C u r r i c u l u m V i t a e

Mgr. Zuzana Benková, PhD.

Born: May 19 1978 in Bratislava (Slovakia)

Marital status: single

Nationality: Slovak

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Education and degrees:

1992-1996 High School, Vazovova 6, Bratislava

1996-2001 Graduate Studies at Faculty of Natural Sciences, Comenius University, Bratislava (Supervisor of diploma thesis: Prof. RNDr. P. Záhradnik, DrSc.)

2001-2005 PhD. Studies at the Department of Organic Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava (Supervisor: Prof. RNDr. P. Záhradnik, DrSc., Supervisor consultant Doc. RNDr. I. Černušák, DrSc., the Department of Physical and Theoretical Chemistry, Comenius University)

16. 2. 2006 The defence of the thesis: *Structure-nonlinear optical properties relationship of organic molecules,* Organic chemistry/Chemical Physics.

Research activities:

During my PhD study I was dealing with quantum-chemical calculations of the electric properties for organic molecules associated with nonlinear optical properties. In order to select the most suitable theoretical method which provides reliable results for relatively large organic molecules and is applicable for these extended systems, I compared various theoretical approaches, as well. The smaller molecules constituting fragments of larger organic molecules, on which more sophisticated methods could be adopted, were also involved into the calculations Theoretical approach corresponding to the above mentioned criteria was partly tailored to extent its applicability on the theoretical study on larger organic systems. These calculations resulted into 7 papers in period 2002-2005 accepted in current journals and one paper currently in press and 6 SCI citations.

I have been employed at the Institute of polymers of Slovak Academy of Sciences since the 1st of December 2005. I work in the Section of Molecular Thermodynamics under supervision of Prof. Ing. T. Bleha, DrSc. and RNDr. P. Cifra, DrSc. I am focused on computer simulations of the elastic and transport properties of synthetic and biological macromolecules.

Study stays

2000 2-months visiting study stay at the Department of Organic Chemistry, Institute of Chemistry, Karl-Franzes University of Graz, Austria (Supervisor: Prof. W. M. F. Fabian) within Central European Exchange Program for University Students (CEEPUS)

2003 2-months visiting study stay at the Department of Organic Chemistry, Institute of Chemistry, Karl-Franzes University of Graz, Austria (Supervisor: Prof. W. M. F. Fabian) within (CEEPUS)

2003-2004 10-months visiting study stay at the Department of Quantum Chemistry, Institute of Chemistry, Nicolaus Copernicus University of Torun, Poland (Supervisor: Prof. A. J. Sadlej), within Visegrad fund

Acquired certificates during the PhD studies:

Intermolecular Interactions

Group Theory

Computational Methods in Chemistry

Other professional activities:

Activities at the Faculty of Natural Sciences, Comenius University

Principal investigator of the grant of the Comenius University, UK-125-2003 „Theoretical study of nonlinear optical properties for organic molecules".

Principal investigator of the grant of the Comenius University, UK-125-2005 „Structure-nonlinear optical properties relationship of organic molecues" .

Grant of the Slovak Research Agency VEGA 1/8207/01 „Computer design and study of new heterocyclic compounds with biological activity and nonlinear optical properties and their synthesis", (principal investigator Prof. RNDr. P. Zahradník, DrSc.)

Grant of the Slovak Research Agency VEGA 1/1374/04 „Heterocyclic compounds with charge transfer-prediction and synthesis of new strutures, study of structure-biological or nonlinear optical properties relationship", (principal investigator Prof. RNDr. P. Zahradník, DrSc.)

Activities at the Institute of Polymers, Slovak Academy of Sciences

Participating on grant APVT-51-044902 „Prediction of properties and functions of biological polymers based on computational modelling", (principal investigator Prof. Ing. T. Bleha, DrSc.)

Participating on grant VEGA 2/6116/06 „Nanoscale simulations of (bio)macromolecular systems with space and phase confinements", (principal investigator RNDr. P. Cifra, DrSc.)

Teaching activities:

Seminars on organic chemistry for various student groups (chemistry, biology, environmentalism, pedagogy).

Excercises on organic chemistry for students of biology, environmental science and pedagogy.

Excercises on laboratory methods for students of chemistry.

Seminar on molecular modelling for students of chemistry.

Language and other skills

English language (scientific and colloquial style)

Quantum-chemical programs Gaussian, Molcas, Gamess, Dalton

List of publications

1. Benkova Z., Kona J., Gann G., Fabian W. M. F.
Redox chemistry of organoselenium compounds: Ab initio and density functional theory calculations on model systems for transition states and intermediates of the redox cycle of selenoenzymes. *International Journal of Quantum Chemistry* **90** (2): 555-565 (2002).
2. Benkova Z., Sadlej A. J.
Electric moments of carbon dichalcogenides. *Molecular Physics* **102** (7): 687-699 (2004).
3. Benkova Z., Sadlej A. J., Oakes R. E., Bell S. E. J.
Reduced-size polarized basis sets for calculations of molecular electric properties. I. The basis set generation. *Journal of Computational Chemistry* **26** (2): 145-153 (2005).
4. Oakes R. E., Bell S. E. J., Benkova Z., Sadlej A. J.
Reduced-size polarized basis sets for calculations of molecular electric properties. II. Simulation of the Raman spectra. *Journal of Computational Chemistry* **26** (2): 154-159 (2005).
5. Benkova Z., Sadlej A. J., Oakes R. E., Bell S. E.
Reduced-size polarized basis sets for calculations of molecular electric properties. III. Second-row atoms. *Theoretical Chemistry Accounts* **113** (4): 238-247 (2005).
6. Benková Z., Černušák I., Zahradník P.
Basis set and electron correlation effects on static electric properties of 1,3-thiazoles and 1,3-benzothiazoles as potential fragments in push-pull NLO chromophores. *Molecular Physics* **104** (13-14): 2011-2026 (2006).
7. Benková Z., Černušák I., Zahradník P.
Theoretical study of static electric properties of benzothiazole containing push-pull systems as potential candidates for NLO materials. *Structural Chemistry* **17** (3): 287-300 (2006).
8. Benková Z., Černušák I., Zahradník P.
Electric properties of formaldehyde, thioformaldehyde, urea, formamide, and thioformamide-post-HF and DFT study. *International Journal of Quantum Chemistry* (accepted).

List of presentations

J. Benko, O. Vollárová, I. Černušák, M. Lácová, Z. Benková, M. Aranyosiová
Preparation and properties of novel derivatives of 2-etoxychromones. *57. Zjazd chemických spoločností ChemZi* 1, 75 (2005).

Z. Benková, I. Černušák, P. Zahradník
Theoretical study of static electric properties of conjugated molecules. *6th European Conference on Computational Chemistry*, September 3-7, 2006.