Curriculum Vitae - Eva Scholtzová

Personal entries:

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

Education:

Scientific degree: philosophiae doctor

1991-1998:
(1991-1994 maternity leave)

Institute of Inorganic Chemistry of Slovak Academy of Sciences,
Department of theoretical chemistry, Bratislava, Slovakia
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. Ladislav Turi Nagy†).

Master's degree:

1983-1988

Slovak Technical University, Bratislava, Slovakia,
Faculty of chemical technology
Department: Technology of silicates
Specialization: Thechnology of glass
Diploma Thesis:

The effect of an alkaline environment on the strength of glass fibers.

Work experiences:

Researcher:

1998 – present — Institute of Inorganic Chemistry, Slovak Academy of Sciences

- 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:

2008 - Chalmers University, Gothenburg, Sweden
2011 - BOKU University, Vienna, Austria
2012 - BOKU University, Vienna, Austria
2022 - University of Patras, Patras, Greece
2023 - University of Patras, Patras, Greece

Teaching experience:

- 2008, 3 month − Supervising BSc. student (Gabriela Orešková - *Modelling of structural units of layered silicates*, Comenius University, Faculty of Natural Sciences, Bratislava (Slovakia)
- 2017-2021 − Supervising PhD student, Slovak Technical University Bratislava (Daniel Moreno Rodriguez, Spain, *Interactions of clay minerals with organic pollutants studied by means of computational methods*),
- 2017-2023 − Supervising PosDoc (Peter Škorňa, *Application of DFT method to clays and organoclays*)
- 2020, 3 months − Supervising PhD student within SAIA project, 3 months (Eleni Gianni, Greece, *Modelling for pilot calculations of halloysite-irinotecan nanocomposites using the solid state DFT method implemented in VASP program*)
- 2020-2024 − Supervising PhD student, Comenius University, Faculty of Natural Sciences, Bratislava (Sanam Bashir, Pakistan, *Theoretical study of clay-polymer hybrids by computational methods*)
- July 2022, August 2023 − lectures for PhD students, Patras University, Greece within the frame of ERASMUS+ (modelling in solid state, computational methods)
- 2024-now – Supervising PhD student, Comenius University, Faculty of Natural Sciences, Bratislava (Ayesha Asbat, Pakistan, *Study of properties of advanced inorganic materials by modelling approach)*
- 2024-now – Supervising Diploma student, Comenius University, Faculty of Natural Sciences, Bratislava (Bc. Emma Mičejová, Slovakia, *Štúdium interakcií fenantrolínu s ílovými minerálmi metódou DFT/Study of the interactions of phenantroline with clay minerals by DFT method*.

Organizational and management skills:

- 2003 – co-organizer of conference: Structure Solution from Powder Diffraction Data (SSPD'03)', Stará Lesná, Slovakia, September 2003
- 2008 - co-organizer of international conference: 8th Solid state chemistry, Bratislava, Slovakia, 6.-11. November 2008
- 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 July 2014
- 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*

09/2024-08/2026 Effect of structural Substitutions on Properties of Inorganic Layered Structures, a basis for atomically designed advanced materials for green technological applications, studied by modelling approach, Recovery plan, 09I03-03-V04-00009, *principal investigator*.

Invited lectures:

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

2014 Computational method - useful tool at characterization of IR spectrum. AnalytiX-2014 , p. 175, Dalian, China

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

2025 Clay minerals – useful adsorbents for drugs. In International Symposium 2025. Molecular modeling in soil science – achievements and perspectives. – Vienna, Austria: Austrian Soil Science Society, 24.9.-26.9.2025, 25.09.2025

Short description of scientific background and skills:

I am focusing on the computational modelling of the structural and physicochemical properties of advanced inorganic materials, with emphasis on their use in environmental and green applications. The fields of study are mainly clay minerals, organoclays, hydrated cement phases, and carbon-based materials. My work has refined the structures of some clay minerals (e.g., TMA-hectorite and halloysite), clarified overlapping bands in the IR spectra of many organoclays, and elucidated the structures of thaumasite and ettringite. Based on the refined halloysite structure, a program for generating nanotubes was developed in collaboration with colleagues at Charles University, Prague. Further, the adsorption mechanism in many hybrid structures was elucidated, along with the factors that influence the stability of adsorbate–adsorbent systems, thereby advancing knowledge of preferred materials for environmental treatment.

Award

2024 Top scientific publications award of the Slovak Academy of Sciences 18.9.2024

YU, Wei - YOSHII, Takeharu - AZIZ, Alex - TANG, Rui - PAN, Zheng-Ze - INOUE, Kazutoshi - KOTANI, Motoko - TANAKA, Hideki - SCHOLTZOVÁ, Eva - TUNEGA, Daniel - NISHINA, Yuta - NISHIOKA, Kiho - NAKANISHI, Shuji - ZHOU, Yi - TERASAKI, Osamu - NISHIHARA, Hirotomo. Edge-Site-Free and Topological-Defect-Rich Carbon Cathode for High-Performance Lithium-Oxygen Batteries. In Advanced Science, 2023, vol. 10, no. 16, art. no. 2300268-1-2300268-10. (2022: 15.1 - IF, Q1 - JCR, 4.086 - SJR, Q1 - SJR). ISSN 2198-3844. Dostupné na: https://doi.org/10.1002/advs.202300268 Typ: ADCA

Publications:

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ResearcherID: R-4691-2019
Scopus ID: 6602260092

As of January 2026, 66 papers and one book chapter have been published in international peer-reviewed journals (CC), which have been cited a total of 788 (644) times, and have a Hirsch index of 16 (source: WOS; without self-citations in parentheses).

Bratislava, 16. January 2026 Ing. Eva Scholtzová, CSc.