Samuel Mathews, Ph.D.

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Career Objective

PhD-trained computational scientist with **8 years of computational research** in molecular simulation and **5+ years managing HPC cluster infrastructure** (Slurm, InfiniBand, CVMFS, Docker). Looking to develop complex models of materials, processes, and engineering problems using cutting-edge techniques and methods. Delivered **29 technical presentations in 4 countries**.

Scientific Investigation & Resource Management

McGill University — Montréal, Canada Jan 2021 – Present

Doctoral Researcher

- Design and execute **molecular dynamics and DFT simulations** generating ∼**10 TB** of data across gas hydrate projects.
- Model **structures and local organizations** present near and far from gas hydrate interfaces.
- Troubleshoot simulation failures, convergence issues, and **force field incompatibilities** for systems up to **38,500 atoms**.
- Collaborate with **Universidad Nacional Autónoma de México (UNAM)**, provide **Spanish-language technical consultation**.
- Develop `lammpslib`, a Python package (**5 submodules,** ∼**20 files**) for simulation analysis used group-wide.
- Train **6 undergraduate researchers** on DFT setup, geometric analysis, and **HPC cluster workflows**.
- Utilize **machine learning** to identify trends and patterns in large datasets, classify structures, and recognize clustering.
- **Implement computational, analytical, and theoretical modeling** of crystalline properties and interfacial processes and phenomena of gas hydrates using high performance computing clusters.

Scientific Systems Administrator

- Onboard users to HPC: provisioning, job submission, and resource optimization across **local and national** systems.
- Provide **frontline technical support**: troubleshoot failed jobs, hardware faults, and software conflicts for all users.
- Document and maintain **Slurm, CVMFS, LDAP**, networking, backup systems across cluster; configure RDMA (**InfiniBand**).
- Architect **external access** solutions and coordinate with university IT on networking and **institutional policy compliance**.
- Deliver proof-of-concept **benchmarks and demonstrations** to justify continued infrastructure investment.
- Assess **parallel performance, optimize resource utilization, and scale simulations** across CPU and GPU.
- **Deploy, configure, debug scientific HPC assets** in a custom research setup; **deliver live demonstrations and training**.

Laboratory Manager

- Manage **vendor relations** and **full-cycle procurement** of hardware and software within institutional guidelines.
- Author **DRAC resource allocation grants** (2021 through 2028), securing ∼**$500k CAD** in compute resources.
- Coordinate multi-stakeholder projects spanning computational chemistry, IT infrastructure, and **license management**.

Graduate Teaching Assistant Sep 2018 – Apr 2026

- Deliver tutorials, lectures, and lab demonstrations across **13 teaching assignments** in **6 courses** (undergrad and graduate).

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.
- Doctoral Research Scholarship - Fonds de recherche du Québec – Nature et technologies (FRQNT)
- McGill Engineering Doctoral Award (MEDA)

Master of Engineering (M.Eng.), 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.
- McGill Engineering Undergraduate Student Master's Award (MEUSMA)

Bachelor of Engineering (B.Eng.), Chemical Engineering, McGill University — Montréal, Canada Sep 2014 – Apr 2018

- Tomlinson Engagement Award for Mentoring (Fluid Mechanics); James McGill Entrance Scholarship

Professional Development

Mathematics of Multiscale and Multiphysics Phenomena in Materials Science — Banff, Canada Jun 2024
Banff International Research Station for Mathematical Innovation and Discovery

- Multiscale and multi-physics problems that emerge in various areas of materials science with the main focus on three themes: Polycrystals and Materials Microstructures; Materials with Unusual Properties; Complex Fluids and Biomaterials.

Computational Materials North Workshop — Kingston, Canada Aug 2023
Queen's University

Moving Ions with VASP (Vienna Ab initio Simulation Package) for the Advanced User Nov 2023
Virtual

HPC Python Jun 2022
Virtual via Compute Ontario Summer School

DAT112: Neural Network Programming Jun 2022
Virtual via SciNet HPC Consortium

- Six-week course: neural network concepts, theory, and techniques using Python 3.9 and Keras framework.

HPC133: Introduction to GPU Programming Apr 2022
Virtual via SciNet HPC Consortium

- GPUs in supercomputing, GPU programming frameworks, accelerating scientific computing with GPUs (Python/C++).

SCMP271: Advanced Linux Command Line Feb 2022
Virtual via SciNet HPC Consortium

- Advanced Linux commands for productivity on HPC systems.

Advanced Materials for Energy Storage and Conversion Summer School Jul 2021
Virtual via Université de Bordeaux

- Thermal energy storage, PEM fuel cells and electrolysis, photocatalysis for solar fuels, photovoltaic systems, supercapacitors, battery technologies, hydrogen storage and metal hydrides, battery recycling, industrial energy systems.

Technical Skills

Programming: Python, MATLAB, Bash, SQL, LaTeX, Jupyter Notebooks.

Materials Modeling: Large Atomic/Molecular Modeling Software Package, Vienna Ab Initio Simulation Package, Phonopy, MDAnalysis, OVITO, VMD, Moltemplate, Packmol, LCAO and Plane-Wave Basis Set Methods, Elastic Constant and Mechanical Property Calculation, Phonon-Based Thermal Property Calculation, Interfacial Tension, Radial Distribution Functions, Density Profiles, Order Parameter Calculation, Equilibrium MD, Exploratory Non-Equilibrium MD (Electric Field, Electrocrystallization).

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

HPC: Installation/Maintenance of Slurm Scheduler, CERN Virtual Machine File System, Ethernet and InfiniBand Network Configuration, CPU/GPU Performance Tuning, Cloud and Edge Compute, Parallel Workflow Optimization, Source Compilation and MPI Library Benchmarking (OpenMPI, Intel MPI), GPU Support Testing, EasyBuild, CMake/Makefile Configuration.

Numerical Methods: Galerkin Finite Elements, Finite Differences, Collocation, Spectral Methods, Method of Weighted Residuals, Gaussian Quadrature, Monte Carlo Integration, Newton-Raphson Iteration, Implicit/Explicit Time Integration, Predictor-Corrector Methods, Bifurcation Theory (Turning Points, Hopf Bifurcations), Arc-Length Continuation (Keller's Method), Mesh Refinement (Adaptive/Moving), Petrov-Galerkin Upwinding, Isoparametric Mapping, Lagrange Interpolation.

Containers & DevOps: Docker, Docker Compose, Git, Gitea.

OS: NixOS, Debian, Home Manager, declarative system configuration.

Technical Writing: Literature Review and Synthesis, Grant Writing (**Awarded**), Review Paper Authorship.

Languages

English: Native fluency in speaking, writing, reading.

French: Native fluency in speaking, writing, reading.

Spanish: Native fluency in speaking, writing, reading.

Portuguese: Beginner level.

Awards & Achievements

Training Mobility Grant/Award - Quebec Center for Advanced Materials (QCAM)	Oct 2025
Doctoral Research Scholarship - Fonds de recherche du Québec – Nature et technologies	Jun 2022 – Dec 2025
Graduate Research Enhanced and Travel Award	Oct 2025
Canadian Association for Computational Science and Engineering Travel Award	Jul 2024
Graduate Research Enhancement and Travel Award	Jul 2024
Presentation Excellence Award — Concordia University CERMM Research Symposium	May 2024
Prize for Best Use of Language (French) — 8th Advanced Materials Annual Meeting of QCAM	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) — Chemical Engineering Research Day	Nov 2019
Tomlinson Engagement Award for Mentoring: CHEE 314 - Fluid Mechanics	Sep 2017
James McGill Entrance Scholarship	Sep 2014
LeClaire Manufacturing Achievement Scholarship	Jul 2014

Publications

Mathews, S.; Zhu, X.; Guerra, A.; Servio, P.; Rey, A. Atomistic Modeling of Methane and Carbon Dioxide Structure I Gas Hydrates under Pressure: Guest Effects and Properties. *Journal of Chemical Theory and Computation* 2026, 22, 6, 3114–3124. 10.1021/acs.jctc.5c01868.

Guerra, A.; Wang, Z.; **Mathews, S.**; Rey, A. D.; France, K. D. Periodic Feature Characterization in Nanostructured Surfaces and Emulsions. *Langmuir* 2025, 41, 37, 25230–25241. 10.1021/acs.langmuir.5c02320.

Mathews, S.; Zhu, X.; Guerra, A.; Servio, P.; Rey, A. Geometric Characterizations of Non-Uniform Structure I Methane Hydrate Behaviors Under Pressure. *Crystals* 2025, 15 (6), 518. 10.3390/cryst15060518.

Mathews, S.; Servio, P.; Rey, A. Multiscale Interfacial Structure and Organization of sII Gas Hydrate Interfaces Using Molecular Dynamics. *Nanomaterials* 2025, 15 (6), 464. 10.3390/nano15060464.

Mathews, S.; Xu, Z.; Servio, P.; Rey, A. Geometric Modeling of Gas Hydrate Structural Properties and Guest-Host Interactions. In *Proceedings of the 16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics*; Scipedia: Vancouver, Canada, 2024. 10.23967/wccm.2024.097

Mathews, S.; Guerra, A.; Servio, P.; Rey, A. Molecular Dynamics Characterization of the Interfacial Structure and Forces of the Methane-Ethane sII Gas Hydrate Interface. *Colloid and Interface Science Communications* 2024, 62, 100800. 10.1016/j.colcom.2024.100800.

Guerra, A.; **Mathews, S.**; Su, J. T.; Marić, M.; Servio, P.; Rey, A. D. 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. *Journal of Molecular Liquids* 2023, 379, 121674. 10.1016/j.molliq.2023.121674.

Guerra, A.; **Mathews, S.**; Marić, M.; Servio, P.; Rey, A. D. 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. *Molecules* 2022, 27 (15), 5019. 10.3390/molecules27155019.

Mathews, S.; Daghash, S.; Rey, A.; Servio, P. Recent Advances in Density Functional Theory and Molecular Dynamics Simulation of Mechanical, Interfacial, and Thermal Properties of Natural Gas Hydrates in Canada. *The Canadian Journal of Chemical Engineering* 2022, 100 (9), 2557–2571. 10.1002/cjce.24516.

Guerra, A.; **Mathews, S.**; Marić, M.; Rey, A. D.; Servio, P. An Integrated Experimental and Computational Platform to Explore Gas Hydrate Promotion, Inhibition, Rheology, and Mechanical Properties at McGill University: A Review. *Energies* 2022, 15 (15), 5532. 10.3390/en15155532.

Mathews, S. L.; Servio, P. D.; Rey, A. D. 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. *Crystal Growth & Design* 2020, 20 (9), 5947–5955. 10.1021/acs.cgd.0c00630.

Presentations & Conferences

29 presentations across 4 countries in English, French, and Spanish

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 of 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 Crystalline 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

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 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

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

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 Laval, Quebec City, Canada
Samuel Mathews, 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

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 Physical 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 Physical 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**, 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