Krystof Brezina, MSc.

PhD Student • Theoretical Physics and Molecular Simulations
Faculty of Mathematics and Physics, Charles University

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Education

Faculty of Mathematics and Physics, Charles University 2019 - present
PhD Student Prague, Czechia

- Accurate *ab initio* molecular simulations of hydrogen-bonded condensed-phase systems including nuclear quantum effects
- Advisor: Dr. Ondrej Marsalek

University of Chemistry and Technology 2017 - 2019
MSc Student Prague, Czechia

- *Ab initio* molecular dynamics insight into solvated electrons in liquid ammonia and their reactivity
- Thesis "Quantum Chemistry Calculations of Solvated Electrons in the Context of the Birch Reduction" defended in June 2019.
- Advisor: prof. Pavel Jungwirth

University of Chemistry and Technology 2014 - 2017
BSc Student Prague, Czechia

- Biosimulations of the complex of arginine with insulin
- Thesis "Interaction of arginine with insulin and effect on its aggregation" defended in June 2017.
- Advisor: prof. Pavel Jungwirth

Research Experience

Institute of Organic Chemistry and Biochemistry AS CR 2014 - present
Student researcher in the group of prof. Pavel Jungwirth Prague, Czechia

Internships

Institute of Organic Chemistry and Biochemistry AS CR 2013 – 2014
Student internship in the group of Dr. Jiri Srogl Prague, Czechia

Emory University August 2014
Student internship in the group of prof. Lanny Liebeskind Atlanta, USA

Selected Publications

Krystof Brezina., Pavel Jungwirth and Ondrej Marsalek*
Benzene Radical Anion in the Context of the Birch Reduction
The Journal of Physical Chemistry Letters 11 (2020)

Christoph Schran, **Krystof Brezina**, Ondrej Marsalek*
Committee Neutral Network Control Generalization Errors and Enable Active Learning
The Journal of Chemical Physics 153 (2020)

Tillmann Buttersack et al.
Photoelectron Spectra of Metal-Ammonia Microjets: from Blue Electrolyte to Bronze Metal.
Science 368 (2020)

Tillmann Buttersack et al.
Valence and Core-Level X-ray Photoelectron Spectra of a Liquid Ammonia Microjet.
The Journal of the American Chemical Society 142 (2019)

Krystof Brezina et al.
Can Arginine Inhibit Insulin Aggregation? A Combined Protein Crystallography, Capillary Electrophoresis and Molecular Dynamics Study
The Journal of Physical Chemistry B 122 (2018)

Selected Conferences

IT4Innovation User's Conference — November 2020
Poster — Ostrava, Czechia

Week of Doctoral Students — September 2020
Talk — Prague, Czechia

IT4Innovation User's Conference — November 2019
Talk — Ostrava, Czechia

Gordon Research Seminar and Conference on Liquids — August 2019
Poster — Holderness, USA

Scholarships and Awards

START Programme Student Research Grant — 2020 - present
Principal Investigator — Prague, Czechia

International Max Planck Research School — 2019 - present
Member — Dresden, Germany

45th International Chemistry Olympiad — July 2013
Bronze Medal — Moscow, Russia