Samuel Mathews, Ph.D. Candidate

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Career Objective

- Detail-oriented, natively-trilingual, computational researcher with 7 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 Jan 2021 – Present

- Characterizing temperature and pressure effects on the interfacial tension and energy of interfaces in sII gas hydrates.
- 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.
- Maintaining Python module for Materials Modeling Research Group installable privately via the pip package manager.

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

- Managing compute infrastructure of the Materials Modeling Research Group: login/compute nodes, auxiliary systems.
- Installing, configuring, and maintaining:
  - Debian login and compute nodes, all memory, CPU, GPU, power supply, and storage operations and replacements.
  - Slurm Workload Manager for job scheduling, resource management, node failure tolerance, job monitoring.
  - CERN Virtual Machine File system on nodes for software distribution and management.
  - MATLAB, COMSOL, COMSOL License Manager implementations, custom software installations for benchmarking.
  - LDAP user authentication for centralized permissions across all cluster related devices and services.
  - Network hardware on rack and desk, DHCP and DNS servers.
  - 3-2-1 backup policy for all research data on a pre-defined schedule.
  - Gitea Docker implementation offsite and remotely accessed for repository version control.
- Integrating and communicating with university IT staff and policies regarding compute resources and networking.
- Making recommendations to research supervisor upgrades, procurement, cost management, technical support.
- Troubleshooting all failed jobs, hardware issues, performance bottlenecks, providing technical support to all users.
- Training lab members in policies, cluster usage and access of local and Digital Research Alliance of Canada clusters.

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 and institutional compliance.
- Assisting principal investigators with grant proposals by preparing computational time records, financial budgets, specific and detailed core-year justifications, and collecting and combining project information from lab members.
- Preparing expense reports for seminars and lab activities, receiving and processing invoices for payment of vendors.
- Scheduling weekly group seminars and meetings, producing attendance lists, noting information for funding agencies.

Graduate Teaching Assistant, McGill University — Montréal,Canada Sep 2018 – Aug 2025

- Graded assignments and exams, led tutorial and lab sessions, invigilated exams for 12 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

PhD Engineering, McGill University — Montréal, Canada Jan 2021 – Apr 2026

- **Thesis:** Computational Modeling of Interfacial Properties and Processes in sII Gas Hydrates
- Employing high performance molecular dynamics for interfacial systems in gas hydrate engineering applications.
- Doctoral Research Scholarship: Fonds de recherche du Québec — Nature et technologies
- McGill Engineering Doctoral Award
- **Relevant Coursework:** Foundations of Fluid Mechanics, Process Dynamics and Control

Master of 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.
- McGill Engineering Undergraduate Student Master's Award
- **Relevant Coursework:** Graduate Thermodynamics, Graduate Computational Methods, Quantum Materials

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

Professional Development

Mathematics of Multiscale and Multiphysics Phenomena in Materials Science — BIRS, Banff, Canada
Computational Materials North Workshop — Queen's University, Kingston, Canada
Moving Ions with Vienna Ab initio Simulation Package for the Advanced User — University of Vienna
HPC Python — Compute Ontario Summer School
Neural Net Programming — SciNet HPC Consortium
Introduction to GPU Programming — SciNet HPC Consortium
Advanced Linux Command Line — SciNet HPC Consortium
Advanced Materials for Energy Storage and Conversion Summer School — Université de Bordeaux
Applied Data Science with Python Specialization — University of Michigan via Coursera

Technical Skills

Tools: MATLAB, Python, Bash, SQL, Excel, Powerpoint, LaTeX.

Operating Systems: NixOS, Nix and home-manager, Debian, Ubuntu, Microsoft Windows, MacOS.

Data Science: NumPy, NumExpr, Multiprocessing Package, Pandas, Scikit-learn, Matplotlib, SciPy, Refactoring for Parallel Execution, Statistical Analysis, Data Cleaning.

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

Materials Modeling: Large Atomic/Molecular Modeling Software Package, Vienna Ab Initio Simulation Package, Phonopy, MDAnalysis.

High Performance Computing: Installation/Maintenance of Slurm Scheduler, CERN Virtual Machine File System, Ethernet and InfiniBand Network Configuration.

Containerization: Docker, Docker Compose, Docker Compose Networking.

Version Control: Git (branching, merging, conflict resolution), Self-Hosted Gitea.

Computer Networking: Nginx Proxy Manager, HTTPS/SSL Provisioning, Traffic Routing, DHCP Server, DNS Server.

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

Awards & Achievements

Doctoral Research Scholarship, Fonds de recherche du Québec — Nature et technologies	Jun 2022 – Dec 2025
Graduate Research Enhancement and Travel Award	Oct 2025
Canadian Association for Computational Science and Engineering Travel Award	Jul 2024
Graduate Research Enhancement and Travel Award	Jul 2025
Presentation Excellence Award	May 2024
Prize for Best Use of Language (French) — Oral Session	May 2024
McGill Engineering Doctoral Award	Jan 2021 – Dec 2023
Graduate Research Enhancement and Travel Award	Jun 2023
Graduate Research Enhancement and Travel Award	Dec 2022
McGill Engineering Undergraduate Student Master's Award	May 2018 – Apr 2020
Outstanding Presentation Award (Masters)	Nov 2019

Publications

Periodic Feature Characterization in Nanostructured Surfaces and Emulsions May 2025
André Guerra, Ziheng Wang, **Samuel Mathews**, Alejandro Rey, Phillip Servio, Kevin De France
10.48550/arXiv.2505.04057

Geometric Characterizations of Non-Uniform Structure I Methane Hydrate Behaviors Under Pressure May 2025
Samuel Mathews, Xiaodan Zhu, André Guerra, Phillip Servio, Alejandro Rey
doi.org/10.3390/cryst15060518

Multiscale Interfacial Structure and Organization of sII Gas Hydrate Interfaces Using Molecular Dynamics Mar 2025
Samuel Mathews, Phillip Servio, Alejandro Rey
doi.org/10.3390/nano15060464

Modeling the Effect of Backbone Instabilities and Guest Occupancies on Interfacial and Structural Processes and Dynamics of sII Gas Hydrate Systems Using Molecular Dynamics Jul 2024
Samuel Mathews, Zijun Xu, Phillip Servio, Alejandro Rey
10.23967/wccm.2024.097

Molecular Dynamics Characterization of the Interfacial Structure and Forces of the Methane-Ethane sII Gas Hydrate Interface Sep 2024
Samuel Mathews, André Guerra, Phillip Servio, Alejandro Rey
10.1016/j.colcom.2024.100800

Molecular Dynamics Predictions of Transport Properties for Carbon Dioxide Hydrates under Pre-Nucleation Conditions Using TIP4P/Ice Water and EPM2, TraPPE, and Zhang Carbon Dioxide Potentials Jun 2023
André Guerra, **Samuel Mathews**, Jennifer Tram Su, Milan Marić, Phillip Servio, Alejandro Rey
10.1016/j.molliq.2023.121674

All-Atom Molecular Dynamics of Pure Water-Methane Gas Hydrate Systems under Pre-Nucleation Conditions: A Direct Comparison between Experiments and Simulations of Transport Properties for the Tip4p/Ice Water Model Jul 2022
André Guerra, **Samuel Mathews**, Milan Marić, Phillip Servio, Alejandro Rey
10.3390/molecules27155019

Recent Advances in Density Functional Theory and Molecular Dynamics Simulation of Mechanical, Interfacial, and Thermal Properties of Natural Gas Hydrates in Canada Jun 2022
Samuel Mathews, Shaden Daghash, Alejandro Rey, Phillip Servio
10.1002/cjce.24516

An Integrated Experimental and Computational Platform to Explore Gas Hydrate Promotion, Inhibition, Rheology, and Mechanical Properties at McGill University: A Review Jun 2022
André Guerra, **Samuel Mathews**, Milan Marić, Alejandro Rey, Phillip Servio
10.3390/en15155532

Heat Capacity, Thermal Expansion Coefficient, and Grüneisen Parameter of CH_4, CO_2, and C_2H_6 Hydrates and Ice I_h via Density Functional Theory and Phonon Calculations Jul 2020
Samuel Mathews, Phillip Servio, Alejandro Rey
10.1021/acs.cgd.0c00630

Presentations & Conferences

Gas hydrate interfacial structures and processes for nanostructure characterization and application to green energy storage Dec 2025
International Bio-Inspiration N.I.C.E. Winter Event — Nice, France
Samuel Mathews, Phillip Servio, Alejandro Rey

Gas hydrate interfaces and bulk: geometric and atomistic perspectives Nov 2025
CHEM 634: Seminar in Advanced Materials Invited Speaker — McGill University, Montréal, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Multiscale Characterisation of sII Gas Hydrate Interfacial Structure and Organisation Oct 2025
Canadian Chemical Engineering Conference — Montréal, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Multiscale Characterisation Gas Hydrates Under Pressure May 2025
Centre for Research in Molecular Modeling Annual Symposium — Concordia University, Montréal, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Characterizing, Classifying and Manipulating Gas Hydrate Crystaline Interfaces and Associated Liquid-Like Layers to Understand Their Nucleation and Growth Dec 2024
Materials Research Society Fall Meeting & Exhibit — Boston, United States
Samuel Mathews, Phillip Servio, Alejandro Rey

Characterizing, Classifying, and Manipulating Gas Hydrate Crystalline Interfaces and Associated Phases & Layers to Understand Nucleation and Growth Nov 2024
Chemical Engineering Research Day — McGill University, Montréal Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Molecular Modeling and Characterisation of Processes and Dynamics of Gas Hydrates in the Presence of Applied Electric Fields and Backbone Instabilities Oct 2024
Canadian Chemical Engineering Conference — Toronto, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Multiscale Modeling of Gas Hydrates and their Interfaces Sep 2024
CHEM 634: Seminar in Advanced Materials Invited Speaker — McGill University, Montréal Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Modeling the Effect of Backbone Instabilities and Guest Occupancies on Interfacial and Structural Processes and Dynamics of sII Gas Hydrate Systems Using Molecular Dynamics Jul 2024
16th World Congress on Computational Mechanics — Vancouver, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Geometric Modeling of Gas Hydrate Structural Properties and Guest-Host Interactions Jul 2024
16th World Congress on Computational Mechanics — Vancouver, Canada
Samuel Mathews, Zijun Xu, Phillip Servio, Alejandro Rey

Molecular Modeling of sII Gas Hydrate Interfacial Structures and Processes Jun 2024
Mathematics of Multiscale and Multiphysics Phenomena in Materials Science — BIRS, Banff, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Interfacial Properties and Processes of Natural Gas Hydrates for Energy Applications May 2024
Centre for Research in Molecular Modeling Annual Symposium — Concordia University, Montréal, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Propriétés et Processus Interfaciaux des Hydrates de Gaz pour des Applications Énergétiques May 2024
Quebec Centre for Advanced Materials Annual Symposium — Université de Laval, Quebec City, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Modeling of Interfacial Growth and Structural Processes and Dynamics of sII Gas Hydrate Systems using Molecular Dynamics and Geometric Techniques Nov 2024
Materials Research Society Fall Meeting & Exhibit — Boston, United States
Samuel Mathews, André Guerra, Phillip Servio, Alejandro Rey

Molecular Modeling and Characterisation of Interfacial Processes, Structures, and Dynamics of sII Gas Hydrate Systems for Engineering Applications Oct 2023
Canadian Chemical Engineering Conference — Calgary, Canada
Samuel Mathews, André Guerra, Phillip Servio, Alejandro Rey

Gas Hydrate Thermal and Interfacial Properties and Processes in Gas Capture and Storage for Energy Applications Jun 2024
11th World Congress of Chemical Engineering — Buenos Aires, Argentina
Samuel Mathews, André Guerra, Phillip Servio, Alejandro Rey

Modeling of Interfacial Processes of Gas Hydrate Systems for Energy and Engineering Applications Mar 2023
Chemical Engineering Research Day — Université de Montréal, Montréal Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Modeling of Interfacial Processes of Gas Hydrate Systems for Engineering Applications at Extreme Conditions Mar 2023
American Phyisical Society March Meeting — Las Vegas, United States

Samuel Mathews, André Guerra, Phillip Servio, Alejandro Rey

Equilibrium molecular dynamics of methane hydrate systems at pre-nucleation conditions to predict system transport properties Mar 2023
American Phyisical Society March Meeting — Las Vegas, United States
André Guerra, **Samuel Mathews**, Phillip Servio, Alejandro Rey, Milan Marić

Molecular Modeling of Interfacial Structure, Kinetics and Processes of sII Gas Hydrate Systems for Engineering Applications Dec 2022
Materials Research Society Fall Meeting — Boston, United States
Samuel Mathews, André Guerra, Phillip Servio, Alejandro Rey

Molecular Dynamics Estimations of Transport Properties of Pure Water and Methane Hydrate Systems at Pre-Nucleation Conditions Dec 2022
Materials Research Society Fall Meeting — Boston, United States
André Guerra, **Samuel Mathews**, André Guerra, Alejandro Rey, Milan Marić, Phillip Servio

All-atom molecular dynamics predictions of transport properties of methane hydrate systems at pre-nucleation conditions using the TIP4P/Ice water OPLS potential Oct 2022
Canadian Chemical Engineering Conference — Vancouver, Canada
André Guerra, **Samuel Mathews**, Milan Marić, Phillip Servio, Alejandro Rey

Molecular Dynamics-based transport and interfacial properties with applications to rheology and crystallization of water-based solutions Aug 2022
McGill-ETH Zurich Synergia Symposium — McGill University, Montréal, Canada
Samuel Mathews, André Guerra

Gas Hydrate Thermal and Interfacial Properties for Natural Gas Capture and Storage via Novel Atomistic-Molecular Dynamics Simulations Dec 2021
Materials Research Society Fall Meeting — Boston, United States
Samuel Mathews, Phillip Servio, Alejandro Rey

Gas Hydrate Thermal and Interfacial Properties via Molecular and Atomic Modeling Techniques Oct 2021
Canadian Chemical Engineering Conference — Virtual
Samuel Mathews, Phillip Servio, Alejandro Rey

Thermal Properties of Structure I Hydrates Using Density Functional Theory and Phonon Calculations May 2021
Quebec Centre for Advanced Materials Annual Symposium — Virtual
Samuel Mathews, Phillip Servio, Alejandro Rey

Thermal Properties of sI Hydrates Using Density Functional Theory Jun 2020
International Conference on Gas Hydrates 10 (Canceled due to COVID-19) — Singapore
Samuel Mathews, Phillip Servio, Alejandro Rey

Thermal Properties of sI Hydrates Using Density Functional Theory Feb 2020
Centre for Research in Molecular Modeling Annual Symposium — Concordia University, Montréal, Canada
Samuel Mathews, Phillip Servio, Alejandro Rey

Thermal Properties of sI Hydrates Using Density Functional Theory Nov 2019
Chemical Engineering Research Day — McGill University, Montréal Canada
Samuel Mathews, Alejandro Rey, Phillip Servio