Transferable Impedance-Grounded Learning for Interfacial Degradation Across Energy Systems

Hithesh Rai Purushothama [1] **Nicholas Rolston** [1]

[1] *Renewable Energy Materials and Devices Lab, School of Electrical, Computer and Energy Engineering (ECEE), Arizona State University, Tempe, AZ, USA*. Correspondence to: Nicholas Rolston Nicholas.Rolston@asu.edu.

1. Introduction

Interfacial degradation governs performance and durability across energy technologies including perovskite photovoltaics (PSCs) and lithium-ion batteries. Despite functional differences, both systems exhibit shared electro-chemo-mechanical degradation mechanisms including ion migration, interfacial charge accumulation, chemical reactivity, defect generation, and mechanical delamination. In PSCs, interfacial processes alter band alignment and accelerate nonradiative recombination losses. In batteries, solid-electrolyte interphase (SEI) evolution and charge-transfer kinetics govern impedance growth and capacity fade. Both represent metastable, nonequilibrium regions where ionic and electronic transport are strongly coupled.

However, modeling and characterization remain largely siloed across device classes. Photovoltaic research often interprets impedance through recombination resistance and chemical capacitance, while battery research focuses on charge-transfer resistance and SEI impedance. Equivalent circuit models are frequently device-specific and heuristic, limiting systematic knowledge transfer between fields.

Electrochemical impedance spectroscopy (EIS) provides a unifying opportunity. Impedance spectra encode frequency-domain responses of coupled ionic-electronic systems governed by drift-diffusion transport and interfacial electrochemical kinetics. While device architectures differ, the mathematical structure of impedance response is closely related. We hypothesize that impedance spectra form a transferable descriptor space for interfacial degradation, enabling physics-grounded machine learning models to generalize across PSCs and lithium-ion batteries.

2. Approach

We develop an impedance-centered learning framework that integrates automated experimentation with multitask transfer learning.

Automated Experimental Platform. For PSCs, potentiostatic impedance measurements are conducted using a PAIOS system under controlled bias, illumination, temperature, and stress conditions. For lithium-ion battery systems, both potentiostatic (PEIS) and galvanostatic (GEIS) impedance measurements are acquired using a BioLogic potentiostat under electrochemical cycling, state-of-charge variation, and temperature control. Both platforms measure impedance over wide frequency ranges under systematically varied stress regimes including elevated temperature and accelerated aging.

Physics-Grounded Feature Representation. Raw impedance spectra are transformed using two complementary strategies. First, constrained equivalent-circuit modeling is performed using predefined circuit topologies (e.g., R_s–($R_{ct}||C_{dl}$)) with parameter bounds enforcing physical admissibility such as positive resistances and capacitances, along with Kramers–Kronig consistency checks to ensure causality and passivity. This yields interpretable descriptors including charge-transfer resistance, recombination resistance, interfacial capacitance, and diffusion-related parameters. Second, the full impedance spectrum is converted into a machine-learning representation by sampling magnitude and phase across logarithmically spaced frequency points to construct frequency-domain embeddings. This approach preserves distributed relaxation behavior that may not be fully captured by simplified circuit models. The hybrid representation balances interpretability with expressive capacity.

Multitask Transfer Learning. A shared encoder architecture first maps impedance-derived features into a common latent representation capturing cross-domain interfacial dynamics. Domain-specific output heads then predict degradation metrics independently for PSC and lithium-ion battery systems. By training jointly across domains, the encoder is encouraged to learn representations that generalize beyond device-specific heuristics. Transfer gain is quantified by comparing predictive performance under single-domain and shared multitask training conditions, particularly under unseen stress regimes and limited-data settings.

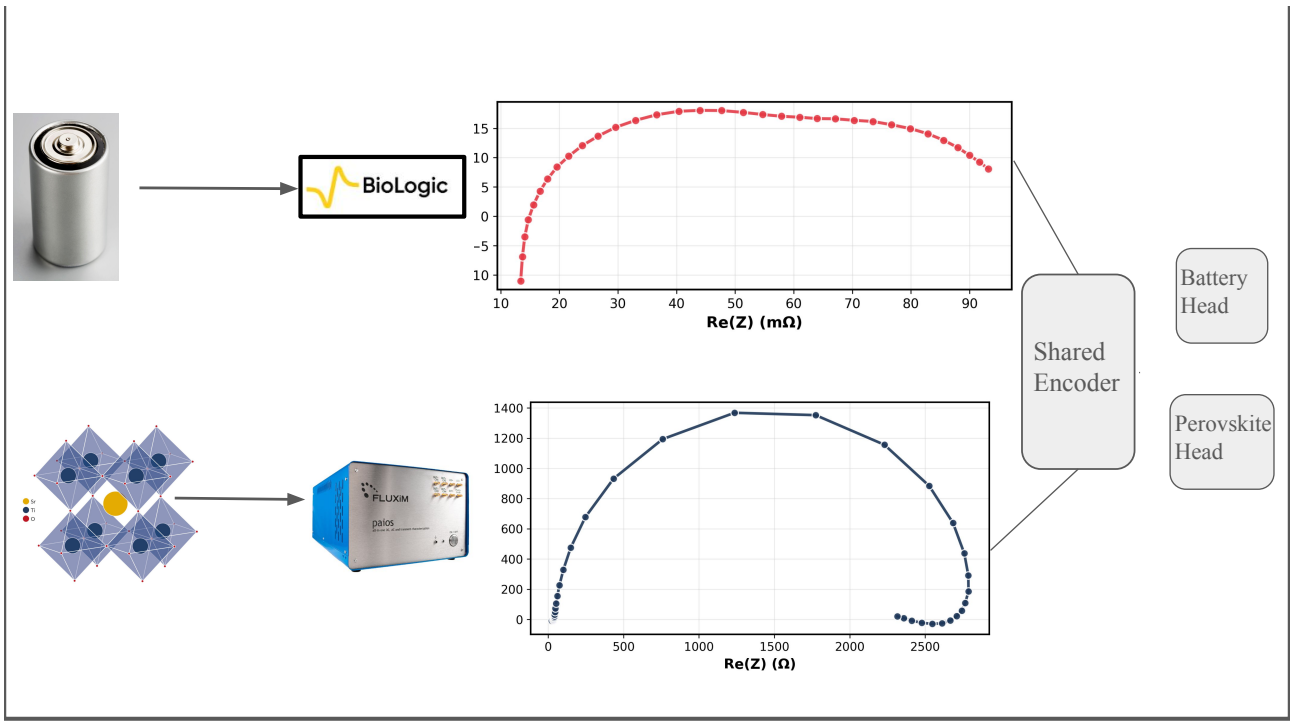

Fig. 1: Impedance-grounded transfer learning framework for cross-domain degradation modeling. (Top) Lithium-ion battery EIS measured via BioLogic potentiostat in milliohm range showing charge-transfer and SEI dynamics. (Bottom) Perovskite solar cell EIS measured via PAIOS system in ohm-kilohm range showing recombination and ionic polarization. Despite four orders of magnitude difference in impedance scale, both exhibit semicircular Nyquist responses. A shared encoder learns common latent representations from physics-constrained features (equivalent circuit parameters and spectral embeddings), while domain-specific heads predict degradation metrics for each system.

3. Expected Impact

This work evaluates whether impedance-derived representations support cross-domain predictive generalization when learned through a shared multitask encoder.

Scientific Impact. The study tests the hypothesis that coupled ionic-electronic interfaces exhibit transferable degradation signatures across optoelectronic and electrochemical systems.

Technological Impact. Integration of automated impedance acquisition with machine learning aims to streamline degradation diagnostics and reduce reliance on manual equivalent-circuit fitting.

Methodological Impact. This work establishes a unified pipeline integrating automated impedance acquisition, physics-constrained feature extraction, and shared multitask predictive modeling. By evaluating transfer gain between PSC and lithium-ion battery domains, we assess whether impedance-derived representations enable cross-domain predictive generalization.

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