an advisory body of the Government of the Slovak Republic (1990-1995; 1998-2002).

Invited lectures, e.g. :

9th Symposium on Problems of Quantum Chemistry, 1978 Kühlungsborn, Germany;
4th and 5th School of Advanced Methods of Quantum Chemistry, 1985 and 1987 Bachotek, Poland;
Congress of the World Association of Theoretical Organic Chemists, 1987 Budapest, Hungary;
Quantum-chemical Micro symposium: Molecules and Solids, Methods and applications, 1993 Berlin, Germany;
1st Congress of the International Society for Theoretical Chemical Physics, 1993 Girona, Spain;
Workshop on electronic structure of complex systems, 1996 Budapest, Hungary
Electron Correlation: From Atoms to Biomolecules. Orenas, Sweden, 1997
9th International Congress of Quantum Chemistry, Atlanta, USA, 1997
11th European Seminar on Computational Methods in Quantum Chemistry, Zakopane, Poland, 1999.
Symposium on Recent developments in Computational Chemistry: Can Theory answer Questions in Applied Natural Sciences? Univ. for Bodenkultur, Wien, 2003
The Systematic Treatment of Electronic Correlation. A Celebration of the Science of Rodney J. Bartlett. Univ. of Florida, Gainesville, St. Simons Island, Georgia, USA; 2004
Response Theory and Molecular Properties. Aarhus Univ. Sonderborg, Denmark, 2004.
2006 International Conference of Computational Methods in Science and Engineering (ICCMSE 2006), Chania, Crete, Greece.

Awards:

1987 State Prize, Czechoslovakia, for research in theoretical chemistry (jointly with S. Biskupič, I. Hubač, V. Kvasnička, V.Kello, V. Laurinc, J.Noga)

1998 "Cristal Wing", an award for achievements in science, Slovakia

2000 Memorial medal of the Faculty of Science, on the occasion of the 60th anniversary of its foundation

2001 The Heyrovský medal, for achievements in chemical science, Czech Academy of Science, Prague, Czech Republic

2002 The Ilkovič medal for achievements in physical chemistry, Slovak Academy of Science,

2002 The Gold medal of the Comenius University, Bratislava

Teaching activities:

Lecturing: Theory of the chemical bond, Quantum chemistry, Quantum physics, Theory of chemical reactivity, Relativistic effects in chemistry

Published papers, 2002 - 2007

1. B. Jansík, V. Kellö, M. Urban; Dipole moments calculations of transition metal mono-nitrides: ScN, TiN, VN, and CrN. Limits of the CCSD(T) method. Int. J. Quantum Chem., **90**, 1240-1248 (2002).
2. P. Neogrády, M. Medveď, I. Černušák, M. Urban; Benchmark calculations of some molecular properties of O_2, CN, and other selected radicals using the ROHF-CCSD(T) method. Mol. Phys. **100**, 541-560 (2002).
3. A. Antušek, M. Urban, A. J. Sadlej; Lone pair interactions with coinage metal atoms: Weak van der Waals complexes of the coinage metal atoms with water and ammonia. J. Chem. Phys. **119**, 7247-7262 (2003).
4. M. Iliaš, V. Kellö, T. Fleig, M. Urban; Electric properties of the hydrogen iodide: Reexamination of correlation and relativistic effects. Theor. Chem. Acc. **110**, 176-184 (2003).
5. J. Raab, A. Antušek, S. Biskupič, M. Urban; A coupled cluster study of van der Waals interactions of the He atom with CN, NO and O_2 radicals. Collection Czech. Chem. Commun. **69**, 189-212 (2004).
6. V. Kellö, A. Antušek, M. Urban; Quasi-relativistic Coupled Cluster calculations of electric dipole moments and dipole polarizabilities of GeO, SnO, and PbO. J. Comp. Meth. Sci. Eng., **4**, 753-764 (2004).
7. M. Iliaš, H. J. Aa. Jensen, V. Kellö, B. O. Roos, M. Urban; Theoretical study of PbO and the PbO anion. Chem. Phys. Letters, **408**, 210-215 (2005).
8. F. Holka, P. Neogrády, V. Kellö, M. Urban, G. H. F. Diercksen; Polarizabilities of confined two-electron systems: The 2-electron quantum dot, the hydrogen anion, the helium atom and the lithium cation. Mol. Phys., **103**, 2747-2761 (2005).
9. P. Neogrády, P. G. Szalay, W. P. Kraemer, M. Urban; Coupled-cluster study of spectroscopic constants of the alkali metal diatomics: Ground and the singlet excited states of Na_2, NaLi, NaK, and NaRb. Collection Czech. Chem. Commun. **70**, 951-978 (2005).
10. P. Neogrády, M. Pitoňák, M. Urban; Optimized virtual orbitals for correlated calculations: an alternative approach. Mol. Phys. **103**, 2141-2157 (2005).
11. M. Urban, V. Kellö; Some trends in relativistic and electron correlation effects in electric properties of small molecules. Adv. Quantum Chem. **50**, 249-269 (2005).
12. F. Holka, M. Urban; The dipole moment and molecular properties of CaH: A theoretical study Chem. Phys. Letters **426**, 252-256 (2006).
13. M. Pitoňák, P. Neogrády, V. Kellö, M. Urban; Optimized virtual orbitals for relativistic calculations: an alternative approach to the basis set construction for correlation calculations. Mol. Phys., **104**, 2277-2292 (2006).
14. M. Pitoňák, F. Holka, P. Neogrády, M. Urban; Optimized virtual orbitals for correlated calculations: Towards large scale CCSD(T) calculations of molecular dipole moments and polarizabilities. J. Mol. Structure (THEOCHEM), **768**, 79-89 (2006).
15. M. Urban, V. Kellö; Relativistic and electron correlation effects as a tool for explaining some trends in molecular properties and interactions. Comput. Lett. **2**, 259 (2006).

16. M. Urban, M. Pitoňák, P. Neogrády; Optimized virtual orbital space (OVOS) as a tool for more efficient correlated and relativistic calculations of molecular properties and interactions. in *Trends and perspectives in modern computational science. Lecture Series on Computer and Computational Sciences*, ed. G. Maroulis and T. Simos, Brill Academic Publishers, Leiden, 2006, p. 265-285
17. F. Holka, P. Neogrády, M. Urban, J. Paldus; Hartree-Fock stability and broken symmetry solutions of O2- and S2- anions in external confinement. Collection Czech. Chem. Commun. **72**, 197-222 (2007).
18. L. Demovič, I. Černušák, G. Theodorakopoulos, I. D. Petsalakis, M. Urban, Improved theoretical calculations of InN in its $X^3\Sigma^-$ ground state and in the first $^3\Pi$ excited state. Chem. Phys. Lett. **447**, 215 – 220 (2007).
19. J. Granatier, M. Urban, A. J. Sadlej, Van der Waals complexes of Cu, Ag and Au with hydrogen sulfide. The bonding character. J. Phys. Chem. A **111**, 13238 -13244 (2007).
20. M. Šulka, M. Pitoňák, P. Neogrády, M. Urban, Electron Affinity of the O_2 Molecule: CCSD(T) Calculations Using the Optimized Virtual Orbitals Space (OVOS) Approach. Int. J. Quantum Chem., in ppress.
21. L. Šimová, D. Tzeli, M. Urban, I. Černušák, G. Theodorakopoulos, I. D. Petsalakis, Structure and Energetics of InN and GaN Dimers, Chem. Phys., in press

Recent scientific projects

– Properties of molecules with complicated electronic structure: Sophisticated calculations and predictions of spectroscopic and electric properties.
– APVV (Research and development Support Agency), project No. 20-018405, 2006-2009.

– Efficient theoretical calculations of molecular properties including electron correlation and relativistic effects: Methods development and applications
– VEGA (Scientific Grant Agency of the Ministry of Education of Slovak Republic) project No.
– 1/3560/06, 2006-2008

– From accurate calculations of small molecules to calculations of properties of larger molecules with a controlled accuracy
– VEGA (Scientific Grant Agency of the Ministry of Education of Slovak Republic) – 1/0115/03
– 2003-2005
– 1 315 000 SKK
– Principal investigator

–Theoretical investigation of group III metal nitrides and their chemisorption on Si(111). Formation of thin films, nanowires and nanoclusters.
– bilateral collaboration Greece – Slovak republic, 2005 – 2007.