ROBY GAUTHIER

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EDUCATION and TRAINING

Carnegie Mellon University, Pittsburgh, PA
Postdoctoral Fellow — November 2022 - May 2024

Developed nuclear magnetic resonance, electrochemical, and computational methods for Lithium-ion cell monitoring, mitigation, and prediction.
Funding: Toyota Research Institute, Stratus Materials
Advisor: Jay Whitacre

Conducted experimental and theoretical research on electrolyte degradation and properties in lithium-ion batteries.
Funding: Toyota Research Institute
Advisor: Venkat Viswanathan

Dalhousie University, Halifax, Canada
Ph.D. in Physics — August 2021
Thesis: Understanding and Preventing Lifetime Failure in Lithium-Ion Batteries
Advisor: Jeff Dahn

Université de Moncton, Moncton, Canada
M.Sc. in Physics — May 2017
Thesis: Effet Casimir, pour des plaques d'aluminium d'épaisseur finie, calculé avec la méthode de pression de radiation
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 — June 2024 - Present
Funding: Arpa-E, Hyundai, Stratus Materials

- Developing fuel cells with improved performance. Developing electrolytes for lithium-ion batteries.

Obrovac Research Group, Dalhousie University, Halifax, Canada
Research Assistant — 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.

Dahn Research Group, Dalhousie University, Halifax, Canada
Graduate Student Research Assistant — September 2016 - August 2021
Funding: Tesla

- Analyzed Li-ion battery failures and researched new electrolyte additives.

- Utilized density functional theory for redox potential predictions.

Beaudoin Research Group, Université de Moncton, Moncton, Canada
Graduate Student Research Assistant September 2013 - May 2017
Funding: New Brunswick Innovation Foundation

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

Ashrit Research Group, Université de Moncton, Moncton, Canada
Undergraduate Student Research Assistant May 2012 - August 2013

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

SKILLS

- **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 and SEI, electrode slurry preparation and coating, building coin cells, cycling 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, 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.

PUBLICATIONS

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 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 24-643: 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

TALKS AND POSTERS

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.
245th Electrochemical Society Meeting (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.
245th Electrochemical Society Meeting (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 236, 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 236, 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

Eugene, CMU PhD student	June 2024 - Present
Hongyi Lin, CMU PhD student	November 2022 - Present
Shang Zhu, CMU PhD student	November 2022 - Present
Matéo Croussette, Polyvalente Alexandre J. Savoie	June 2022 - Present
Adriana Reitano, Dalhousie University B.Sc. Student	September 2018 - December 2018

SPECIAL TRAINING AND CLASSES

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

VOLUNTEERING AND OUTREACH

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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