# ROBY GAUTHIER

# **Research Scientist, Carnegie Mellon University**

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#### **EDUCATION & TRAINING**

## Carnegie Mellon University, Pittsburgh, PA

Postdoctoral Fellow May 2024

Developed nuclear magnetic resonance, electrochemical, and computational methods to study electrolyte degradation and properties for Lithium-ion cell monitoring, mitigation, and prediction.

Funding: Toyota Research Institute, Stratus Materials

Advisors: Jay Whitacre, Venkat Viswanathan

#### Dalhousie University, Halifax, Canada

Ph.D. in Physics August 2021

Analyzed Li-ion battery failures, researched new electrolyte additives, and utilized density functional theory for redox potential predictions. **Thesis:** Understanding and Preventing Lifetime Failure in Lithium-Ion Batteries

Funding: Tesla Advisor: Jeff Dahn

#### Université de Moncton, Moncton, Canada

M.Sc. in Physics May 2018

Formulated mathematical models of the Casimir effect for thin aluminum plates, leveraging electromagnetism and quantum physics principles.

Thesis: Effet Casimir, pour des plaques d'aluminium d'épaisseur finie, calculé avec la méthode de pression de radiation

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

#### Université de Moncton, Moncton, Canada

B.Sc. in Physics with distinction August 2013

#### **RESEARCH EXPERIENCE**

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

Research Scientist

Findings Area F. Haundei Banartmant of Facus & Street

June 2024 - Present

Funding: Arpa-E, Hyundai, Department of Energy, Stratus Materials

- Developing ionomer-free fuel cells with improved oxygen transport and oxygen reduction reaction kinetics using functionalized mixed conductors. This will enable fuel cells with higher performance, lower cost, and longer lifetimes.
- Collaborating on developing characterization techniques to study ionomer degradation in fuel cells using NMR, Fluoride selective electrode, Nano-CT, and SAXS.
- · Advising Stratus Materials for the development of high-performance electrolytes for lithium-rich batteries.

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

Research Scientist

September 2021 - September 2022

- **Funding:** Novonix
  - Oversaw laboratory operations, including chemical and equipment procurement, safety protocols, and equipment maintenance.
  - · Led examination and modeling of amorphous materials for battery electrode applications.

#### Ashrit Research Group, Université de Moncton, Moncton, Canada

Undergraduate Student Research Assistant

May 2012 - August 2013

Funding: Natural Sciences and Engineering Research Council (NSERC)

• Executed impedance studies on tungsten trioxide thin films produced via physical vapor deposition.

## **PUBLICATIONS**

## **WORKING PAPERS**

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-lon 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. Journal of The Electrochemical Society, 169(8), 2022, 080531.

# In Situ Imaging of Electrode Thickness Growth and Electrolyte Depletion in Single-Crystal vs Polycrystalline LiNixMny-CozO2/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.

#### **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, Canada

Graduate Student Instructor for PHYC1190 & PHYC1290 -

Introduction to Physics September 2016 - December 2020

## Université de Moncton, Moncton, Canada

Teaching Assistant for PHYS2523 - Introduction à la physique

moderne et à l'optique January 2014 - April 2015

#### **SKILLS**

# **Laboratory Skills:**

- Equipment and Methods: NMR, Micro-CT, Neware/Maccor cyclers, UHPC cyclers, EIS, XRD, SEM, 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

Janurary 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

2022

Collaborated on an article to promote information sharing on battery technology research.

Provided technology and emotional support for stroke recovery patients.

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

Physics Department, Dalhousie University, Halifax, Canada

2019

2021

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

Physics Department, Dalhousie University, Halifax, Canada

2019

#### **REFERENCES**

LinkedIn

#### Shawn Litster, Ph.D.

March of Dimes Canada

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## Venkat Viswanathan, Ph.D.

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

Associate Professor in Battery Technology

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

**Professor Emeritus** 

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Dalhousie University Email: jeff.dahn@dal.ca Phone: 902-494-2991

Website: https://www.dal.ca/diff/dahn.html