

DR. MONIKA GEŠVANDTNEROVÁ

PERSONAL INFORMATION

Date of birth: 14.12.1995
Sex: Female
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EDUCATION

Study of Theoretical and Computational Chemistry at the Comenius University in Bratislava, Faculty of Natural sciences

2020 - 2024

PhD. study programme: Theoretical and Computational Chemistry

Dissertation thesis: Mechanisms, kinetics and thermodynamics of catalytic reactions from computer simulations: cutting edge methodology and its applications

Supervision: Dr. Tomáš Bučko

Study of Theoretical and Computational Chemistry at the Comenius University in Bratislava, Faculty of Natural sciences

2018 - 2020

Master study programme: Theoretical and Computational Chemistry

Master's thesis: Ab Initio Simulations of Heterogenous Catalysis Processes

Supervision: Dr. Tomáš Bučko

Study of Chemistry at the Comenius University in Bratislava, Faculty of Natural sciences

2015 - 2018

Bachelor study programme: Chemistry

Bachelor's thesis: Computer Simulations of Important Catalytic Reactions

Supervision: Dr. Tomáš Bučko

PROFESSIONAL EXPERIENCE

Laboratory technician

2023

Comenius University in Bratislava, Faculty of Natural Sciences, Department of Physical and Theoretical Chemistry

Postdoctoral researcher at University of Lorraine, CNRS, L2CM, Metz

2024 - present

Topic: Contribution of Machine Learning in atomic-scale simulations in catalysis: Case of the dehydration of butanols on acidic zeolites

Supervision: Prof. Michael Badawi

Researcher at Comenius University in Bratislava, Faculty of Natural Sciences

2024 - present

Department of Physical and Theoretical Chemistry

LICENSES AND CERTIFICATIONS

Drivers licenses

AM, A1, A2, B1, B

AWARDS

Dean's award (2021)

For exceptional scientific publication in category: Chemical and biological sciences

Rector's award (2020)

For excellent diploma thesis

Academic praise of the Rector of Comenius University (2020)

For excellent fulfillment of study obligations during the entire study at the university

PUBLICATIONS

M. Gešvandtnerová, P. Raybaud, C. Chizallet, T. Bučko: Importance of Dynamic Effects in Isobutanol to Linear Butene Conversion Catalyzed by Acid Zeolites Assessed by AIMD, *ACS Catalysis*, 14 (2024) 7478-7491.

M. Gešvandtnerová, T. Bučko, P. Raybaud, C. Chizallet: Monomolecular mechanisms of isobutanol conversion to butenes catalyzed by acidic zeolites: Alcohol isomerization as a key to the production of linear butenes, *Journal of Catalysis* 413 (2022) 786-802.

M. Gešvandtnerová, D. Rocca, T. Bučko: Methanol carbonylation over acid mordenite: Insights from ab initio molecular dynamics and machine learning thermodynamic perturbation theory, *Journal of Catalysis* 396 (2021) 166-178.

T. Bučko, M. Gešvandtnerová, D. Rocca: Ab Initio Calculations of Free Energy of Activation at Multiple Electronic Structure Levels Made Affordable: An Effective Combination of Perturbation Theory and Machine Learning, *J. Chem. Theory Comput.* 16 (2020) 6049-6060.

INTERNSHIPS

Scientific stay in IFP Energies nouvelles, France (2022)

Supervision: Dr. Céline Chizallet

INVITED LECTURES

Ab initio calculations of free energy of activation at multiple electronic structure levels made affordable

Seminar at prof. Sauer's group (Humboldt University in Berlin), 28.1.2021

Mechanisms, kinetics and thermodynamics of catalytic reactions from computer simulations: cutting edge methodology and its applications

Seminar at prof. Badawi's group (University of Lorraine, IUT de Moselle-Est), 10.7.2024

RESEARCH PROJECTS

Towards reliable finite temperature ab initio calculations of molecules and materials
APVV-20-0127

PEER REVIEW

Review activity for **Nature communications** (1)

PERSONAL SKILLS

Mother language	Slovak language
Foreign languages	English (C1 UNICert certificate), Russian (basics), French (beginner)
Computational chemistry software	VASP, ORCA, Molcas
Programming	Python, Bash, C++ (beginner)

FURTHER QUALIFICATION

Attended ORCA workshop at Slovak Academy of Sciences (2024)

Was a member of organization committee for 17th International Congress of Quantum chemistry (2023)

Lead a seminar session in IFPEN: Gadget hands-on: Searching for transition states Seminar in IFP
Energies nouvelles (Lyon), 1.12.2022

Attended Summer school of condensed matter physics (2022, 2023)

Attended PRACE Spring school on Modelling materials using AI/ML (2021)

Attended Machine learning in Physics, VDSP-ESI Winter School (2020)

Attended language school in Trenčín, English language (2009-2015)

Attended Art school of J. Krén in Nové Mesto nad Váhom (2009-2011)