# **ROBY GAUTHIER**

# **Research Scientist - Electrochemical Energy Storage & Carbon Materials**

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### **SUMMARY**

Research scientist with 10+ years of experience in carbon-based electrochemistry for energy storage. Expertise in structure, synthesis, functionalization, and multi-scale characterization of carbon material, with proven success advancing Li-ion and fuel cell technologies through collaborations with Tesla, Toyota, Hyundai, Los Alamos National Laboratory, and ARPA-E, among others.

#### RESEARCH EXPERIENCE

#### Litster Research Group, Carnegie Mellon University, Pittsburgh, PA

Research Scientist

June 2024 - Present

Funding: Arpa-E, Hyundai, Power to Hydrogen (P2H2)/Department of Energy (DoE), Stratus Materials

- Developing ionomer-free fuel cells with improved oxygen transport and oxygen reduction reaction kinetics using functionalized carbon mixed conductors by collaborating with Los Alamos National Lab and UC Irvine.
- Characterizing the electrochemical properties of new functionalized carbon mixed conductors using cyclic voltammetry, electrochemical impedance spectroscopy, and polarization curve measurement, among other techniques.
- Collaborating on developing characterization techniques to study ionomer degradation in fuel cells using NMR, fluoride-selective electrode-based analysis, Nano-CT, FTIR, Raman, XPS, and SAXS.
- Analyzing electrode and membranes degradation using micro-CT and SEM-EDS.
- Advancing high-performance electrolytes for lithium-rich batteries.

# Whitacre Research Group, Carnegie Mellon University, Pittsburgh, PA

Postdoctoral Fellow

October 2022 - May 2024

Funding: Toyota Research Institute, Stratus Materials

• Developed nuclear magnetic resonance, electrochemical, and computational methods to study electrolyte degradation at graphite interfaces of lithium-ion cells, enabling monitoring, mitigation, and prediction of degradations.

#### Obrovac Research Group, Dalhousie University, Halifax, NS, Canada

Research Scientist

September 2021 - September 2022

Funding: Novonix

- Assembled coin cells from active material powder and polymer binders.
- Performed characterization of synthesized electrode material using electron microscopy, surface area analyzer, and XRD.
- Led synthesis of amorphous materials for battery electrode applications.
- Oversaw laboratory operations, including chemical and equipment procurement, safety protocols, and equipment maintenance.

#### Dahn Research Group, Dalhousie University, Halifax, NS, Canada

Doctoral Researcher

August 2016 - August 2021

- Funding: Tesla
  - Gained advanced knowledge of carbon synthesis and structure from Jeff Dahn, including graphite turbostratic misalignment and its impact on anode capacity, hard carbons and graphite/soft carbon synthesis methods, the falling cards model, and the role of hydrogen functional groups in anode capacity.
  - Characterized graphite-based coin cells and pouch cells using galvanostatic charge discharge, electrochemical impedance spectroscopy, long-term storage at high temperature, and gas production measurement.
  - Analyzed Li-ion battery failures, researched new electrolyte additives, and utilized density functional theory for redox potential predictions.

#### **EDUCATION**

Dalhousie University, Halifax, NS, Canada

Ph.D. in Physics August 2021

Thesis: Understanding and Preventing Lifetime Failure in Lithium-Ion Batteries

Funding: Tesla Advisor: Jeff Dahn Université de Moncton, Moncton, NB, Canada

M.Sc. in Physics May 2018

**Thesis:** Casimir effect, for thin aluminium plates, calculated with the radiation pressure method (Translated from

French)

**Funding:** New Brunswick Innovation Foundation **Advisors:** Normand Beaudoin, Claude Gauthier

Université de Moncton, Moncton, NB, Canada

B.Sc. in Physics with distinction

#### **PUBLICATIONS**

#### **WORKING PAPERS**

A Guide to Predict Redox Potentials of New Electrolyte Components for Li-ion Batteries and Beyond *Roby Gauthier*, Shang Zhu, Venkatsubramanian Viswanathan, and Jay Whitacre. In Preparation, 2025

Reproducible Determination of 3D Model and Porosity of Fuel Cell Cathode Layers from pFIB-SEM Data.

*Roby Gauthier*, Nicole Wang, Enora Petry, and Aryan Mehta. In Preparation, 2025

Formation Accelerated Stress Test (FAST): A New Technique to Study Anode Passivation in Lithium-ion Cells using Differential Capacity, Low Salt Concentration and Low Temperature.

*Roby Gauthier*, Hongyi Lin, Haotian Chen, Venkatsubramanian Viswanathan, and Jay Whitacre. ChemRxiv, 2025

One-Dimensional Casimir Force at Short and Long Ranges Between Two Parallel Plates of Finite Thickness.

Roby Gauthier, Ahcène Brahmi, Claude Gauthier, and Normand Beaudoin.

Physical Review A (In Review), 2025

#### **PEER-REVIEWED**

Nuclear Magnetic Resonance Spectroscopy and Differential Capacity Analysis as Tools to Study Electrolyte Consumption During the Formation Cycle of Li-Ion Pouch cells.

*Roby Gauthier*, Hongyi Lin, Venkatsubramanian Viswanathan, and Jay Whitacre. Journal of Power Sources, 657, 2025, 238134.

The Complex and Spatially Heterogeneous Nature of Degradation in Heavily Cycled Li-ion Cells

Toby Bond, *Roby Gauthier*, Graham King, Reid Dressler, Jeffin James Abraham and Jeff R Dahn Journal of The Electrochemical Society, 171(11), 2024, 110514.

The Amorphization of Crystalline Silicon by Ball Milling

*Roby Gauthier*, B. Scott, J. Craig Bennett, Mina Salehabadi, Jun Wang, Tariq Sainuddin, and M.N. Obrovac. Heliyon, 10(15), 2024, E34881.

How Do Depth of Discharge, C-Rate, and Calendar Age Affect Capacity Retention, Impedance Growth, the Electrodes, and the Electrolyte in Li-Ion Cells?

*Roby Gauthier*, Aidan Luscombe, Toby Bond, Michael Bauer, Michel Johnson, Jessie Harlow, AJ Louli, and Jeff R Dahn. Journal of The Electrochemical Society, 169(2), 2022, 020518.

In-Situ Computed Tomography of Particle Microcracking and Electrode Damage in Cycled NMC622/Graphite Pouch Cell Batteries.

Toby Bond, Roby Gauthier, Sergey Gasilov, and JR Dahn.

August 2013

# In Situ Imaging of Electrode Thickness Growth and Electrolyte Depletion in Single-Crystal vs Polycrystalline LiNixMnyCozO2/Graphite Pouch Cells using Multi-Scale Computed Tomography.

Toby Bond, *Roby Gauthier*, A. Eldesoky, Jessie Harlow and JR Dahn. Journal of The Electrochemical Society, 169(2), 2022, 020501.

#### Lithium Difluoro (dioxalato) Phosphate as an Electrolyte Additive for NMC811/Graphite Li-ion Pouch Cells.

Wentao Song, *Roby Gauthier*, Tina Taskovic, Dongxu Ouyang, Harrison A Ingham, Ahmed Eldesoky, Saad M Azam, Eniko S Zsoldos, Zhe Deng, Dylan H Heino, and Jeff R. Dahn.

Journal of The Electrochemical Society, 169(11), 2022, 110513.

#### Ultrasonic Scanning to Observe Wetting and "Unwetting" in Li-Ion Pouch Cells.

Zhe Deng, Zhenyu Huang, Yue Shen, Yunhui Huang, Han Ding, Aidan Luscombe, Michel Johnson, Jessie E. Harlow, *Roby Gauthier*, and Jeff R. Dahn. Joule, 4(9), 2020, 2017-2029.

#### Effect of Duty Cycle on the Lifetime of Single Crystal LiNi0.5Mn0.3Co0.2O2/Graphite Lithium-Ion Cells.

JH Cheng, JE Harlow, MB Johnson, *Roby Gauthier*, and JR Dahn. Journal of The Electrochemical Society, 167(13), 2020, 130529.

#### Impact of Functionalization and Co-Additives on Dioxazolone Electrolyte Additives.

*Roby Gauthier*, David S Hall, Katherine Lin, Jazmin Baltazar, Toren Hynes, and JR Dahn. Journal of The Electrochemical Society, 167(8), 2020, 080540.

#### New Chemical Insights into the Beneficial Role of Al2O3 Cathode Coatings in Lithium-Ion Cells.

David S Hall, *Roby Gauthier*, Ahmed Eldesoky, Vivian S Murray, and JR Dahn. ACS Applied Materials & Interfaces, 11(15), 2019, 14095–14100.

# A Joint DFT and Experimental Study of an Imidazolidinone Additive in Lithium-ion Cells.

Roby Gauthier, David S Hall, T Taskovic, and JR Dahn. Journal of The Electrochemical Society, 166(15), 2019, A3707.

#### **TEACHING EXPERIENCE**

#### Carnegie Mellon University, Pittsburgh, PA

Guest Instructor for 24-642 / 06-644: Electrochemical Decarbonization Technologies (with Shawn Litster)

January 2025 - May 2025

#### Carnegie Mellon University, Pittsburgh, PA

Guest Instructor for 24-643 / 27-700: Energy Storage Materials and Systems (with Jay Whitacre)

August 2024 - December 2024

### Carnegie Mellon University, Pittsburgh, PA

Guest Lecturer for 24-653: Special Topics: Materials and Their Processing for Mechanical Engineers
(with B. Reeja Jayan)

January 2024 - May 2024

#### Dalhousie University, Halifax, NS, Canada

Graduate Student Instructor for PHYC1190 & PHYC1290 - Introduction to Physics

September 2016 - December 2020

#### Université de Moncton, Moncton, NB, Canada

Teaching Assistant for PHYS2523 - Introduction à la physique

#### **SKILLS**

#### **Laboratory Skills:**

- Equipment and Methods: NMR, Micro-CT, Neware/Maccor cyclers, UHPC cyclers, EIS, XRD, SEM-EDS, Pycnometer, In-Situ/Ex-Situ gas apparatus, Scribner fuel cell test system, cyclic voltammetry, linear sweep voltammetry.
- Tasks: Li-ion pouch cell electrolyte filling, NMR analysis of battery electrolyte, anode SEI, and fuel cell ionomer degradation, electrode slurry preparation and coating, building coin cells, ball milling, and post-mortem cell analysis. Fuel cell characterization, membrane electrode assembly (MEA) construction. Lab management (ordering equipment and chemicals, safety, and equipment maintenance) and gas cylinder replacement.

#### **Data Analysis, Prediction, and Reporting**

- Experienced practitioner in Li-ion battery failure analysis, including modeling the state of health versus cycle number and time, dV/dQ analysis, and data fitting.
- Fitting amorphous and crystalline phase contributions in XRD patterns.
- Density functional theory to predict reduction potentials and Gibbs free energy of reactions.
- Electrolyte property prediction (density, dielectric constant, diffusion constant, radial distribution function, etc.) using molecular dynamics (Gromacs) and the Advanced Electrolyte Model (AEM) from Idaho National Laboratory.
- Reporting data to industrial and governmental partners (Tesla, Novonix, the Toyota Research Institute, Hyundai, ARPA-E).

#### **Collaborations**

- Collaborated on X-ray CT imaging of pouch cells performed at the Canadian Light Source, lithium-ion differential thermal analysis, scanning ultrasonic imaging of pouch cells.
- Collaborated with Los Alamos National Laboratory to develop fuel cells with improved performance.
- Collaborated on developing characterization techniques to study ionomer degradation in fuel cells using NMR, Fluoride selective electrode, Nano-CT, and SAXS.

# **Computational Skills**

- Simulation: DFT (Gaussian, Gpaw, Psi4, Abinit, VASP), Molecular dynamics (Gromacs), Advanced Electrolyte Model (AEM).
- Languages: Python, Matlab, Bash.
- Tools/Frameworks: Azure, PyTorch, TensorFlow, Scikit-learn, Pandas, NumPy, Matplotlib, Git.

#### Languages

- French: Native language.
- · English: Fluent, professional proficiency.

#### **TALKS AND POSTERS**

# Low Salt Concentration and Temperature during Formation as a Tool to Characterize the Passivation of the Anode Solid Electrolyte Interface.

*Roby Gauthier*, Hongyi Lin, Haotian Chen, Venkatasubramanian Viswanathan, and Jay Whitacre. Electrochemical Society Meeting Abstracts 247, 2025.

# Development of Characterization Techniques to Study Chemical and Ionomer Degradation in Proton-Exchange Membrane Fuel Cells.

Roby Gauthier, Eugene Jeong, Chanho Jeong, and Shawn Litster.

Electrochemical Society Meeting Abstracts 247, 2025.

# A Coupled NMR and Differential Capacity Study of the Consumption of Electrolyte and Additive Components during the Formation Cycle of Li-Ion Pouch Cells.

Roby Gauthier, Hongyi Lin, Venkatasubramanian Viswanathan, and Jay Whitacre.

Electrochemical Society Meeting Abstracts 224, 2024.

# A Study on the Kinetics and Structural Changes of Silicon during Ball Milling.

Roby Gauthier, J. Craig Bennett, Benjamin Scott, and M.N. Obrovac.

Electrochemical Society Meeting Abstracts 408, 2024.

#### **Understanding Lifetime Failure in Lithium-ion Batteries**

UC Berkeley Invited Lecture (February 2021).

# New Chemical Insights into the Beneficial Role of Al2O3 Cathode Coatings in Lithium-ion Cells.

Roby Gauthier, David S Hall, Ahmed Eldesoky, Vivian S. Murray, and Jeff R Dahn.

Batteries Gordon Research Conference (2020).

# Probing the Effect of the Depth of Discharge Range and C-Rate on the Lifetime of Li-Ion Cells at Different Temperature.

Roby Gauthier, Alexander J Louli, and Jeff R Dahn.

Electrochemical Society Meeting Abstracts 446, 2019.

#### The Effect of Functional Groups and Co-Additives on the Performance of an Electrolyte Additive for Li-Ion Cells.

Roby Gauthier, David S Hall, Toren Hynes, and Jeff R Dahn.

Electrochemical Society Meeting Abstracts 313, 2019.

#### The Effect of 1,3-Dimethyl-2-Imidazolidinone (DMI) as an Additive in Lithium-ion Cells.

Roby Gauthier, David S. Hall, and Jeff R. Dahn.

CAP Congress, 2018.

# Propriétés Électriques de Couches Minces de WO3 Amorphes et Polycristallins Lithiés.

Roby Gauthier.

2013 Atlantic Universities Physics & Astronomy Conference, 2013.

#### **MENTORSHIP**

#### Abigail Hempy, CMU PhD student

January 2025 - Present

Advising on the fabrication, assembly, and testing of new fuel cell technologies.

#### **Eugene Jeong**, CMU PhD student

June 2024 - Present

Advising on best practices for using NMR and leading through the experimental study of ionomer degradation in fuel cells.

#### **Hongyi Lin**, CMU PhD student

November 2022 - Present

Advising on best practices for using NMR and directing the choice of electrolyte and charging-discharging protocol for lithium-ion battery studies.

#### **Shang Zhu**, CMU PhD student

November 2022 - Present

Instructing on performing density functional theory (DFT) calculations with experimental accuracy by teaching the inclusion of polarizable continuum models. Also guided on how to compare theoretical results to published experimental research.

#### Matéo Croussette, Polyvalente Alexandre J. Savoie

June 2022 - Present

Guiding on potential career paths, answering science-related questions, and encouraging passion for the sciences.

#### Adriana Reitano, Dalhousie University B.Sc. Student

September 2018 - December 2018

Mentored through the introduction to physics class by building confidence and fostering a passion for the subject.

#### **SERVICE & OUTREACH**

Organized and hosted a laboratory visit for our Hyundai research sponsors for a week. The visit consisted of demonstrating our laboratory method and discussing its potential impact on the ongoing research partnership.

Carnegie Mellon University, Pittsburgh, PA

2024

Supported OurCS 2024, a 3-day research-focused workshop aimed at improving gender balance in computing research. The event encourages undergraduate students from the USA and across the globe to explore research opportunities and develop skills in computing disciplines.

Carnegie Mellon University, Pittsburgh, PA

2024

Offered expertise in chemistry to a research team focused on using generative AI for the advancement of learning materials and educational resources.

Carnegie Mellon University, School of Computer Science, Pittsburgh, PA

2023

Provided technology and emotional support for stroke recovery patients.

March of Dimes Canada 2021

Planetary Shows: Hosted high school students to explore educational opportunities about astronomy.

Physics Department, Dalhousie University, Halifax, NS, Canada

2019

Physics Fun and Discovery Days: Hosted high school students to explore educational opportunities about physics.

Physics Department, Dalhousie University, Halifax, NS, Canada

2019

### **REFERENCES**

#### Shawn Litster, Ph.D.

Professor of Mechanical Engineering
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Website: https://www.meche.engineering.cmu.edu/di-

rectory/bios/litster-shawn.html

#### Jay F. Whitacre, Ph.D.

Trustee Professor in Energy

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### Venkat Viswanathan, Ph.D.

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ple/viswanathan-venkat/

#### David Scott Hall, Ph.D.

Associate Professor in Battery Technology Faculty of Science and Technology Department of Energy and Petroleum Engineering

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#### B. Reeja Jayan, Ph.D.

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rectory/bios/jayan-reeja.html

### Jeff Dahn, Ph.D., FRSC, O.C.

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