

# ROBY GAUTHIER, PH.D.

## Research Scientist, Carnegie Mellon University

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### EDUCATION & TRAINING

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#### **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 and 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

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

Research Scientist

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.

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

## **PEER-REVIEWED PUBLICATIONS**

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### **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, 2024, Accepted.

### **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 LiNi<sub>x</sub>Mn<sub>y</sub>Co<sub>z</sub>O<sub>2</sub>/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 LiNi<sub>0.5</sub>Mn<sub>0.3</sub>Co<sub>0.2</sub>O<sub>2</sub>/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 Al<sub>2</sub>O<sub>3</sub> 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.

## OTHER PUBLICATIONS

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**Analyzing the Formation of the Solid Electrolyte Interfaces under Low Salt Concentrations and Low Temperature to Better Understand Graphite Passivation and Accelerate Electrolyte Discovery.**

*Roby Gauthier*, Hongyi Lin, Venkatsubramanian Viswanathan, Jay Whitacre.

In Review, 2024

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

*Roby Gauthier*, AHCÈNE BRAHMI, Claude Gauthier, Normand Beaudoin.

In Review, 2024

**NMR and dQ/dV Analysis as Tools to Study Electrolyte Consumption During the Formation Cycle of Li-ion Pouch Cells.**

*Roby Gauthier*, Hongyi Lin, Venkatsubramanian Viswanathan, Jay Whitacre.

In Preparation, 2024

## TEACHING EXPERIENCE

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**Carnegie Mellon University**, Pittsburgh, PA

Guest Instructor for 24-643 / 27-700: Energy Storage Materials and Systems

(with Jay Whitacre)

August 2024 - Present

**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

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**Laboratory Skills:**

- Equipment and Methods: NMR, 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.

## 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

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### **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 Al<sub>2</sub>O<sub>3</sub> 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 WO<sub>3</sub> Amorphes et Polycristallins Lithiés.**

*Roby Gauthier.*  
2013 Atlantic Universities Physics & Astronomy Conference, 2013.

## **MENTORSHIP**

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**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 on 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 guiding 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 passion for the subject.

## **SPECIAL TRAINING AND CLASSES**

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|--|------------------|
| 11-637: Foundations of Computational Data Science                  | 2023             |
| NMR Spectrometer Training  | 2017, 2019, 2023 |
| ACENET & Compute Canada Training                                   | 2019             |
| CHEM 2401: Introductory Organic Chemistry                          | 2019             |
| CHEM 6363: Electronic Structure Theory of Solids (Abinit Software) | 2018             |
| CHEM 6353: Density-Functional Theory                               | 2018             |
| CHEM 5301: Theory of Chemical Bonding (Gaussian Software)          | 2017             |

## **SERVICE & OUTREACH**

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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

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

*LinkedIn* 2022

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, Canada* 2019

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

*Physics Department, Dalhousie University, Halifax, Canada* 2019

## REFERENCES

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### **Shawn Litster, Ph.D.**

Professor of Mechanical Engineering  
Department of Mechanical Engineering  
Carnegie Mellon University  
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### **Jay F. Whitacre, Ph.D.**

Trustee Professor in Energy  
Department of Materials Science and Engineering  
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### **Venkat Viswanathan, Ph.D.**

Associate Professor of Aerospace Engineering  
University of Michigan  
College of Engineering  
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Website: <https://aero.engin.umich.edu/people/viswanathan-venkat/>

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

Associate Professor in Battery Technology  
Faculty of Science and Technology  
Department of Energy and Petroleum Engineering  
University of Stavanger  
Email: [david.s.hall@uis.no](mailto:david.s.hall@uis.no)  
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### **B. Reeja Jayan, Ph.D.**

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CMU Engineering Dean's Early Career Fellow  
Carnegie Mellon University  
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### **Jeff Dahn, Ph.D., FRSC, O.C.**

Professor Emeritus  
Principal Investigator - NSERC/Tesla Canada  
Industrial Research Chair/Dalhousie Alliance Grant  
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