

Curriculum Vitae - Eva Scholtzová

Personal entries:



e-mail: eva.scholtzova@savba.sk
Citizenship: Slovak
Date of Birth: 24th June 1965

Education:

Scientific degree: philosophiae doctor

1991-1998: Institute of Inorganic Chemistry of Slovak Academy of Sciences,
Department of theoretical chemistry, Bratislava, Slovakia

(1991-1994 maternity leave)

Study program: Physical chemistry
PhD. Thesis: *The effect of substitution of central cations in brucite sheet on the electronic structure of trioctahedral layer silicates*
(supervisor: Dr.LadislavTuri Nagy†).

Master's degree:

1983-1988 Slovak Technical University, Bratislava, Slovakia,
Faculty of chemical technology

Department: Technology of silicates
Specialization: Technology of glass
Diploma Thesis: *The effect of an alkaline environment on the strength of glass fibres.*

Work experiences:

Researcher:

1998 – present Institute of Inorganic Chemistry, Slovak Academy of Sciences
Department of theoretical chemistry, Bratislava, Slovakia

- Application of computational methods for study of advanced materials based on inorganic structures

PhD study:

1991 – 1998: Institute of Inorganic Chemistry, Slovak Academy of Sciences,
Department of theoretical chemistry, Bratislava, Slovakia

Researcher:

1991-1988: Common laboratory for basic research of glass, Centre of chemical research,
Slovak Academy of Sciences, Bratislava, Slovakia

- Experimental and theoretical study of siloxanes

Short-stays:

04/2008 (2 weeks)	Chalmers University, Gothenburg, Sweden
05/2011(2 weeks)	BOKU University, Vienna, Austria
06/2012 (3 weeks)	BOKU University, Vienna, Austria
07/2022 (1 week)	University of Patras, Patras, Greece
08/2023 (1 week)	University of Patras, Patras, Greece

Teaching experience:

2008, 3 months	Supervising BSc. Student (Gabriela Orešková - <i>Modelling of structural units of layered silicates</i> , Comenius University, Faculty of Natural Sciences, Bratislava (Slovakia)
2017-2021	Supervising PhD student, Slovak Technical University Bratislava (Daniel Moreno Rodriguez, Spain, <i>Interactions of clay minerals with organic pollutants studied by means of computational methods</i>)
2017-2023	Supervising PosDoc (Peter Škorňa , <i>Application of DFT method to clays and organoclays</i>)
2020, 3 months	Supervising PhD student within SAIA project, (Eleni Gianni, Greece, <i>Modelling for pilot calculations of halloysite-irinotecan nanocomposites using the solid state DFT method implemented in VASP program</i>)
2020-2024	Supervising PhD student, Comenius University, Faculty of Natural Sciences, Bratislava (Sanam Bashir, Pakistan, <i>Theoretical study of clay-polymer hybrids by computational methods</i>)
July, 2022	lectures for PhD students, Patras University, Patras, Greece within the frame of ERASMUS+, one week (modelling in solid state, computational methods)
August, 2023	lectures for PhD students, Patras University, Patras, Greece within the frame of ERASMUS+, one week (mechanical properties of clay minerals)

Organizational and management skills:

- 2003 co-organizer of conference: Structure Solution from Powder Diffraction Data (SSPD'03), Stará Lesná, Slovakia, 14.– 19. September 2003
- 2008 co-organizer of international conference: 8th Solid state chemistry, Bratislava, Slovakia, 6.-11. November2008
- 2009-2010 vice-president of the Scientific technical society IIC SAS
- 2014 co-organizer of international conference: 11th Solid state chemistry, Trenčianske Teplice, Slovakia, 6-11 July2014
- 2016 co-organizer of international conference: 8th Mid-European Clay Conference (MECC2016) ,4. - 8. July 2016, Košice, Slovakia
- 2022 Main organizer of the international workshop: 2nd Annual meeting of AtomDeC project – V4-Japan, JRC; Smolenice, Slovakia

Managed projects:

- 01/2009-12/2011 Structure and dynamics of hydrogen bonds in solids by diffraction methods, quantum chemistry and inelastic neutron spectroscopy (INS). VEGA - 2/0150/09, Deputy of principal investigator
- 01/2011-12/2012 Molecular simulations of selected organoclays - characterization of structure and properties. SK-AT-0020-10, principal investigator
- 01/2012-12/2014 The influence of the water content in cementitious minerals on their structural, physical, chemical and mechanical properties – Model and experimental study, VEGA- 2/0021/19, principal investigator
- 01/2019-12/2022 Insight into the mechanism of interactions of pollutants adsorbed on the surface of aluminosilicate structures, VEGA- 2/0021/19, principal investigator
- 11/2021-10/2024 Atomic Design of Carbon-Based Materials for New Normal Society (AtomDeC). V4-Japan/JRP/2021/96AtomDeC, principal investigator IIC SAS
- 01/2023-12/2026 Advanced materials based on the inorganic layered structures studied by model and experimental approaches, VEGA-2/0026/23, principal investigator

Invited lectures:

- 2004 Substitutions in lizardite, 262. Rozhovory, Bratislava, Slovakia
- 2008 Hydrogen bonding and vibrational spectra in kaolinite-dimethylsulfoxide and -dimethylselenoxide intercalates – a solid state computational study, IIC SAS, Bratislava, Slovakia
- 2009 NBO analýza - užitočný nástroj pri spresňovaní kryštálovej štruktúry látok (NBO analysis – useful tool at the refinement of crystal structure of compounds). 279. Rozhovory. Prague, Czech Republic
- 2012 Využitie výpočtových metód pri riešení problémov experimentálnych meraní/ Use of computational methods in solving problems of experimental measurements, IIC SAS, Bratislava, Slovakia
- 2014 Computational method - useful tool at characterization of IR spectrum. AnalytiX-2014, p. 175, Dalian, China
- 2015 Laws of conservation, IIC SAS, Bratislava, Slovakia
- 2017 Problematic Parts of IR Spectrum and Stability of Organoclays - DFT Study. AnalytiX-2017, p. 117, Fukuoka, Japan
- 2019 Insight into the stability of beidellite intercalates, 7th AnalytiX-2019, p. 78, Singapore
- 2022 DFT method - a useful tool for characterisation of clay minerals and organoclays, University of Patras, Dept of Geology, Patras, Greece, 12.07.2022
- 2023 DFT study of the structural behaviour of montmorillonite under different pressure and temperature conditions, University of Patras, Dept of Geology, Patras, Greece, 21.8.2023

Short description of scientific background and skills:

My focus is to study the properties of advanced materials by computational approach. This requires skills in quantum chemistry, crystallography, spectroscopic methods (e.g., FTIR, Raman) and computational science (e.g., modelling, methods, UNIX). In particular, one needs to master the preparation of models of solid- state materials in both ways (cluster and periodic) and be able to decide which computational method is suitable to use for calculations. Moreover, one should be able to compare the obtained results with experimental data and be familiar with the limits of both computational and experimental methods with the aim to add new information for the characterization of advanced materials.

I study mainly inorganic layered structures (clay minerals, graphene, and the hybrids based on them because these materials are widely studied for their useful properties applicable in green chemistry, wastewater and soil treatment, drug carriers, and catalytic properties. For examination of advanced materials, I predominantly use ab initio Density Functional Theory (DFT) method for solid state (e.g., to study of stability of hybrid systems, to analyse of problematic parts of overlapped bands in FTIR/Raman spectra, further to examine optical, magnetic, electrical, mechanical properties and to refine the newly synthesized structures.

Publications:

ORCID:	0000-0001-8281-6713
ResearcherID:	R-4691-2019
Scopus ID:	6602260092

As of October 2023, 57 papers and one book chapter, have been published in international peer-reviewed journals (CC), that have been cited a total of 529 (412) times, and have a Hirsch index of 13. (source: WOS; without self-citations in parentheses)

Bratislava, 15th November 2023

Ing. Eva Scholtzová, CSc.