

Dr. Behnam Ghalami Choobar

Multiscale Battery Modeling | SOC/SOH Estimation | Electrolyte Simulation

Email: Ghalamichoobar@Guilan.ac.ir | Ghalamichoobar@gmail.com

Location: Rasht, Iran

[Google Scholar](#) | [ORCID](#)

Research Metrics:

- ◇ Total Publications: $\approx 20+$
- ◇ h-index: 11 (Google Scholar)
- ◇ Citations: 350 (Google Scholar)

RESEARCH PROFILE

Faculty member specializing in multiscale modeling of lithium-ion batteries, integrating electrochemical modeling, observer-based SOC/SOH estimation, and molecular simulation of electrolytes.

My research aims to bridge molecular-scale transport phenomena with system-level battery management algorithms through physics-informed and data-driven approaches.

I have authored 20+ peer-reviewed publications in journals including *Journal of Energy Storage*, *Journal of Energy Chemistry*, *ChemElectroChem*, and *Small*.

RESEARCH INTERESTS

Battery Management Systems (SOC/SOH estimation)
Physics-informed machine learning for battery diagnostics
Multiscale modeling of lithium-ion batteries
Molecular dynamics simulation of electrolytes
Electrochemical transport and degradation mechanisms

SELECTED PUBLICATIONS

Battery Management Systems & SOC/SOH Estimation

- ◇ **Behnam Ghalami Choobar***, A Fereydooni, “Adaptive sliding mode observer for joint state-of-charge and state-of-health estimation in lithium iron phosphate batteries using a hysteresis-inclusive dual-polarization model”, *Journal of Energy Storage*, 2023
- ◇ **Behnam Ghalami Choobar**, Hamid Hamed, Mohammadhosein Safari*, “Sliding mode observer with adaptive switching gain for estimating state of charge and internal temperature of a commercial Li-ion pouch cell” *Journal of Energy Storage*, 2024
- ◇ **Behnam Ghalami Choobar***, Hamid Hamed, Abolfazl Moghadam, Quanquan Pang, Mohammadhosein Safari “Fractional-Order Derivatives to Elevate the Physics-Awareness of the Data-Driven Battery Health Estimators” *Journal of Energy Storage* (Under Revision)

Electrochemistry & Battery Physics

- ◇ **Behnam Ghalami Choobar**, Hamid Hamed, Mohammadhosein Safari*, “Morphological peculiarities of the lithium electrode from the perspective of the Marcus-Hush-Chidsey model” *Journal of Energy Chemistry*, 2023
- ◇ **Behnam Ghalami Choobar**, Hamid Hamed, Saeed Yari, Mohammadhosein Safari*, “Theoretical and Experimental Insights into Dendrite Growth in Lithium-Metal Electrode” *ChemElectroChem*, 2024
- ◇ Hamid Hamed, AC Reis, **Behnam Ghalami Choobar**, Quanquan Pang, Rebeca Killick, Mohammadhosein Safari* “Changeoint detection as a light data-driven approach to battery state-of-health prediction”, *Cell Reports Physical Science*, 2026

Molecular Simulation & Electrolytes

- ◇ **Behnam Ghalami Choobar**, Hamid Modarress*, Rouein Halladj, Sepideh Amjad-Iranagh, “Multiscale Investigation on Electrolyte Systems of [(Solvent + Additive) + LiPF₆] for Application in Lithium-Ion Batteries” *Journal of Physical Chemistry C*, 2019
- ◇ Maryam Molashahi, Hamid Modarress*, Bahram Nasernejad, Sepideh Amjad-Iranagh, **Behnam Ghalami Choobar**, ‘Structural and Transport Properties of Novel High-Transference Number Electrolytes Based on Perfluoropolyether-block-Poly(ethylene oxide) for Application in Lithium-Ion Batteries: A Molecular Dynamics Simulation Study, *Macromolecules*, 2022
- ◇ Haniyeh Akbari-Kiasaraei, **Behnam Ghalami Choobar***, and Neda Gilani*, “ Ion Correlation Governs Transport in LiTFSI Electrolytes: Role of Moderate Solvation ” *Physical Chemistry Chemical Physics*(Under review)

RESEARCH EXPERIENCE

- 2021-2023 **Hasselt University, Belgium** — Postdoctoral Researcher
- ◇ Developed multiscale electrochemical models connecting molecular-level electrolyte transport to macroscopic battery performance.
 - ◇ Conducted DFT investigations to decode lithium metal deposition/stripping asymmetry, addressing critical stability challenges in next-generation batteries.
 - ◇ Engineered advanced degradation models to accurately capture battery aging mechanisms, significantly improving SOH prediction algorithms.
- 2015-2021 **Amirkabir University of Technology (AUT)** — PhD Researcher (2015–2021)
- ◇ Conducted MD simulations of electrolyte systems and transport properties
 - ◇ Developed MATLAB codes for ionic conductivity and diffusion analysis
 - ◇ Successfully coupled DFT, MD, and P2D models to create a comprehensive, multiscale framework for holistic battery simulation
- 2012-2014 **Sharif University of Technology** — Graduate Researcher (2012–2014)
- ◇ Designed and implemented adaptive nonlinear controllers to maintain the performance of complex dynamic systems.
 - ◇ Formulated advanced fuzzy logic and optimization-based control strategies

MENTORSHIP EXPERIENCE

- ◇ Supervised and mentored several MSc and BSc students within the Chemical Engineering Departments at both institutions.
- ◇ Guided graduate-level research projects focused on the multi-scale simulation and performance optimization of LIBs

CURRENT RESEARCH DIRECTION

Developing **physics-informed frameworks** that connect electrolyte molecular behavior with battery degradation and SOC/SOH estimation. Current focus includes:

- ◇ Formulating fractional-order models to accurately capture non-ideal behaviors in complex electrochemical systems.
- ◇ Integrating physics-based modeling with AI/ML techniques for robust, data-driven battery diagnostics and prognostics.
- ◇ Establishing direct analytical correlations between electrolyte solvation structures and long-term battery aging trajectories.

EDUCATION

PhD, Chemical Engineering — Amirkabir University of Technology (2015–2021)

GPA: 18.63/20

Dissertation: Multiscale simulation of lithium-ion battery electrolytes

MSc, Chemical Engineering (Modeling & Control) — Sharif University (2012–2014)

GPA: 17.4/20

BSc, Chemical Engineering — Sharif University (2008–2012)

GPA: 17.0/20

TEACHING EXPERIENCE

2023–Present **University of Guilan** — Lecturer

- ◇ Process Control
- ◇ Advanced Fluid Mechanics
- ◇ Engineering Mathematics
- ◇ MATLAB Programming

2016–2019 **University of Tehran** — Visiting Lecturer

- ◇ Process Control
 - ◇ Thermodynamics
 - ◇ Advanced Thermodynamics
-

SKILLS

Modeling & Simulation:

MATLAB, Python, COMSOL, Aspen Plus, HYSYS

Molecular Simulation:

GROMACS, Materials Studio, Gaussian

Methods:

Electrochemical modeling, DFT, MD simulation, control systems, machine learning

HONORS, AWARDS & SCHOLARSHIPS

HONORS & AWARDS

- ◇ Ranked 1st in PhD comprehensive exam (AUT)
- ◇ National Elite Foundation member
- ◇ Ranked 1st in national MSc entrance exam (Iran)
- ◇ Top ranks in national Olympiad and competitions

SCHOLARSHIPS & GRANTS

- ◇ MSc Research Grant, Sharif University of Technology (1 Year)
 - ◇ Parseh Institute Scholarship (5 Years)
-

PROFESSIONAL EXPERIENCE

2016–2017 **SEPDco** — Process Design Engineer
Dynamic simulation and control of DME production plant

2021-2025 **NIPC — Part-time Process Design Engineer**
Optimization of separation unit of Methanol-to-Propylene process and refrigeration cycles using heat integration and exergy analysis



INTERNATIONAL COLLABORATION

Postdoctoral research at Hasselt University (Belgium)

Co-authorship with international research groups in battery science
