Bharathy S. Parimalam

Battery research scientist versed in battery materials, electrochemistry, chemical characterization, imaging techniques, scientific python stack, and machine learning

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Professional Highlights

- Over 10 years of research experience in lithium-ion batteries, focused on electrolytes, and silicon anodes along with lithium metal systems, zinc-air batteries, and fuel cells. Experienced in coating electrodes, cell construction, electrochemical testing, disassembly, and electrolyte extraction.
- Versed in a range of characterization and imaging techniques such as electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), gas chromatography mass spectrometry (GCMS), nuclear magnetic resonance spectroscopy (NMR), Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), nano computed tomography (Nano-CT), and micro computed tomography (Micro-CT).
- Several impactful publications in the domain of lithium-ion anode SEI, electrolyte-SEI interactions, and lithium metal anodes with 1000+ citations.
- Experienced in processing, quantifying, and visualizing large datasets using scientific python stack; building numerical, machine learning, and deep learning models; and segmenting complex and noisy images and extracting quantitative insights.

Education

Research Advisor: Prof. Brett L. Lucht

University of Rhode Island Kingston, RI, USA Ph.D. in Chemistry 2012 - 2017

Central Electrochemical Research Institute

B.S. in Chemical and Electrochemical Engineering

Research Advisor: Dr. T. Prem Kumar

Karaikudi, TN, India 2008 - 2012

Work Experience

Research Scientist

E-one Moli Energy (Canada) Ltd.

Nov 2021 - Present Maple Ridge, BC

Modeled lithium-ion cells to synthesize electrochemical data for method development and validation purposes. Developed a python library to extract aging parameters such as silicon state of health, slippage, and resistance growth from the electrochemical performance data of lithium-ion cells, using pandas, numpy, scipy, and matplotlib. Published a detailed documentation of the library using Sphinx. Evaluated the consumption rate of crucial electrolyte components using gas chromatography-mass spectrometry (GCMS). Maintained my domain knowledge current through reading relevant literature and attending scientific conferences. Provided recommendations to improve electrolyte formulations using the understanding obtained with experiments. Evaluated the significance of various factors in an experiment using Design Expert (DOE). Participated in regular discussions among colleagues with different domains and levels of expertise.

Postdoctoral Fellow

Simon Fraser University

Jan 2020 - Sep 2021 Surrey, BC

Studied pore size distribution, porosity on zinc-air battery, and water/ionomer distribution in fuel cell cathodes. Designed and fabricated custom fixtures with humidity and temperature controls using Solidworks(CAD). Acquired high-resolution 3D images using nano/micro X-ray computed tomography (Nano-CT/Micro-CT) and scanning electron microscopy (FIB-SEM). Carried out image processing with ImageJ, and python(scikit-image, numpy). Segmented the 3D images for quantitative analysis using machine learning methods with python (scikit-learn, tensorflow, pandas, numpy). Conducted quantitative analyses on images with python using the porespy library. Mentored graduate and undergraduate researchers with varying levels of expertise.

Postdoctoral Researcher

Carnegie Mellon University

Jun 2018 - Nov 2019 Pittsburgh, PA

Designed, fabricated, and optimized custom electrochemical coin cells to suit specific goals. Studied the impact of current density, temperature, and electrolytes, on lithium electroplating and dendrite growth in lithium-ion/lithium metal battery anodes, using a combination of electrochemical techniques, and nano X-ray computed tomography (Nano-CT). Studied the reversal tolerant anodes and OER catalyst failure mechanisms in fuel cells using various electrochemical techniques. Designed, and fabricated custom holders to acquire high-resolution images of polymer electrolyte membrane (PEM) in nano XCT under controlled humidity. Mentored graduate and undergraduate researchers with varying levels of expertise.

Graduate Research/Teaching Assistant

University of Rhode Island

Aug 2012 - Mar 2018 Kingston, RI

Studied the formation and decomposition reactions of anode SEI components originating from electrolyte solvents, salts, and additives of lithium-ion batteries, using a combination of nuclear magnetic resonance spectroscopy (NMR), Fourier transform infrared spectroscopy (FTIR), gas chromatography-mass spectrometry (GCMS), liquid chromatography-mass spectrometry (LCMS), and X-ray photo electron spectroscopy (XPS). Fabricated electrodes, built and tested lithium-ion batteries using various electrochemical techniques. Delivered brief lectures on theoretical concepts and calculations pertaining to the experiments. Taught and supervised the general chemistry experiments, safe lab practices, and waste management to undergraduate students. Evaluated the academic performance of the students through lab reports.

Projects

Lithium-ion Electrolyte Optimization

Research Scientist

Nov 2021 - Present Maple Ridge, BC

JupyterPythonmolicelpandasmatplotlibSciPyNumPycyclersmaccorGCMSDOECVEIS

Screened additives and solvents to improve silicon retention and high-rate performance. Designed experiments using optimal mixture method to determine optimal fraction of various solvents in the electrolyte to meet the performance goals. Determined optimal electrolyte volume to achieve a balanced performance profile for cylindrical cells. Estimated the influence of various factors and designs on FEC consumption rate using GCMS.

Molicel Python Module

Research Scientist

Nov 2021 - Present Maple Ridge, BC

Python pandas matplotlib SciPy NumPy reST Sphinx

Written a Python library to automate parsing, processing, and plotting large sets of electrochemical

data. Developed novel methods to monitor silicon state-of-health, and slippage from cycling data and implemented them as part of the module. Published a detailed API reference, examples, and usecases internally using the documentation generator Sphinx.

Numerical Model of Lithium-ion Battery

Nov 2021 - Oct 2022 Maple Ridge, BC

Research Scientist

Python

pandas matplotlib SciPv

/ NumPy

cyclers

pouch cells

Developed a numerical model of lithium-ion battery using half cell voltage curves, and simple Python functions. Generated challenging datasets to aid in various method development through method validation. Published a detailed API reference, examples, and usecases internally using the documentation generator Sphinx.

Composite Silicon Anode Health Estimation

Nov 2021 - Apr 2022 Maple Ridge, BC

Research Scientist

Python pandas matplotlib

SciPv

NumPy

cyclers maccor

Developed a novel, simple, yet robust method to measure silicon active mass loss. Validated the method using challenging simulted datasets. Implemented the method as part of a Python module for the ease of automation and distribution within the company. Studied an array of conditions, protocols, additives, solvents for their impact on silicon health and provided useful recommendations to improve

3D Analysis of Air Electrode Interactions

the durability of the lithium-ion cells.

Jan 2020 - Sep 2021

Postdoctoral Fellow

Surrey, BC

Python ImageJ scikit-image scikit-learn

TensorFlow

pandas

NumPy

matplotlib

porespy Micro-CT Nano-CT FIB-SEM

Studied pore size distribution, porosity on zinc-air battery, and water/ionomer distribution in fuel cell cathodes. Designed and fabricated custom fixtures with humidity and temperature controls using Solidworks(CAD). Acquired high-resolution 3D images using nano/micro X-ray computed tomography (Nano-CT/Micro-CT) and scanning electron microscopy (FIB-SEM). Carried out image processing with ImageJ, and Python(scikit-image, NumPy). Segmented the 3D images for quantitative analysis using machine learning methods with Python (scikit-learn, TensorFlow, pandas, NumPy). Conducted quantitative analyses on images with Python using the porespy library. Mentored graduate and undergraduate researchers with varying levels of expertise.

3D Analysis of Fuel Cell Membrane

Mar 2018 - Nov 2019

Postdoctoral Researcher

Pittsburgh, PA

ImageJ Avizo MATLAB Python Nano-CT potentiostat

Studied the reversal tolerant anodes and OER catalyst failure mechanisms in fuel cells using various electrochemical techniques. Designed, and fabricated custom holders to acquire high-resolution images of polymer electrolyte membrane (PEM) in nano XCT under controlled humidity. Mentored graduate and undergraduate researchers with varying levels of expertise.

3D Analysis of Lithium Metal Anodes

Jun 2018 - Mar 2019

Postdoctoral Researcher

Pittsburgh, PA

ImageJ Avizo MATLAB Python Nano-CT potentiostat

Designed, fabricated, and optimized custom electrochemical coin cells to suit specific goals. Studied the impact of current density, temperature, and electrolytes, on lithium electroplating and dendrite growth in lithium-ion/lithium metal battery anodes, using a combination of electrochemical techniques, and nano X-ray computed tomography (Nano-CT). Mentored graduate and undergraduate researchers

with varying levels of expertise.

Understanding Formation and Evolution of Lithium-ion Anode SEI

Graduate Research Assistant

Aug 2012 - Dec 2017 Kingston, RI

Mnova XPSPEAK Avantage MS Excel ChemDraw GIMP NMR GCMS FTIR XPS LCMS

glove box synthesis Arbin

Investigated the components of lithium-ion anode SEI through novel methods. Identified the initial components resulting from common solvents, salts, and additives, and their subsequent degradation products. These works were published through a series of academic papers and garnered over 800 citations.

Intermetallic Lithium-ion Anode Development

Research Assistant

Jan 2010 - May 2012 Karaikudi, TN, India

MS Excel synthesis Arbin

Studied coppper-bismuth nanoparticulate composite material as anodes for lithium-ion batteries. The material was synthesized through chemical reduction of respective metal ions in an aqueous solution. Electrochemical performance of the materials were evaluated in coin cell format. The compsite electrodes outperformed pure silicon electrode in capacity retention and reversibly cycled several hundred times with the specific capacity of 300 mAh/g.

Publications

- [In Preparation] **Bharathy S. Parimalam**, Paul Choi, Dan Velez, Yubai Li, and Shawn Litster. *Lithium Electroplating Patterns Revealed with Nano XCT Imaging using Coin-cell Configuration*.
- J. Power Sources (2023) 564, 232820. Fabusuyi Aroge, **Bharathy S. Parimalam**, John MacDonald, Francesco Orfino, Monica Dutta, and Erik Kjeang. *Analysing operando 2D X-ray transmission images for liquid water distribution in polymer electrolyte fuel cells*.
- ACS Energy Lett. (2021) 6, 11, 3788–3792. Chamithri Jayawardana, Nuwanthi Rodrigo, **Bharathy S.** Parimalam, and Brett L Lucht. Role of Electrolyte Oxidation and Difluorophosphoric Acid Generation in Crossover and Capacity Fade in Lithium Ion Batteries.
- ACS Applied Energy Materials (2021) 4, 2, 1657-1665. Paul Choi, Bharathy S. Parimalam, Laisuo Su, B Reeja-Jayan, Shawn Litster. Operando Particle-Scale Characterization of Silicon Anode Degradation during Cycling by Ultrahigh-Resolution X-ray Microscopy and Computed Tomography.
- MethodsX (2021) 8, 101562. Laisuo Su, Paul Choi, Bharathy S. Parimalam, Shawn Litster, B Reeja-Jayan. Designing reliable electrochemical cells for operando lithium-ion battery study.
- Journal of the Electrochemical Society(2018) 165 (10) A1991-A1996. K. W. D. Kaveendi Chandrasiri, Cao Cuong Nguyen, **Bharathy S. Parimalam**, Sunhyung Jurng ,and Brett L. Lucht. *Citric Acid Based Pre-SEI for Improvement of Silicon Electrodes in Lithium Ion Batteries*
- Journal of the Electrochemical Society(2018) 165 (2) A251-A255. Bharathy S. Parimalam, and Brett L. Lucht. Reduction Reactions of Electrolyte Salts for Lithium-Ion Batteries: LiPF₆, LiBF₄, LiDFOB, LiBOB, and LiTFSI.
- Journal of Physical Chemistry C (2017) 121 (41), 22733-22738. Bharathy S. Parimalam, Alex D. MacIntosh, Rahul Kadam, and Brett L. Lucht. Decomposition Reactions of Anode Solid Electrolyte Interphase (SEI) Components with LiPF₆.

- Electrochimica Acta (2017) 250, 285-291. KWD Kaveendi Chandrasiri, Cao Cuong Nguyen, Yuzi Zhang, Bharathy S. Parimalam, and Brett L. Lucht. Systematic Investigation of Alkali Metal Ions as Additives for Graphite Anode in Propylene Carbonate Based Electrolytes.
- Journal of Electroanalytical Chemistry (2017) 799, 181-186. Yue Pan, Yuzi Zhang, Bharathy S. Parimalam, Cao Cuong Nguyen, Guiling Wang, and Brett L. Lucht. Investigation of the Solid Electrolyte Interphase on Hard Carbon Electrode for Sodium-Ion Batteries.
- Chemistry of Materials (2017) 29 (7), 3237-3245. Taeho Yoon, Mickdy S. Milien, Bharathy S. Parimalam, and Brett L. Lucht. Thermal Decomposition of the Solid Electrolyte Interphase (SEI) on Silicon Electrodes for Lithium-Ion Batteries.
- Chemistry of Materials (2016) 28, (22) 8149-8159. Alison L. Michan, Bharathy S. Parimalam, Michal Leskes, Rachel N. Kerber, Taeho Yoon, Clare P. Grey, and Brett L. Lucht. Fluoroethylene Carbonate and Vinylene Carbonate Reduction: Understanding Lithium-Ion Battery Electrolyte Additives and Solid Electrolyte Interphase Formation.
- ECS Electrochemistry Letters (2014) 3 (9), A91-A93. Daniel M. Seo, Dinesh Chalasani, Bharathy S. Parimalam, Rahul Kadam, Mengyun Nie, and Brett L. Lucht. Reduction Reactions of Carbonate Solvents for Lithium-Ion Batteries.

Presentations

- 242nd ECS Meeting, Atlanta. Sara Abouali, Bharathy S. Parimalam, Fabusuyi Aroge, Francesco Orfino, Monica Dutta, Erik Kjeang. Visualization of Water Distribution in Fuel Cell Microporous and Catalyst Layers with 3D Nanoscale X-Ray Imaging (2022).
- 240th ECS Meeting, Orlando. Fabusuyi Aroge, Bharathy S. Parimalam, Francesco Orfino, Monica Dutta, Erik Kjeang. Method for Analyzing 2D X-Ray Transmission Images for Operando Liquid Water Distribution in a Polymer Electrolyte Fuel Cell (2021).
- 236th ECS Meeting, Atlanta. Bharathy S. Parimalam, Yubai Li, Paul Choi, Shawn Litster. Lithium Plating Patterns on Lithium Anode Revealed with Operando Nanoscale X-Ray Imaging (2019).
- 233rd ECS Meeting, Seattle. Brett L. Lucht, KWD Kaveendi Chandrasiri, Sunhyung Jurng, Bharathy S. Parimalam, Cao Cuong Nguyen, Benjamin Young, David Heskett. Surface Functionalization of Silicon Nanoparticles with Citric Acid for Enhanced Performance As Lithium Ion Battery Anodes (2018).
- 250th ACS national meeting, Boston. **Bharathy S. Parimalam**, Mengyun Nie, Brett L. Lucht. *Comparison of the Reduction Products: Vinylene Carbonate vs. Fluoroethylene Carbonate* (2015).
- 224th ECS Meeting, San Francisco. Brett L Lucht, Dinesh Chalasani, Bharathy S. Parimalam, Daniel M Seo, Rahul Kadam, Mengqing Xu. Lithium Alkyl Carbonates: Preparation and Investigation of Stability (2013).

Posters

- 256th ACS national meeting, Boston. Kaveendi Chandrasiri, Sunhyung Jurng, **Bharathy S. Parimalam**, Cao Cuong Nguyen, Benjamin Young, Brett Lucht, David Heskett. *Use of citric acid to form an artificial SEI on silicon nanoparticles to enhance the performance of lithium-ion battery anodes* (2018).
- 233rd ECS Meeting, Seattle. Brett L Lucht, Dilni Kaveendi Chandrasiri, Sunhyung Jurng, Bharathy S. Parimalam, Cao Cuong Nguyen, Benjamin Young and David Heskett. Surface Functionalization of Silicon Nanoparticles with Citric Acid for Enhanced Performance As Lithium Ion Battery Anodes (2018).

- 68th Meeting of International Society of Electrochemistry, Providence. **Bharathy S. Parimalam**, and Brett L Lucht. *Insights into the Stability of Lithium-Ion Battery SEI Components in LiPF6 Containing Electrolytes* (2017).
- 18th International Meeting on Lithium Batteries, Chicago. Bharathy S. Parimalam, Mengyun Nie, Brett L Lucht. Reduction Products of Vinylene Carbonate and Fluoroethylene Carbonate (2016).
- International Symposium on Energy Materials. Kolkata. **Bharathy S. Parimalam**, Chinnathambi S., SriDeviKumari T., PremKumar T. *Nanoscale Bismuth-Copper Composite as a Lithium Insertion Anode Material* (2011).

Skills

- Evaluating the significance of various factors in an experiment using design of experiment (DOE) software, such as Design Expert
- Electrode fabrication, cell building and electrochemical testing of lithium-ion batteries
- Multiscale *operando/in situ* imaging of electrochemical cells and components using micro and nano X-ray computed tomography
- X-ray Photoelectron Spectroscopic analysis of electrically insulating air-sensitive powder samples
- Fourier Transform Infrared Spectroscopic analysis of air-sensitive powder samples and electrodes
- Gas Chromatography-Mass Spectrometric analysis of liquids and gases
- Nuclear Magnetic Resonance Spectroscopic analysis of water/air-sensitive samples
- Operando/in situ nano and micro XCT imaging of electrochemical cells, electrodes, and membranes
- Processing and segmentation of microscopy images using traditional and machine-learning methods (python/pandas, tensorflow, scikit-image; Image))
- Computing pore/crack/particle size distributions, phase fractions, and other properties from 2D/3D images using python (porespy, scikit-image)
- Numerical simulation of battery cycling and aging behavior using python (pandas, numpy, scipy)
- Documenting python modules using document generator, Sphinx
- Familiar with Jupyter Lab/Notebook
- Computer-aided design using and fabrication of custom XCT fixtures for operando/in-situ analysis
- Design and fabrication of custom electrochemical cells and samples with high X-ray transparency for operando/in situ imaging
- Technical communication in the forms of presentations, reports, white papers, and publications
- Mentored graduate and undergraduate researchers with varying levels of expertise.
- Collaborated both within and outside the team on several research projects