2020 OE Peer Review Session Summary

Redox Flow Battery Status and Challenge

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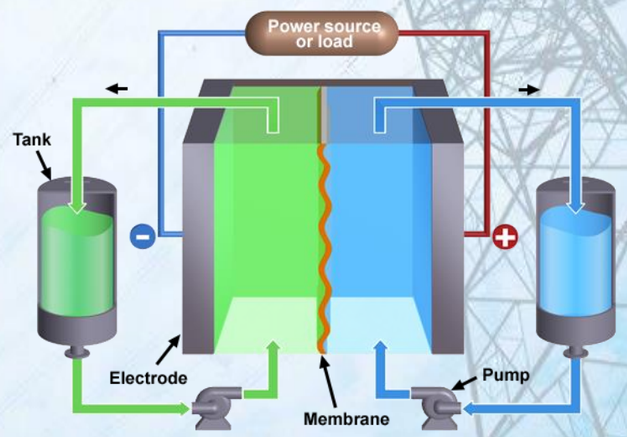
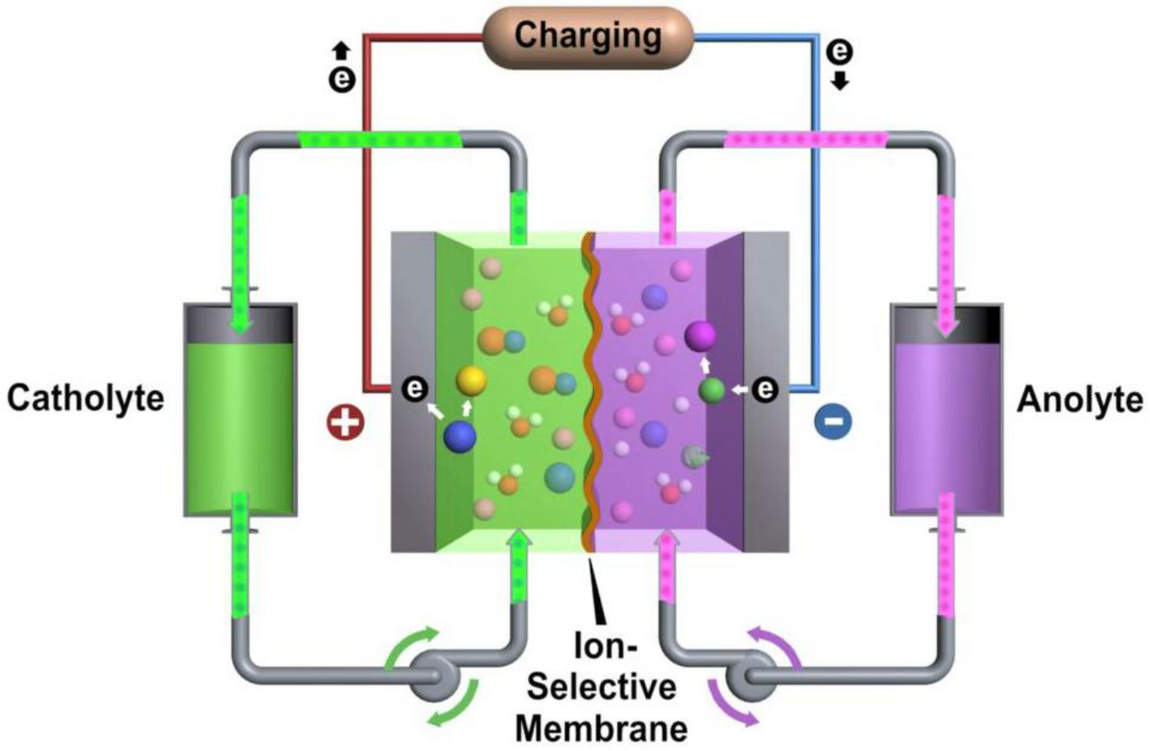
Richland, WA 99354, USA



PNNL is operated by Battelle for the U.S. Department of Energy

Redox Flow Batteries



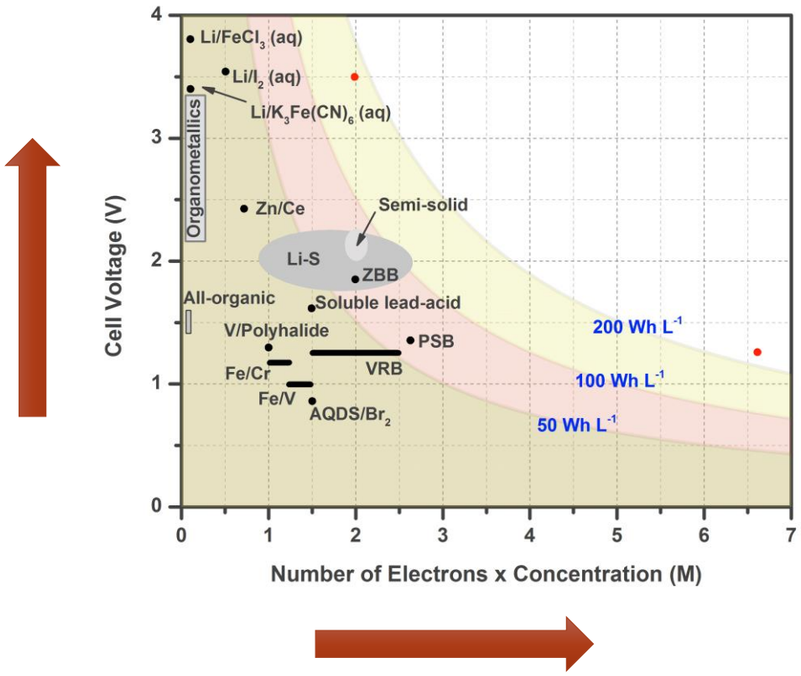
Key Aspects

- ***Power and Energy are separate enabling greater flexibility and safety.***
- ***High safety***
- Suitable for wide range of applications 10's MW to ~ 5 kw
- Wide range of chemistries available.
- Low energy density ~ 30 Whr/kg

Major Challenge of the current RFB technology

Low energy density:

$$E = \frac{NC_aFV}{n}$$



Other key performance parameters

- Capacity decay
- Efficiencies
- Operation temperature window

Adv. Mater. 2014, DOI: 10.1002/adma.201403746

Focused R&D in OE energy storage program towards advanced RFB systems

Nonaqueous systems:

Higher Voltage Iron Bipyridines for Non-Aqueous Redox Flow Battery	Travis Anderson	SNL
Ambient Temperature Non-Aqueous Sulfide Based Redox Flow Batteries and Membrane Development	Jagjit Nanda	ORNL

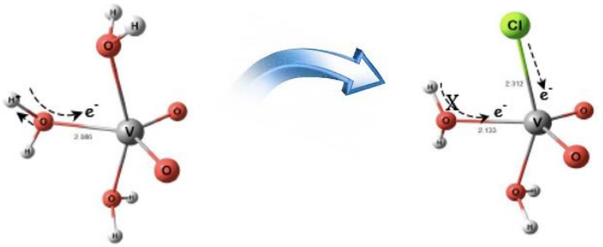
Aqueous systems:

Phenazine-Based Anolyte Materials in Aqueous Redox Flow Batteries	Aaron Hollas	PNNL
Advanced Membranes for Flow Batteries	Cy Fujimoto	SNL
Towards Building Optimal Electrolytes for Pb-Acid Battery Through Tunable Solvation Chemistry	Vijayakumar Murugesan	PNNL
Flow Battery Capacity Fade and Power Density With Redox-Active Aqueous-Soluble Organics	Michael Aziz	Harvard
Probing Components and Durability in Redox Flow Batteries	Tom Zawodzinski	ORNL

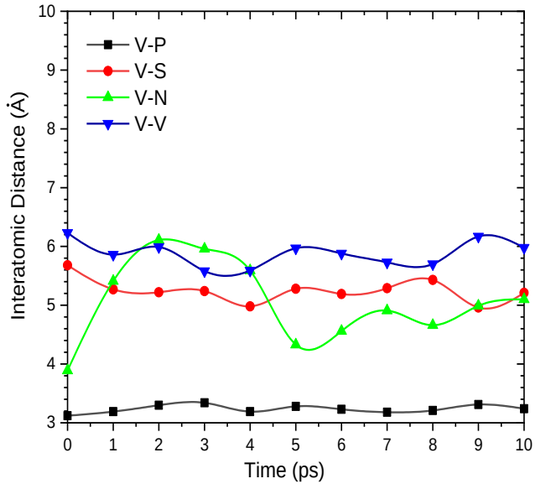
Current status of the RFB technology

Electrolyte development

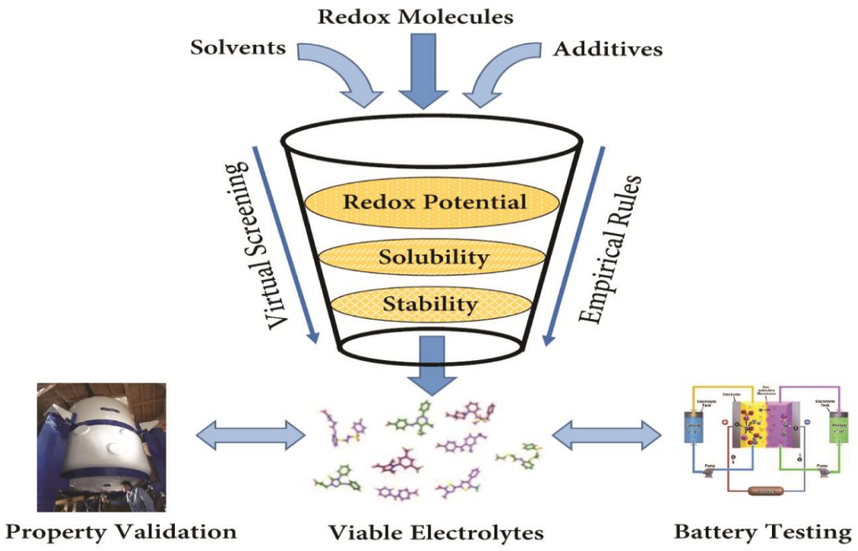
Mixed-acid vanadium electrolyte



Bi-additive vanadium electrolyte



Electrolyte Design Module

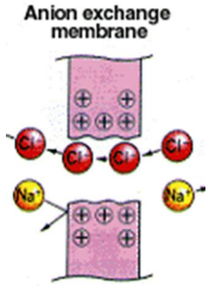


Phenazine-Based Anolyte Materials in Aqueous Redox Flow Batteries	Aaron Hollas	PNNL
Towards Building Optimal Electrolytes for Pb-Acid Battery Through Tunable Solvation Chemistry	Vijayakumar Murugesan	PNNL

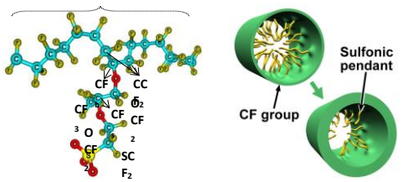
Current status of the RFB technology

Component and system

Advanced membrane development

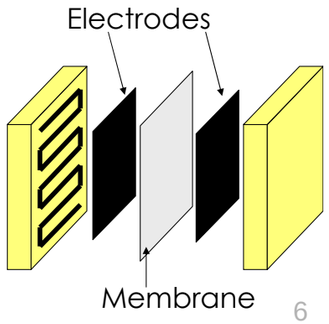


Cy Fujimoto, SNL

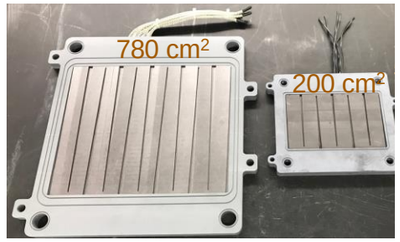


PNNL, UET, Chemours, and LLNL

System development

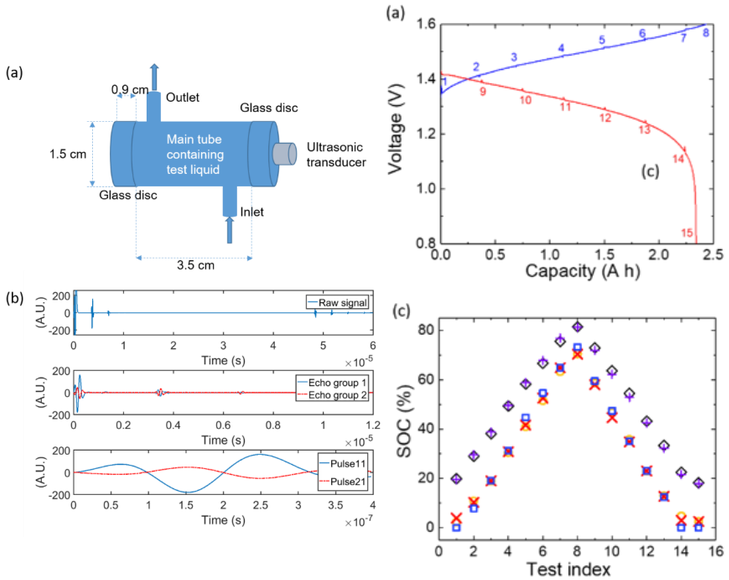


Tom Zawodzinski, ORNL

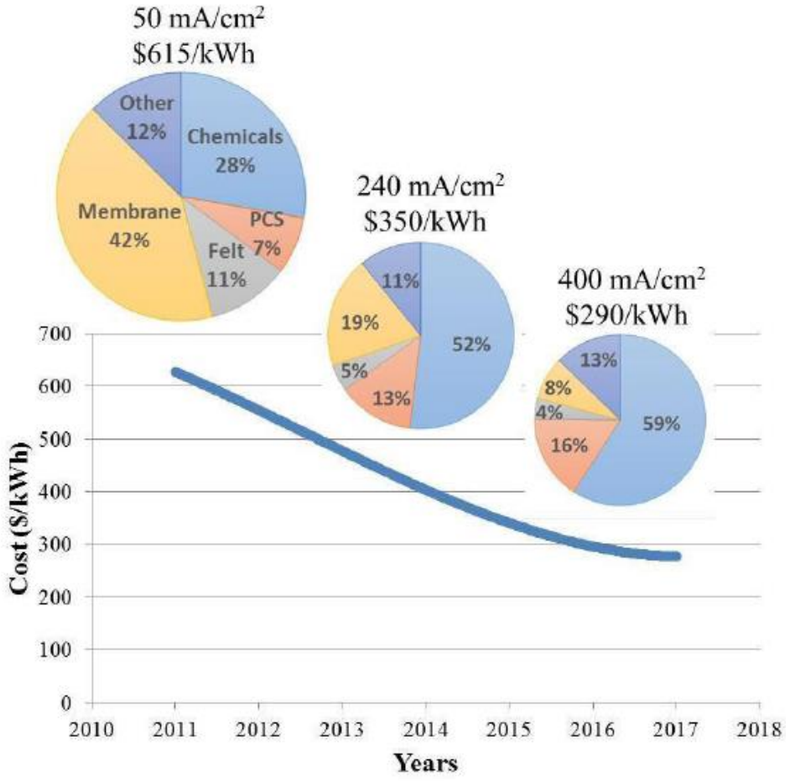


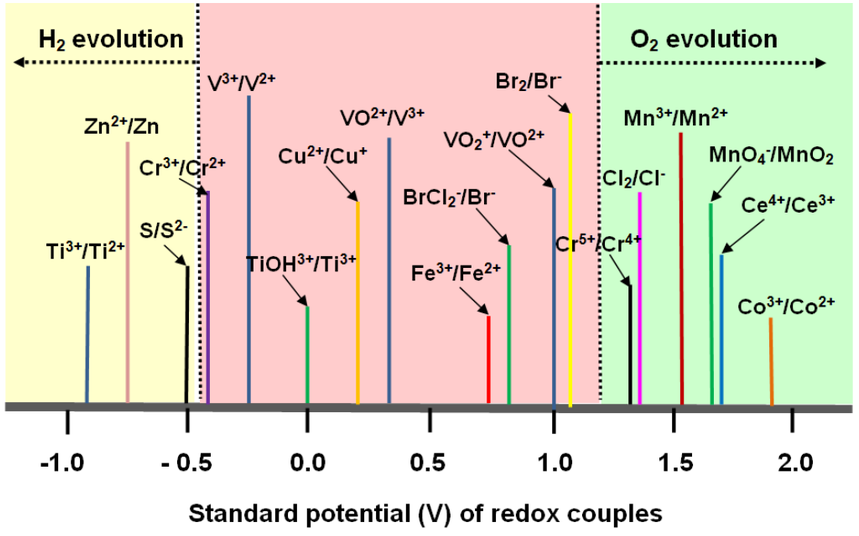
PNNL

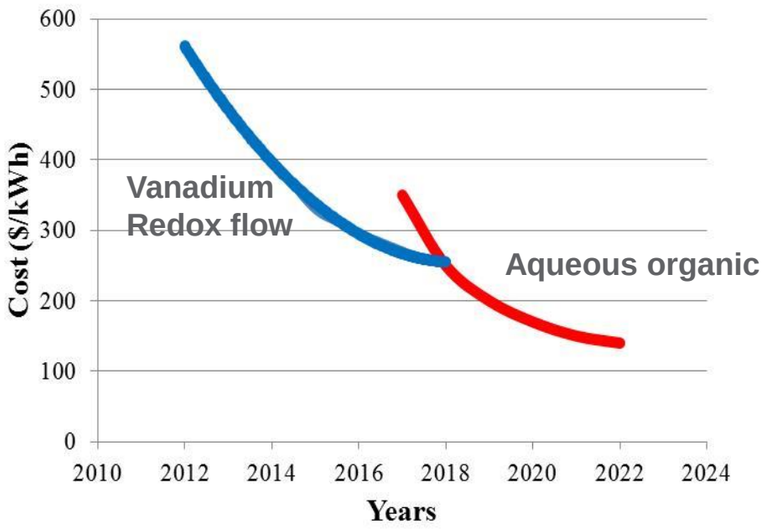
Characterization
Acoustic SOC monitoring



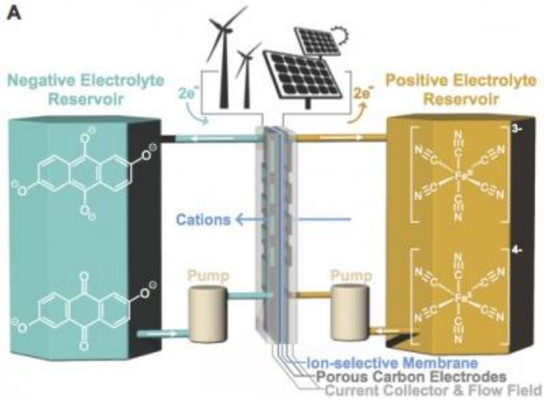
Transition to aqueous organic RFBs



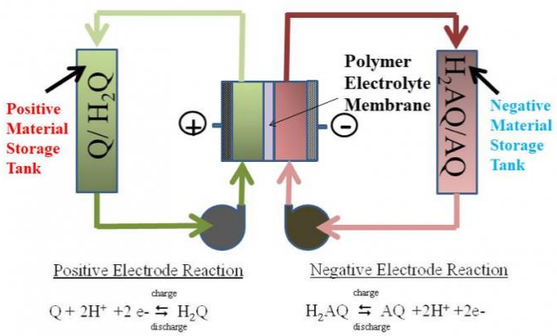




Advanced aqueous organic RFBs



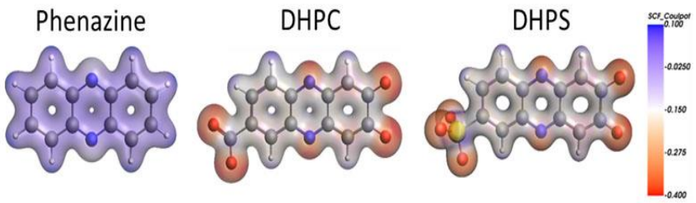
Michael Aziz, Harvard



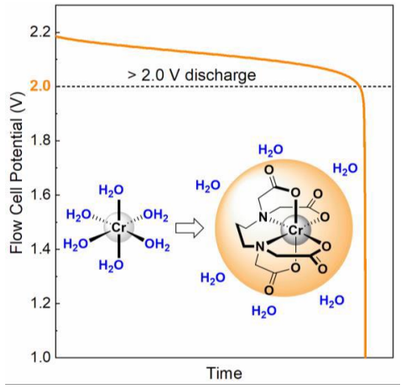
Sri Narayan, USC

Key technical challenges

- Lack of mature chemistry
- Stability

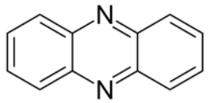


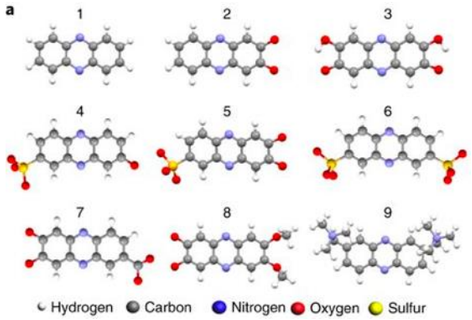
PNNL

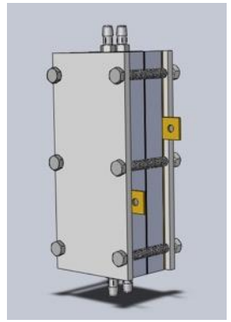


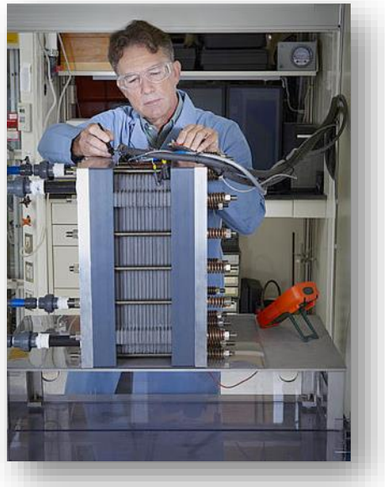
Michael Marshak, UC

Current fragmented research through trial-and-error approach slows the innovation









Prototyping in 1kW stack

A Hollas, X Wei, V Murugesan, Z Nie, B Li, D Reed, J Liu, V Sprenkle, W Wang
Nature Energy **3**, 508–514, 2018

Current fragmented research through trial-and-error approach slows the innovation

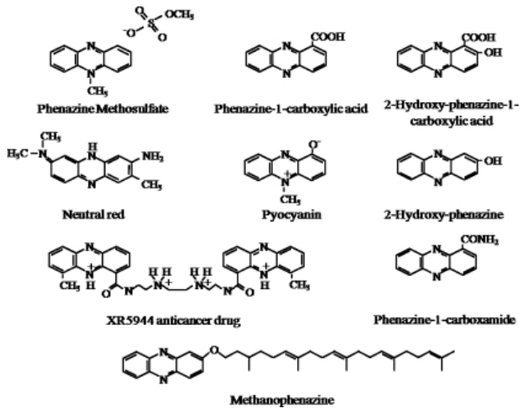
2 years to screen the 8 molecules and develop the best one to prototype

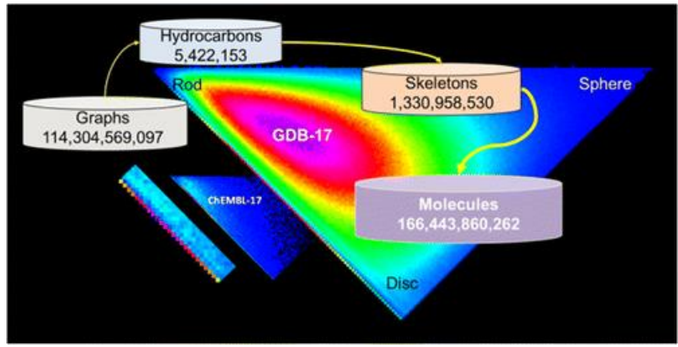
You are 10 times better: 80 molecules

You have 10 times more resource: 800 molecules

10 such groups: 8000 molecules

Known Phenazine derivatives: >6000





The largest small molecule data-base GDB-17 contains 166.4 billion molecules.

A Hollas, X Wei, V Murugesan, Z Nie, B Li, D Reed, J Liu, V Sprenkle, W Wang
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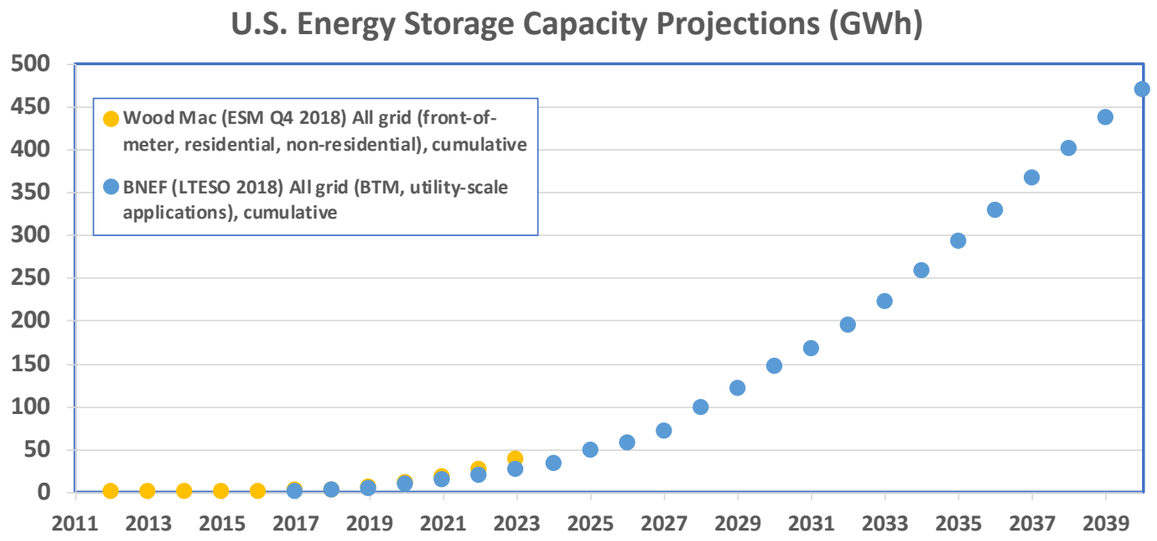
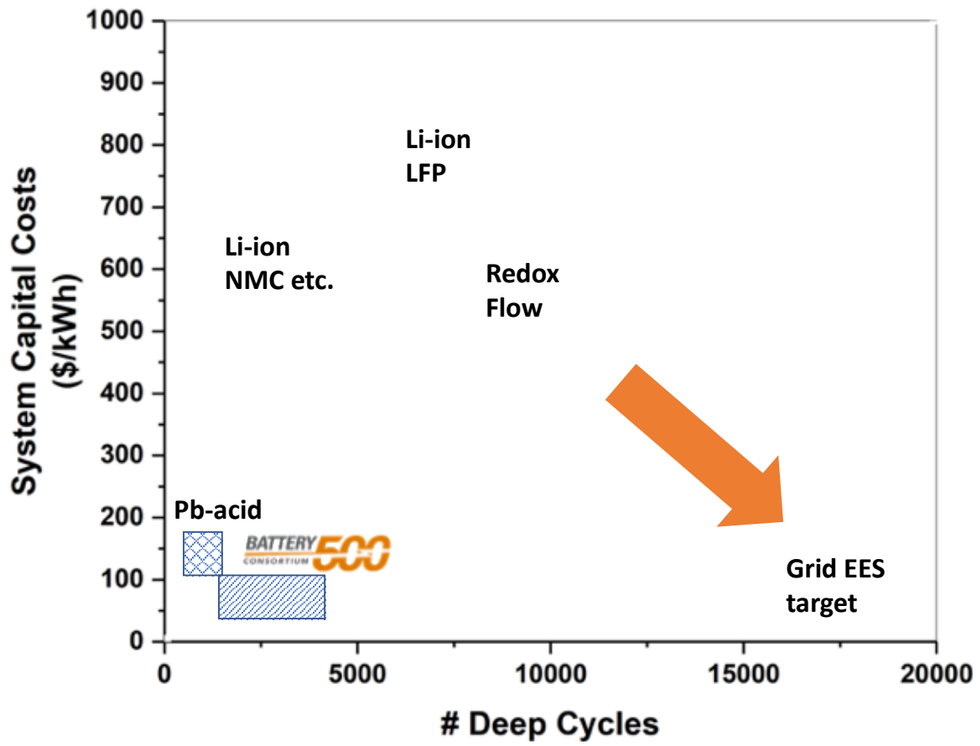
Market and Technology Challenges



The energy density of lithium-ion battery was improved < 2% per year over the last 40 years.



- Close to 500GWh by 2040, equivalent to the capacity of 75 Hoover dams.

Assuming 100wh/kg at system level, 5 million metric tons of batteries are needed

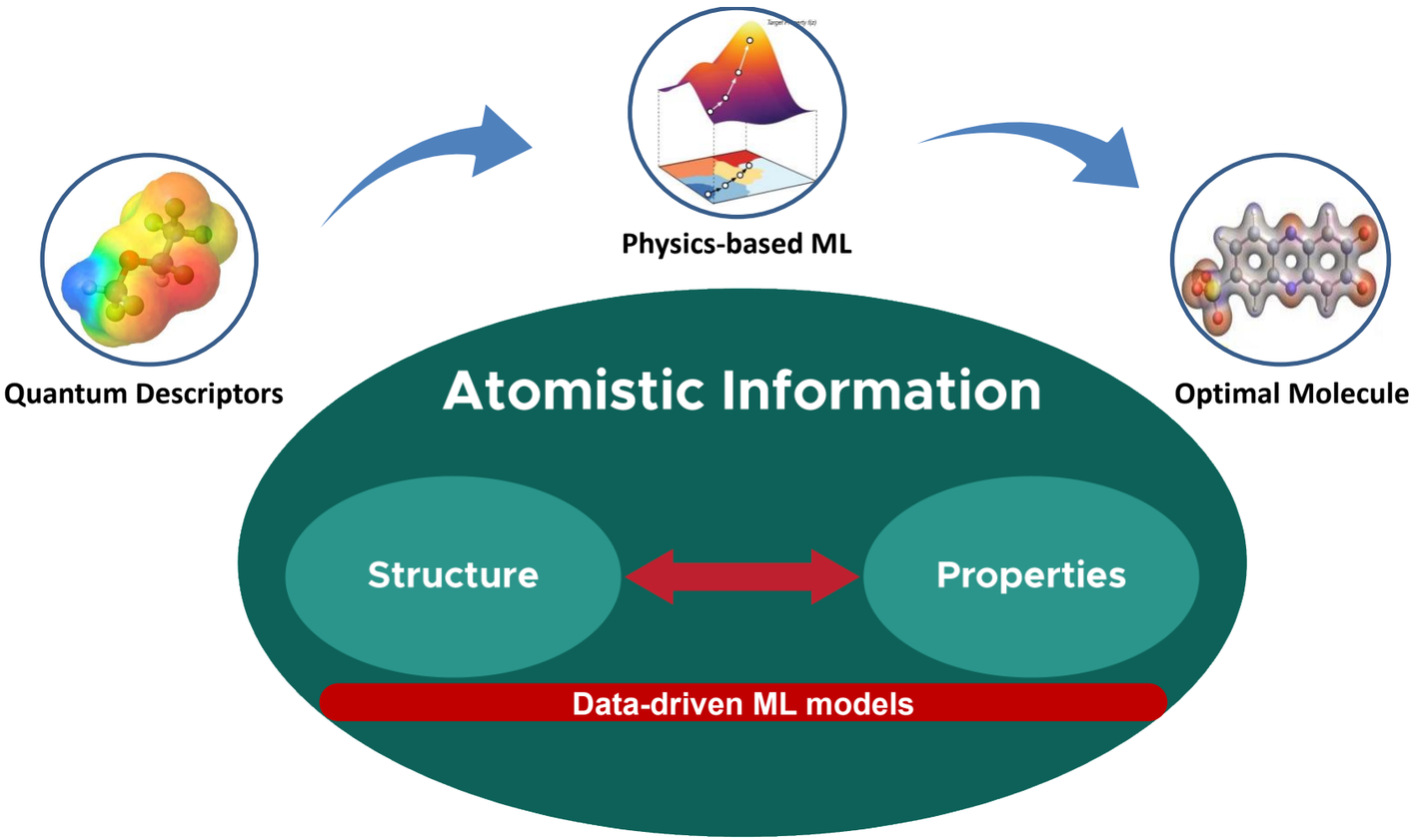
- No current technologies can satisfy such rapid growing demand!

Can we predict material property before synthesis?

Atomistic information

Predictive material design:

By establishing correlation between material structure and material properties.

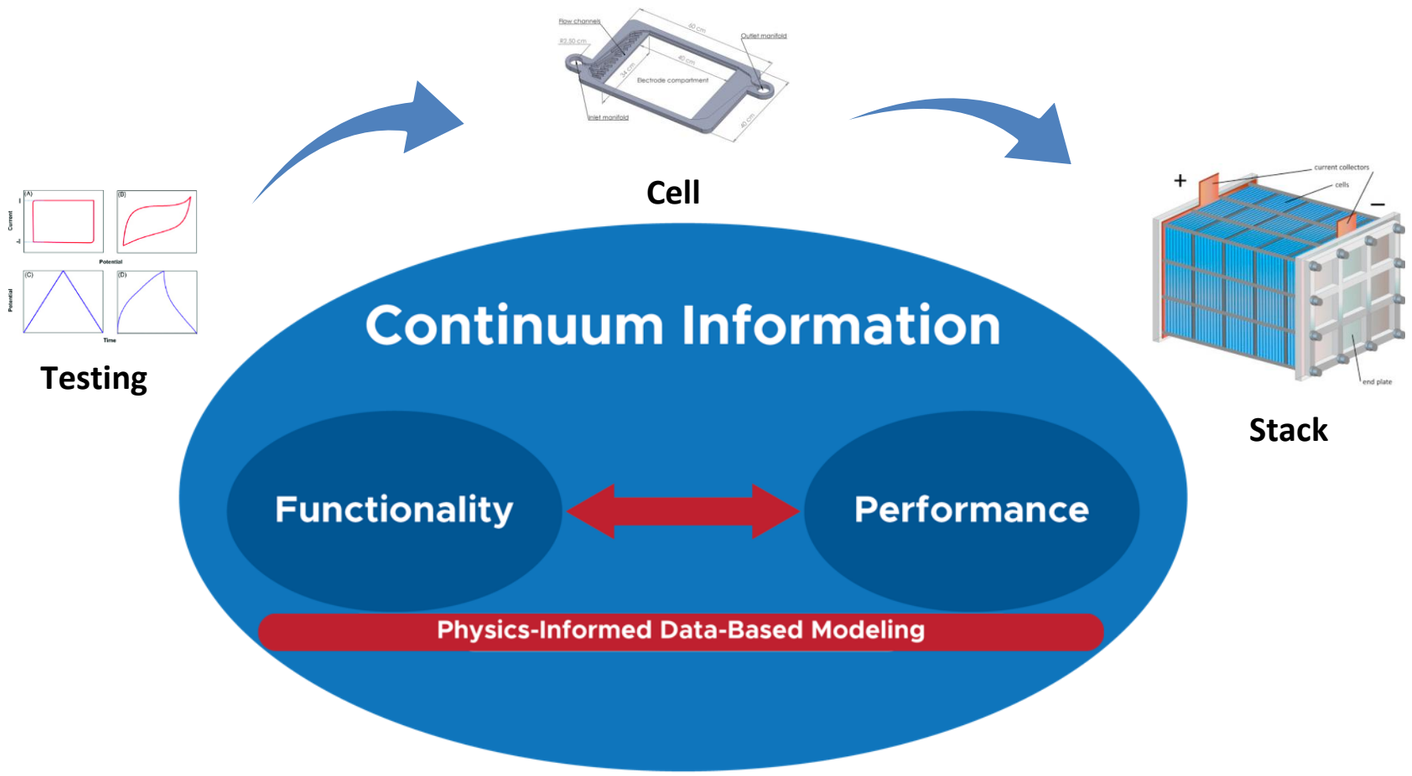


Can we predict device performance before assembly?

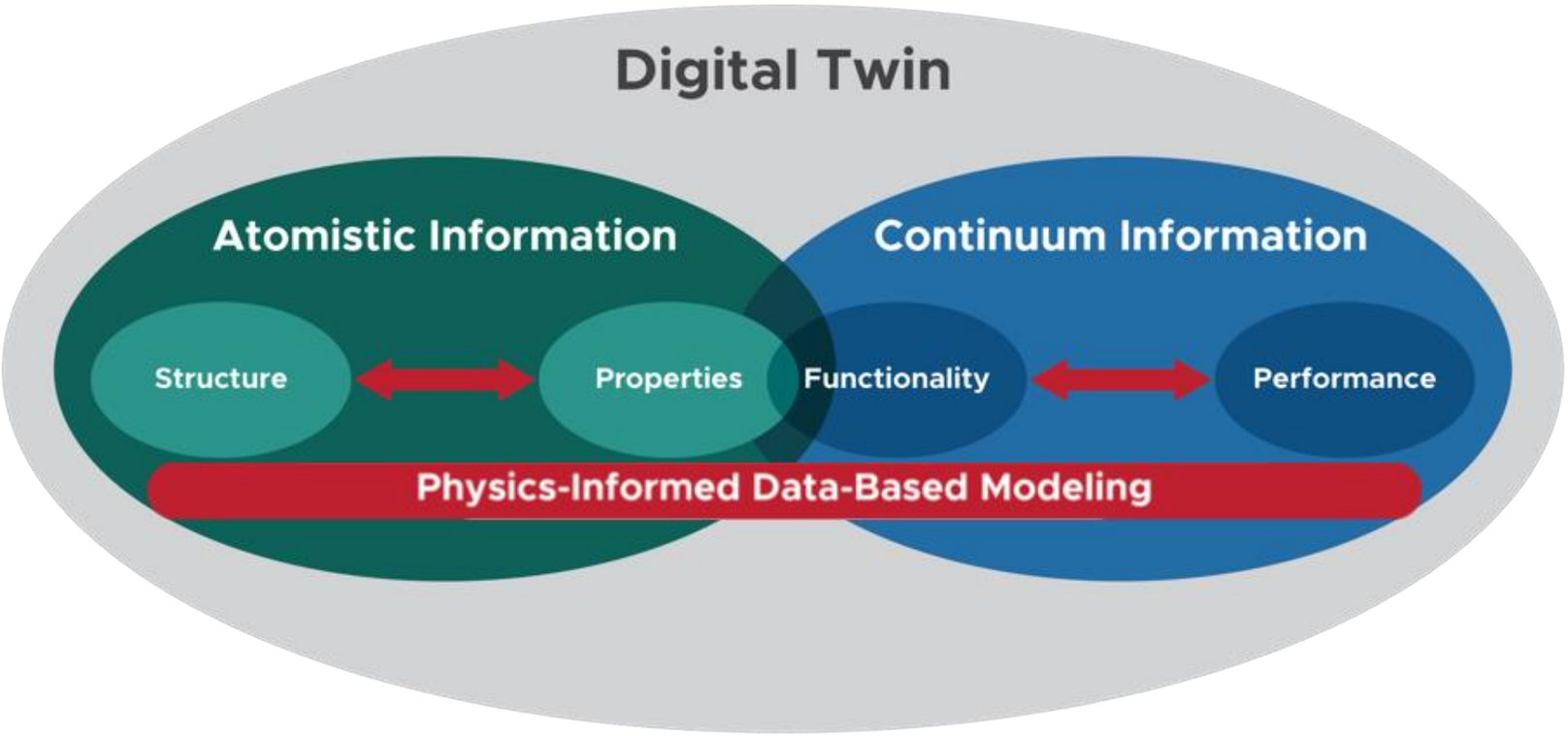
Continuum information

Rapid prototyping validation

By linking material properties and device performance across temporal and spatial scales.



A Paradigm Shift:
From Trial-and-Error to Digital Twin

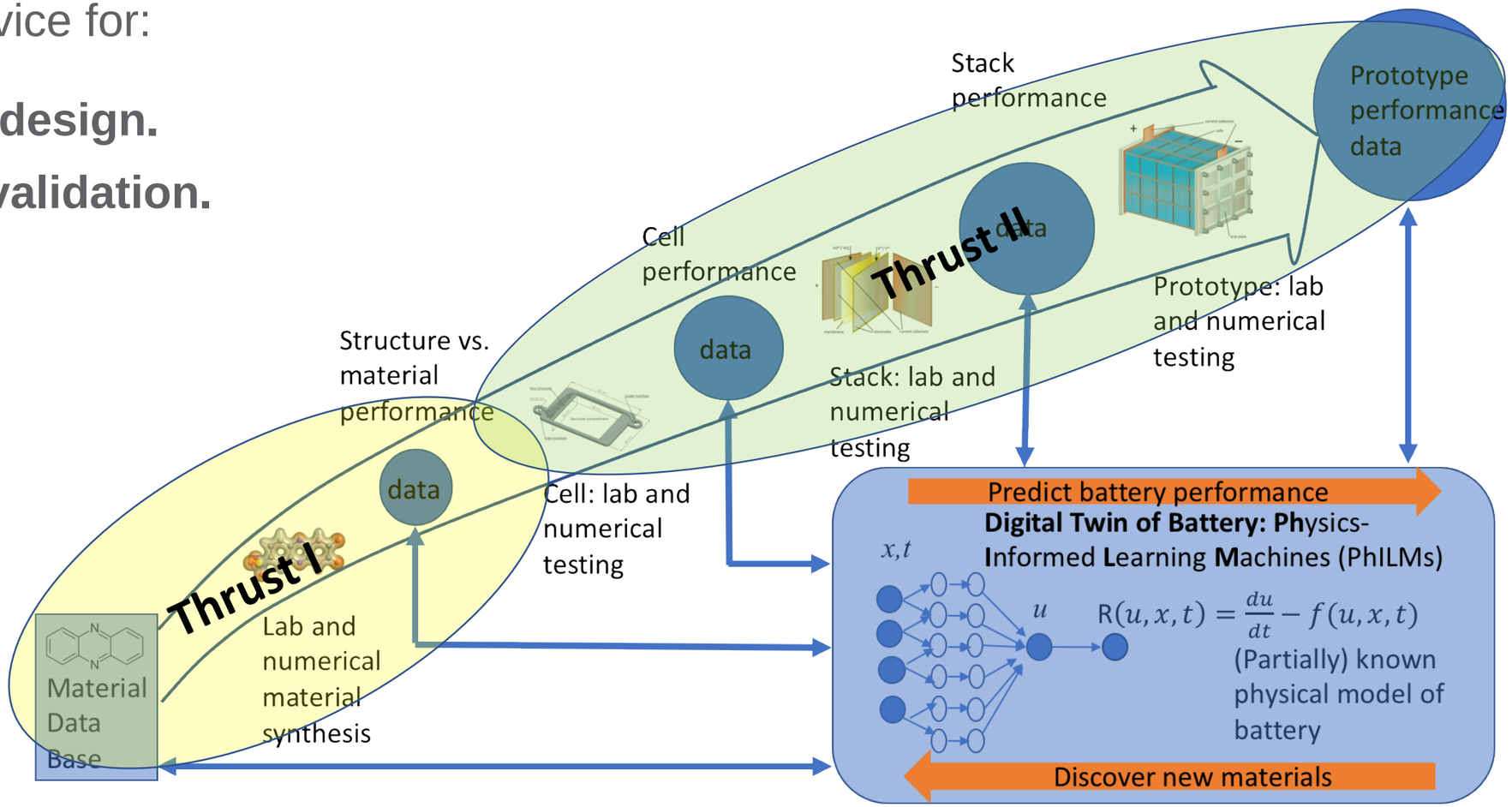


ESMI will pioneer the digital twin approach for an accelerated design of complex systems such as batteries through physics-informed data-based models that integrate experimentation and modeling across traditionally siloed scales to accelerate energy storage development.

Digital Twin of Battery

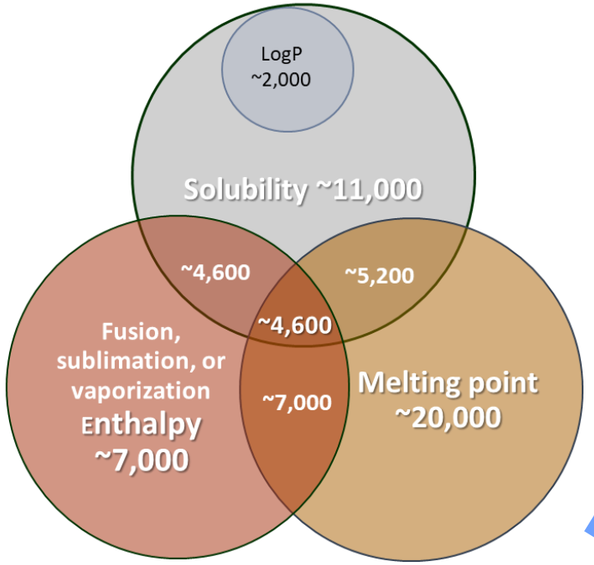
Linking atomistic to device for:

- **Predictive material design.**
- **Rapid prototyping validation.**



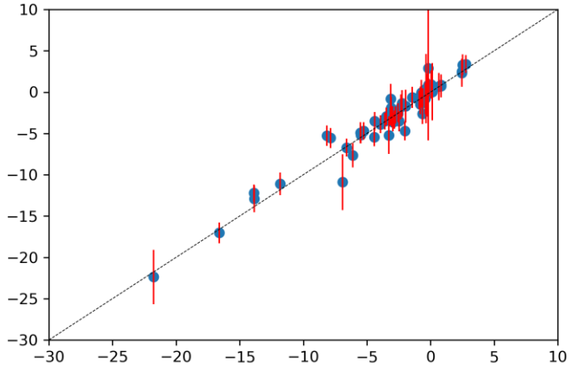
From Trial-and-Error to Predictive design

ESMI Redox Molecules Experimental Databases



High fidelity data from high throughput system

Prediction of solvation free energy

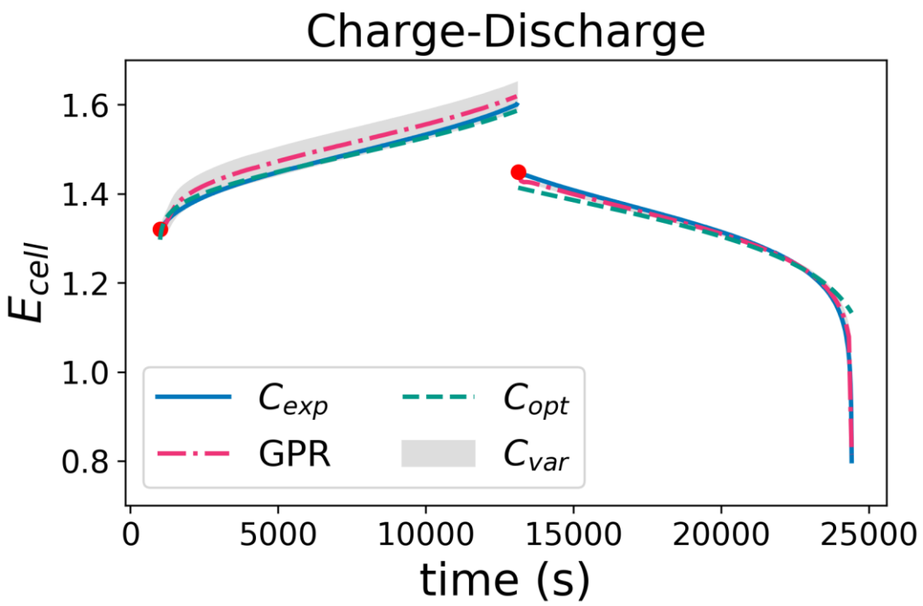


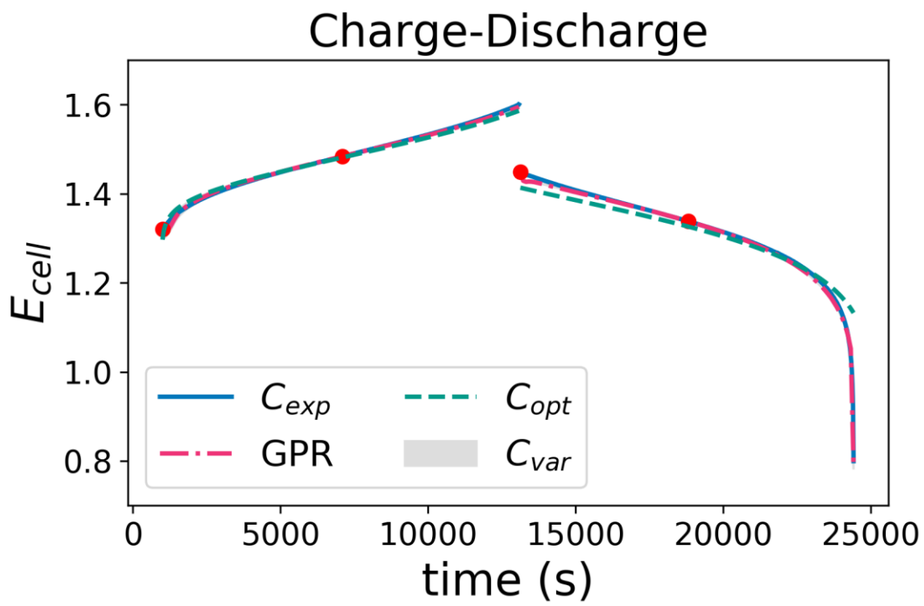
The new GP model achieve similar prediction accuracy using <25% of data

From Trial-and-Error to Performance Prediction

First PINN model of a sophisticated electrochemical device

Multi-fidelity ML model based on physics-informed Gaussian process method





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- Vijay Murugesan, Aaron Hollas, Zimin Nie, Vish Viswanatha, David Reed, Vincent Sprenkle, Ed Thomsen, Zhijie Xu, Jie Bao, Emily Saldanha, Alex Tartakovsky, George Muntean.