

PEI SUN

PhD. student in Applied Mathematics, Computational Chemistry & Physics

PROFILE

I am a PhD researcher specializing in AI-assisted scientific computing for materials and battery manufacturing. My work combines physics-based simulations, microstructure characterization, and data-driven modeling to study how processing parameters influence performance-critical properties. I have hands-on experience with DEM/FEM simulations, numerical experimentation, and ML-based analysis, and I am particularly interested in using AI to accelerate simulations, extract scientific insight from complex datasets, and address open problems in materials science. I aim to contribute to AI for Science by bridging domain expertise, computational modeling, and advanced AI/ML tools for high-impact research and industrial applications.

SKILLS

- **Programming skills (advanced level):** Python, C and C++, Matlab, Octave
- **Molecular and mesoscopic modeling:** LAMMPS, LIGGGHTS, Materials Studio, Ovito
- **Finite Element Method modeling:** Abaqus, Geodict, MeshLab, Z-set
- **Experimental background:** Physics/Chemistry experiments, membrane technology at pilot scale, instrumentation, Electricity control, optimization
- **Engineering:** chemical (ASPEN), CFD and coupled heat and mass transfer (Comsol Multiphysics), Mechanical design (AutoCAD)
- **Data-driven modeling & AI tools:** PyTorch, GitHub, Linux System, etc.

INTERSHIPS

- **Computational Modeling of Food Processes** 2022.03 – 2022.09
SayFood, University of Paris-Saclay & INRAE (Palaiseau, France)

Supervisor: Dr. Olivier Vitrac

- Developed Smoothed Particle Hydrodynamics (SPH) methods in LAMMPS and Python to simulate mechanical and rheological behavior during oral processing.
- Performed Dissipative Particle Dynamics (DPD) simulations to model hydrophobic mass transfer in the small intestine.
- Contributed to building theoretical and computational methodologies for industrial biological process simulation.

- **Microstructure Modeling of Paper Materials** 2023.03 – 2023.09
Lab PIMM, CNRS/CNAM/ENSAM (Paris, France)

Supervisor: Dr. Justin Dirrenberger

- Conducted numerical modeling of paper microstructure to reproduce real mechanical behavior through virtual mechanical tests.
- Developed a homogenized material model using the finite element method (FEM) and characterized mechanical properties based on Representative Elementary Volume (REV) morphology.
- Performed thermodynamic simulation of a 3D random fiber model to analyze structure-property relationships.

PUBLICATIONS

1. **Sun, P.**, Vigneaux, P. and Franco, A.A. (2026), Discrete Element Method Modeling of an Extrusion Process with Recirculation for Dry Manufacturing of Lithium-Ion Battery Electrodes. Batteries & Supercaps 2500211. <https://doi.org/10.1002/batt.202500211>
Cover Feature of this study: <https://doi.org/10.1002/batt.70274>
2. S.Saravanan, I.Cardenas-Sierra, **P.Sun**, et al. "Assessing Mesoscale Heterogeneities in Hard Carbon Electrodes Through Deep Learning-Assisted FIB-SEM Characterization, Manufacturing and Electrochemical Modeling." Advanced Energy Materials (2026): e06765. <https://doi.org/10.1002/aenm.202506765>
3. Accelerated Parameter Optimization of Granular Models of Battery Manufacturing (Preprint and Under Review). <https://doi.org/10.26434/chemrxiv.15001277/v1>
4. (Review paper) Solvent-Free Extrusion of Polymer-based Solid-State Electrolytes: Formulation, Processing and Modeling (Accepted by Chemical Engineering Journal)
5. Machine Learning Surrogate Modeling of Materials Extrusion for Lithium-Ion Battery Electrode Dry Manufacturing (Preprint and Under Review). <https://doi.org/10.26434/chemrxiv.15005025/v1>
6. Perspective paper on modeling the polymer-based electrolyte (In Preparation)
7. Modeling of 3D printing battery electrode (In Preparation)



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📍 Amiens, France

EDUCATION

2024.02 – 2027.01

CNRS, LRCS, LAMFA

- PhD. of Applied Mathematics

2021.09 – 2023.06

UNIVERSITY OF PARIS-SACLAY

- Master of Process, Energy and Environment

2017.09 – 2021.06

NORTHEASTERN UNIVERSITY

- Bachelor of Environment Engineering

LANGUAGES

- English (Fluent)
- French (Fluent)
- German (Basic)
- Japanese (Basic)
- Chinese (Native speaker)

INTERESTS

- Tennis
- Marathon
- Videography

CONFERENCES

- Swiss Battery Day 2025 (Oral presentation)
- MRS Fall 2025 (Oral presentation)
- MRS Fall 2025 Symposium Assistant

EVENTS

- Abilympics, Metz 2023
- Olympic Paris 2024
- Paralympic 2024
- UNESCO For Women in Science, Paris 2025