Data-Efficient Machine-Learned Potentials for Solid-State Ion Conductors

From Doctoral Research to an Autonomous Discovery Platform

Dr. Elena Marsh
Ph.D. Candidate, Department of Materials Science, Vertex University

Postdoctoral Fellowship Interview
Nimbus Computational Energy Materials Lab ▪ Apex University

August 4, 2026

Talk Overview

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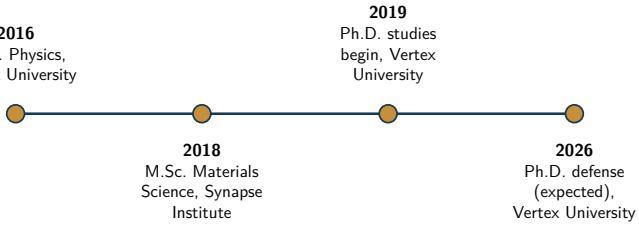
About Me

Background & Training

Physics to computational materials science, with an experimental thread



- Thesis: *"Data-Efficient Machine-Learned Potentials for Accelerated Discovery of Solid-State Li-Ion Conductors"* (advisor: Prof. Aaron Whitfield)
- Visiting researcher, Synapse Battery Materials Consortium (2022–2024): joint computation–synthesis validation studies
- Maintainer of **IonForge**, an open-source machine-learned potential framework (MIT license, 4 external adopting groups)

Doctoral Research

The Problem

Ab initio accuracy is too slow for the size of the search space

Solid-state electrolytes are the bottleneck for safe, high-energy-density batteries, but:

- Ab initio molecular dynamics (AIMD) is accurate but far too slow to screen ionic conductivity across candidate chemistries
- Classical force fields are fast but too inaccurate for the disordered, defect-rich structures that make good conductors
- Existing machine-learned potentials need thousands of labeled structures per chemistry – a cost few labs can absorb

Research Question

Can we build a machine-learned potential that reaches AIMD-level accuracy on ionic transport while needing an order of magnitude less training data?

Key Contributions

Three results from the doctoral thesis

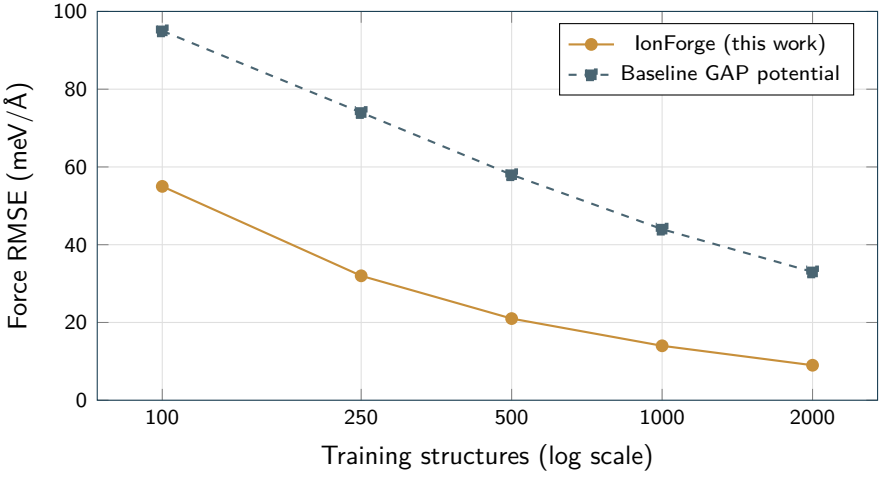
Contribution	Venue / Validation	Impact
IonForge machine-learned potential framework	*Journal of Computational Materials Science*, 2024	40× speedup vs. AIMD; <2 meV/atom force error
Active-learning sampling protocol	*Computational Energy Materials*, 2025	Cut required training structures by 65%
Discovery of 12 candidate garnet-type conductors	Synapse Battery Materials Consortium, Annual Meeting 2025	3 candidates validated experimentally by partner labs

Headline result

IonForge matches AIMD force accuracy on Li-ion conductors while training on 65% fewer structures than the strongest published baseline.

Prediction Accuracy vs. Training-Set Size

IonForge reaches lower error with far fewer labeled structures



Fit with the Host Lab

Why the Nimbus Lab, Apex University

Direct overlap between my toolset and the lab's roadmap

Nimbus Lab focus area	Candidate's aligned expertise
High-throughput DFT screening pipelines	Built and maintain a 500-node autonomous DFT workflow underlying IonForge
Machine-learned force fields for ionic transport	Three years developing equivariant MLIPs; thesis focus
Experimental validation partnerships	Led a joint validation study with the Synapse Battery Materials Consortium
Open-source tooling for the community	IonForge released under the MIT license; adopted by 4 external groups

Why now

The Nimbus Lab's new **AutoSynth** robotic synthesis platform and IonForge's screening speed are complementary halves of a closed discovery loop that neither group can build alone.

Proposed Postdoctoral Project

Aims

An autonomous discovery loop for halide solid electrolytes

Aim 1

Extend IonForge to halide chemistries (Cl, Br, I frameworks) beyond the oxide and sulfide systems covered in my thesis.

Aim 2

Couple IonForge screening with the Nimbus AutoSynth robotic platform for closed-loop candidate validation.

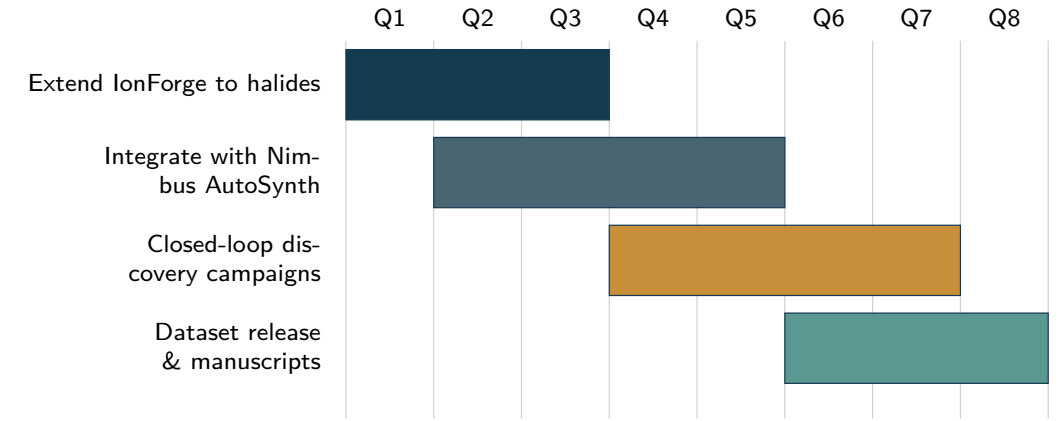
Aim 3

Release an open benchmark dataset for halide solid electrolytes for the wider community.

- Target output: 5–8 experimentally validated halide conductor candidates within the fellowship period
- Deliverable: IonForge-Halide, released alongside the benchmark dataset

24-Month Timeline

Proposed schedule for the fellowship period



Bars indicate active phases; overlaps reflect iterative, not sequential, execution.

Broader Impact

Funding, Dissemination & Community Value

Positioning the project beyond a single lab

Funding fit

- Directly addresses the Meridian Foundation Energy Grand Challenge priority area on solid-state battery materials
- Builds a competitive case for a joint Nimbus Lab / Vertex University follow-on proposal

Dissemination

- Open dataset and code release under a permissive license
- Workshop contribution at the Synapse Solid-State Energy Symposium
- Shared benchmark suite to accelerate reproducible comparisons across labs

Why this matters for the field

Halide solid electrolytes are under-explored relative to oxides and sulfides largely because no fast, transferable screening tool exists. Closing that gap benefits every group working on solid-state batteries, not just ours.

Closing

Selected Publications

1. E. Marsh, A. Whitfield. "IonForge: A Data-Efficient Framework for Machine-Learned Interatomic Potentials in Solid Electrolytes." *Journal of Computational Materials Science*, 2024.
2. E. Marsh, R. Okafor, A. Whitfield. "Active-Learning Sampling for Rapid Force-Field Convergence in Disordered Ionic Conductors." *Computational Energy Materials*, 2025.
3. E. Marsh et al. "Twelve Candidate Garnet-Type Solid Electrolytes from High-Throughput Screening." *Proceedings of the Synapse Battery Materials Consortium Annual Meeting*, 2025.
4. A. Whitfield, E. Marsh. "Benchmarking Machine-Learned Potentials Against AIMD for Superionic Conductors." *Journal of Computational Materials Science*, 2023.

Thank You

I would welcome the chance to bring IonForge into the Nimbus Lab's discovery pipeline.

elena.marsh@vertex.edu

+1 (555) 019-2247

github.com/emarsh/ionforge

Department of Materials Science, Vertex University