Samuel Mathews, Ph.D.

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Career Objective

- Detail-oriented, natively-trilingual, computational researcher with 8 years of experience in materials modeling, data science and analytics, and high performance computing looking to develop engineering solutions to complex problems.

Experience

Graduate Researcher, McGill University — Montréal, Canada — May 2018 – Present

- Characterizing temperature and pressure effects on the interfacial tension and energy of interfaces in sII gas hydrates.
- Determining the evolving material properties and behaviors in sI gas hydrates under changing pressure conditions.
- Using machine learning to identify trends and patterns in large datasets, classify structures, recognize clustering.
- Developing processing pipelines using numpy, pandas, numexpr, multiprocessing, scikit-learn on HPC clusters.

Scientific Systems Administrator, McGill University — Montréal, Canada — Jan 2021 – Present

- Managing compute infrastructure of the Materials Modeling Research Group: login/compute nodes, auxiliary systems.
- Configuring nodes, hardware operations, storage requirements, networking, LDAP authentication, DHCP, DNS.
- Configuring Slurm Workload Manager, CERN Virtual Machine File System for software and workload distribution.
- Maintaining MATLAB, COMSOL, COMSOL License Manager implementations, custom software installations.
- Recommending upgrades, procurements, cost management, technical support, providing technical support and training.

Laboratory Manager, McGill University — Montréal, Canada — Jan 2021 – Present

- Managing all lab software licenses and cloud computing credit grants on Digital Research Alliance of Canada resources.
- Overseeing and coordinating all hardware and software procurement while adhering to institutional regulations.
- Maintaining records of lab activities for funding agencies, institutional compliance, and fund restrictions.
- Preparing core-year records, budgets, resource justifications, multiple projects' of researchers for multi-year grants.
- Scheduling weekly group seminars and meetings, producing attendance lists, noting information for funding agencies.

Graduate Teaching Assistant, McGill University — Montréal,Canada — Sep 2018 – Apr 2026

- Graded assignments and exams, led tutorial and lab sessions, invigilated exams for 13 advanced courses.
- Lectured on advanced mathematics, programming techniques in Python and MATLAB, optimization, high performance calculations, heat and mass transfer, energy systems engineering, process modeling.

Education

Doctor of Philosophy (Ph.D.), Chemical Engineering, McGill University — Montréal, Canada — Jan 2021 – Apr 2026

- **Thesis:** Multiscale Characterization of Gas Hydrates: Interfacial and Structural Aspects
- High performance modeling of gas hydrate systems and applications with molecular dynamics and density functional theory.

Master of Engineering, Chemical Engineering, McGill University — Montréal, Canada — May 2018 – Jun 2020

- **Thesis:** Thermal Properties of Gas Hydrates Using Density Functional Theory
- Predicted thermal properties of sI gas hydrates from first principles using density functional theory.

Bachelor of Engineering, Chemical Engineering, McGill University — Montréal, Canada — Sep 2014 – Apr 2018

Professional Development – for a complete list of continuing education, please refer to: smphd.com/education.

Awards & Achievements — for a complete list, please refer to: smphd.com/awards.

Publications & Talks — **7 first-author**, **4 second-author**: smphd.com/publications, **29 presentations**: smphd.com/talks.

Technical Skills

Data Science: NumPy, NumExpr, Multiprocessing, Pandas, Scikit-learn, Matplotlib, SciPy, Statistics, Version Control.

Artificial Intelligence: Classifiers, Regression, Support Vector Machine, Text Mining, Neural Network Programming.

Materials: Large Atomic/Molecular Modeling Software Package, Vienna Ab Initio Simulation Package, Phonopy, MDAnalysis, Molecular Dynamics, Density Functional Theory, Nucleation, Elecrocrystallization, Material Strength, Interfacial Phenomena.

Tools: MATLAB, Python, Bash, SQL, Excel, Powerpoint, LaTeX, NixOS, Nix and home-manager, Debian, Windows.

Languages: English (Native), French (Native), Spanish (Native).