Samira Baghbanbari

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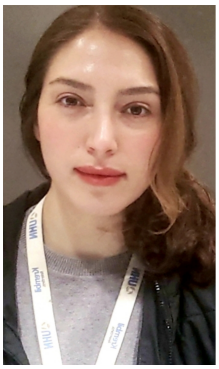

About me

I am a Master's graduate with a strong foundation in computational chemistry, data science, and materials-focused modeling, and molecular simulations. During my MSc, I applied Density Functional Theory (DFT), and molecular dynamics simulations to investigate charge transfer mechanisms and molecular interactions in neuronal gap junctions. My primary analytical tool is Python, which I use to develop custom scripts for data processing, automation, and visualization. I also have extensive experience with Bash and command-line tools for managing large-scale computational workflows on high-performance computing (HPC) clusters.

Education

Sep 2022 - Oct 2024 — *MSc in Computational Science, University of Toronto, Ontorio, Weaver's lab*

- *MSc Thesis: Computational Characterization of Electronic Charge Transfer in Interfacial Phospholipid–Water Layers Using Quantum Mechanical Methods, and Design of Arginase-I Inhibitors as Potential Therapeutics in Alzheimer's Disease*
- *Evaluation of Proton Binding Energies, Acidities, using Ligand Electrochemical Parameters with Application to Nitrogen Fixation*

Sep 2018 - Sep 2022 — *BSc in Chemistry, York University of Toronto, Ontorio, Lever's lab*

- *BSc thesis: Ligand electrochemical parameter approach to molecular design: σ-donation, π-back donation and other metrics in molybdenum dinitrogen complexes*

Academic Positions

Feb 2025 - Present — *Academic Guest at Universität Zürich, Dr. Marcella Iannuzzi's lab*

- *Electronic Structure, Ab Initio Molecular Dynamics and Spectroscopy in Porphyrin in water system, Coumarin 6 isomers and converstion of CO2 to Ethanol on RhFe alloys @SiO2*

Oct 2024 - July 2025 — *Research Assistant at University of Waterloo, Dr. Leonenko's Lab*

- *Biophysical study of neuronal lipid membrane*
  - *Effect of trehalose and NaCl on the structure and electrostatic properties of Langmuir lipid monolayers studied by Scanning Probe Microscopy and Density Functional Theory Computation*

Dec 2022 - May 2024 — *Teaching Assistant at University of Toronto*

- *Medicinal Chemistry and de-novo drug design.*
  - *contribute to the development of appropriate teaching materials based on An introduction to Medicinal Chemistry 6th Edition, Graham Patrick textbook.*

Aug 2023 - May 2024 *Teaching Assistant at University of Toronto*

- *Chemical Pharmaceutical Laboratories*
  - *Play a role in advancing suitable laboratory techniques, particularly in the realm of physical chemistry, encompassing the calculation of specific physical properties within diverse solutions featuring fluid and gel-like mediums.*

Recent Projects *(to be published)*

Effect of trehalose and NaCl on the structure and electrostatic properties of Langmuir lipid monolayers studied by Scanning Probe Microscopy and Density Functional Theory Computation (ready for submission)

Evaluation of Proton Binding Energies, Acidities, using Ligand Electrochemical Parameters with Application to Nitrogen Fixation (Submitted)

Computational Characterization of Electronic Charge Transfer in Interfacial Phospholipid-Water Layers using QM calculations (Submitted)

Contributed Presentations and Invited Talks

May 2023 *Pharmacutical and Biophysical Chemistery seminar (PBC)*

Jan 2024 *Biomedical Sciences seminar (BMS)*

Feb 2024 *AFPC poster competition*

Feb 2024 *3MT competition-3-minute Presentation*

April 2024 *Chemical Biophysics Symposium (CBS)*

June 2024 *International Computational Chemistry and Molecular Modeling (ICCMM)*

June 2024 *Graduate Research in Progress (GRIP)*

March 2025 *Quantum Biology Gordon Research Conference*

Courses Highlights

Introduction to Machine Learning (A^+)

Statistical Methods I (A)

Instrumental Methods of Chemical Analysis (B^+)

Analytical Chemistry (A)

Biochemistry (CHEM2050) (B^+)

Advanced Physical Chemistry-Thermodynamics statistical and kinetics based on Thomas Engle and Philip Reid textbook(A)

Research Project in Chemistry (Applications of Machine Learning in Computational Chemistry under supervision of Dr.René Fournier (B^+)

Research Bsc thesis Project- Quantum chemistry theories- A computational Chemistry study (Under supervision of Dr. Lever) (A)

Theoretical Chemistry (Schrodinger equation and DFT (Prof. Fournier)) (A)

Skills

Programming Language: Python, Fortran

Designing and Computational Softwares: CP2K, Gaussian16, GaussView6, GROMACS, MOE, VMD, Avogadro, Docking, QSAR, Chem Draw, AOMix

Language Skills: English (Fluent), German (Limited Working Proficiency), Persian

References

Marcella Iannuzzi (Current Internship Supervisor at University of Zurich, Chemistry Department): marcella.iannuzzi@chem.uzh.ch

Zoya Leonenko (Research Assistant Supervisor at University of Waterloo): zleonenk@uwaterloo.ca

Donald Weaver (Master's Supervisor, University of Toronto): donald.weaver@uhn.ca

A.B.P. Lever (Bachelor's thesis Supervisor and Master's Co-Supervisor): blever@yorku.ca