JCESR Joint Center for Energy Storage Research

# JCESR Scientific Progress and Technological Impact

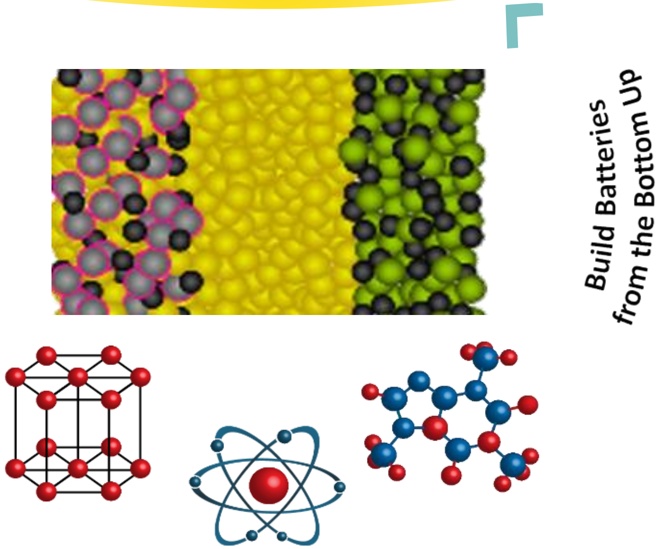
*George Crabtree*

*Director, Joint Center for Energy Storage Research (JCESR)*

*Argonne National Laboratory*

*University of Illinois at Chicago*

***Transformative Materials, Chemistries and Architectures***




Outline

JCESR vision and mission grow with the field

Shrinking costs, growing markets and climate change

Themes: Solvation, Redoxmers and Multivalent Materials

JCESR Alums: Industry, Academia, National Labs

Outreach, Publications, User Facilities

*Basic Energy Sciences Advisory Committee*
*April 5, 2022*

U.S. DEPARTMENT OF ENERGY

# *The Energy Storage Landscape in 2012*

JCESR

Li-ion: one-size-fits-all battery
for personal electronics

*A thriving commercial enterprise since 1991*

Electric Vehicles and Electricity Grid

*Promising opportunities, many commercial barriers*

Electric Vehicles

Three models: Nissan Leaf, Tesla Roadster, Tesla Model S

High cost, low range, no charging infrastructure, tiny market

Electricity Grid

High cost: Battery $825/kWh / Solar $225/MWh

*Natural gas combined cycle: $100/MWh*

Battery storage: short lifetime, no deployment at scale

JCESR Vision

A single low-cost, high-energy density, beyond Li-ion battery
enabling EV and electricity grid markets
5x energy density, 1/5 cost

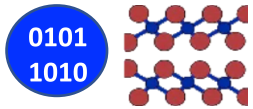
# JCESR Initial Five Years . . .

BLUE CURRENT JCESR

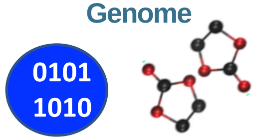
**Vision: an all-purpose battery for EVs and grid**
**Focus exclusively on beyond Li-ion batteries**

**Innovative tools**

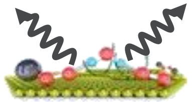
Simulation before Synthesis




Electrolyte Genome

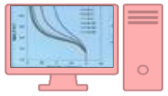



Multi-modal Characterization



*X-ray, Raman, FTIR, LEIS, NMR, STEC*

Techno-Economic Modeling



**Frontier Science Advances**

- Technoeconomic modeling
  - *Batteries → component materials*
  - *Full analysis of Li-O energy density*
- Comprehensive simulation of multivalent cathodes and solid-state electrolytes
- Anode stripping and plating in multivalent electrolytes
- Redoxmers - Introduction and rational design
- PIM polymer membranes for size and charge separation
- Li-S lean electrolytes and alternate reaction pathways

Redoxmer Flow

Air-Breathing Aqueous Sulfur

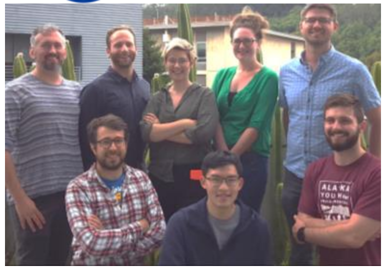
Multivalent Mg++

Li-Sulfur

**Transformative Next Generation Batteries**

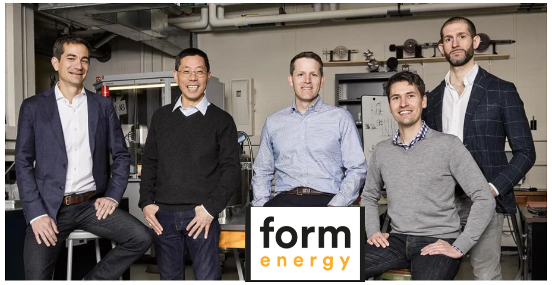
Solid State Electrolytes

SEPION TECHNOLOGIES



Size-selective PIM polymer membranes

Secretary of Energy Achievement Award
*August 29, 2018*



form energy

Many-day discharge batteries

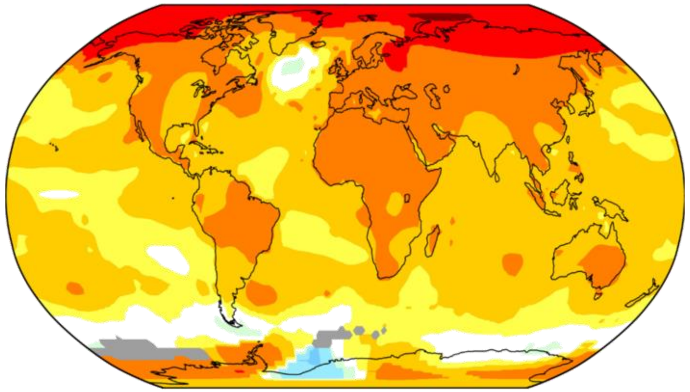
**Fundamental Science Outcomes** → **Four Laboratory Demonstrations** → **Three Startups**

# 2018 Renewal: Energy Storage Outgrew Original JCESR Vision

## Electric Vehicles
Range and cost gaps narrowed or closed
14 models in 2018, 100 new models in 2024

## Electricity Grid
5x cost reduction achieved by Li-ion
*\$181/kWh (2018); \$137/kWh (2021)*

Clean electricity market boom
*1300 MWh in 2018*
*11,000 MWh in 2021*

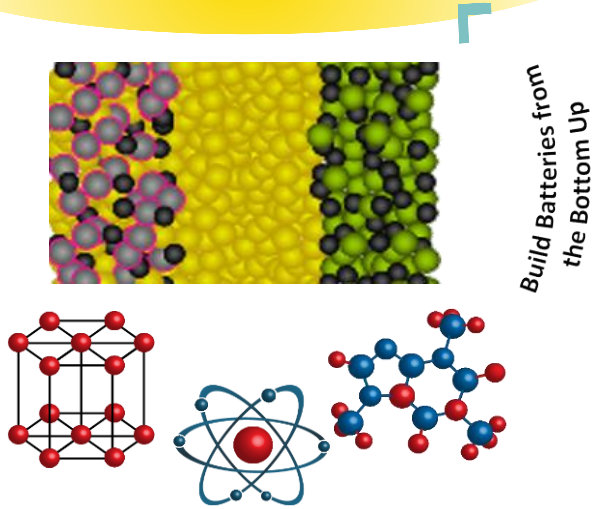


## New Player: Climate Change
Paris Accords 2015
International consensus
Warming well below 2°C (→ 1.5°C)
Decarbonize by 2050

## Energy storage
Opportunity → Necessity
*Fundamental science advances needed to meet 2050 decarbonization goals*

## JCESR Renewal Vision
*Fundamental Science*

***Transformative Materials, Chemistries and Architectures***




*A predictive understanding of electrochemical phenomena at atomic and molecular levels*

*"Bottom up" design and build to meet targeted performance metrics*

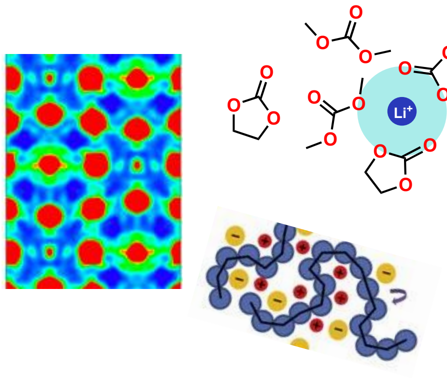
*Serves all next-generation batteries and applications*

# JCESR Mission

*Fundamental Science Mission*

***Three Primary (L1) Milestones***

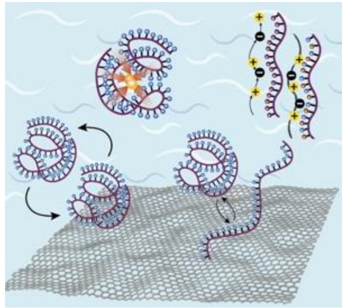
*Solvation*
*at Atomic and Molecular Levels*




Solids, Liquids, Glasses, Polymers,

*Controls static and dynamic electrochemistry of batteries*

*Redoxmer Design*

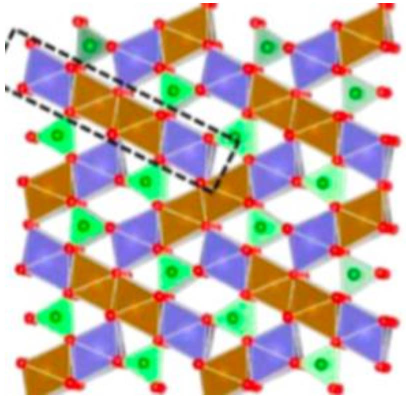


Redox-active mers
for flow batteries

*Broad molecular design space*

*High voltage, high solubility, stability, multi-electron transfer self-reporting, self-healing*

*Multivalent Ion Materials Design*



$Mg^{++}$, $Ca^{++}$, $Zn^{++}$
working ions

*Earth-abundant, safer, less expensive alternatives to Li-ion*

Guiding Principles

Extensive use of "simulation before synthesis"

*Electrolyte Genome, Materials Project, Machine Learning*

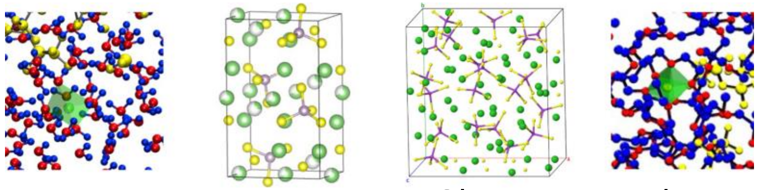
Collaborative theory and experiment at atomic and molecular level

Engage BES User Facilities

Cross-institutional collaboration

# Solvation

## Unified Framework for Solvation and Transport



Liquids
Moveable solvation shells

Crystals
Fixed lattice environment

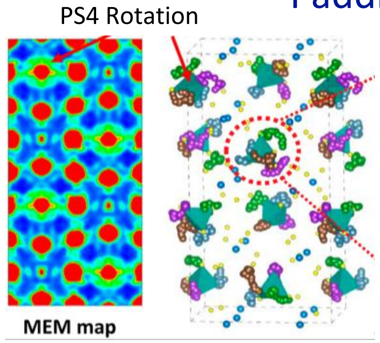
Glasses

Polymers

**Establishing a unified framework for ion solvation and transport in liquid and solid electrolytes**
D. Siegel, L. Nazar, Y-M.Chiang, C. Fang, N. Balsara 2021

Cation velocity depends on surrounding solvation dynamics
Liquids: solvent and anion translation
Solids and polymers: vibration and rotation of fixed neighbors
Vision: Predictive understanding in a single framework

## Paddlewheels



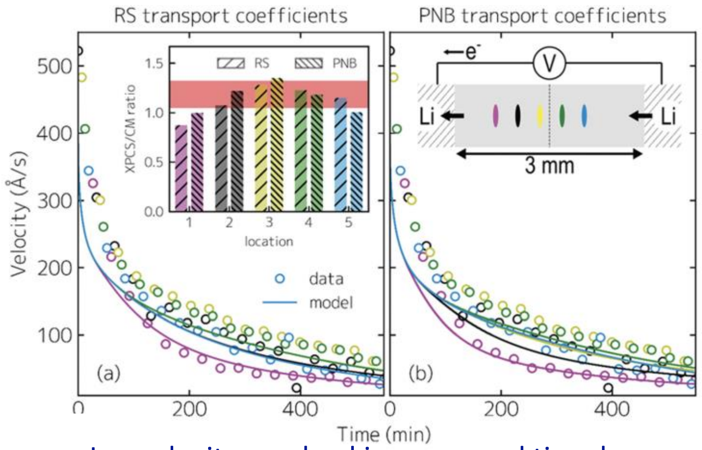

Glassy 75$Li_2S$–25$P_2S_5$
Crystalline $Li_2OHCl$
Crystalline $Na_{11}Sn_2PS_{12}$
Crystalline $Li_3PS_4$

*Ab initio Molecular Dynamics*
*Neutron/X-Ray*
*Diffraction/Spectroscopy*
*Ionic Conductivity*

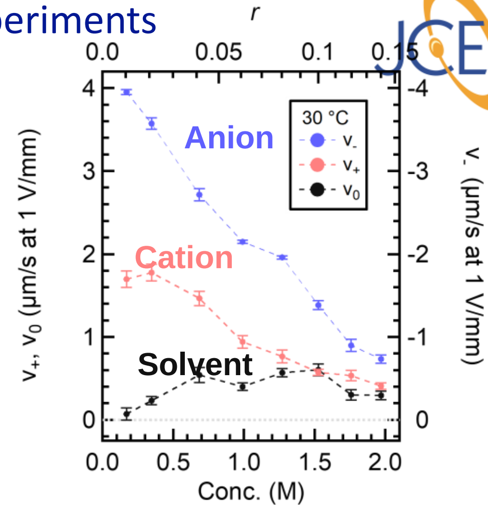
Anion rotation onset → 10x increase in ionic conductivity
Anion substitution stabilizes rotor at room temperature
Cooperative transport among cations contributing factor

*Zhang et al, JACS 141, 19360 (2019)*
*Smith et al, Nature Comm11, 1483 (2020)*
*Wang et al, Chem Matls3 2, 8481 (2020)*
*Zhang et al, Matter 2, 1667 (2020)*
*Zhang et al, Nature Reviews Materials, Early Access, Jan 2022*

## Incisive New Transport Experiments




Ion velocity resolved in space and time by
X-Ray Photon Correlation Spectroscopy (XPCS)



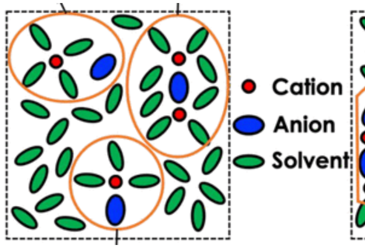

Initial ion velocity by
Electrophoretic NMR

*Detailed motion of all constituents*

*Enables full development of unified framework for solvation*

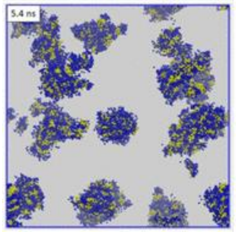
Steinruck et al, Energy Envron Sci 13, 4312 (2020)
Halat et al, Chem Mater 33, 4915. (2021)
Choo et al, JECS 169, 020538 (2022)

## Nanometric Aggregation in Concentrated Electrolytes




Dilute
Isolated Solvation Shells

Concentrated
Shared Solvent Shells



Phase Separated
Liquid

Water-in-Salt, Redox-Flow, Multivalent, Polymer, and Ionic Liquid-based electrolytes

Effect on dynamics of transport, de-solvation, SEI formation, degradation, reaction electrochemistry

*Qian et al, Energy Storage Materials 41, 222 (2021)*
*Shkrob et al, J Molecular Liquids 334,116533 (2021)*
*Qian et al, Energy Fuels 35, 23, 19849 (2021)*
*Yu et al, ACS Energy Lett. 7, 1, 461 (2022)*

>250 Papers, 12 Highly Cited, 1 Hot, 24 Reviews, 11,500 Citations

# *Redoxmers*

*Opportunity*

Wide design space to satisfy multiple performance metrics

High voltage, multi electron, long lifetime, high solubility (energy density), low cost, self-reporting, self-healing

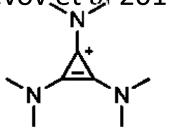
*Challenge*

discover monomers and oligomers that satisfy multiple performance metrics simultaneously

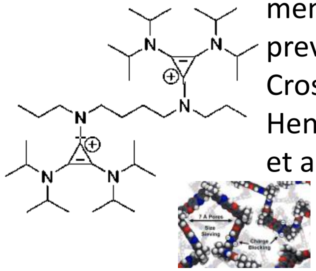
2014
Darling et al
*Technoeconomic models of aqueous and non-aqueous flow batteries,*
Energy Environ Sci 7, 3459 (2014)
398 Citations

2015 | 2017 | 2018 | 2019 | 2020 | 2021

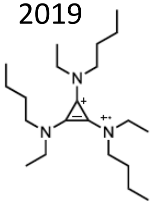
Cyclopropenium (CP) Catholyte
Sevov et al 2017



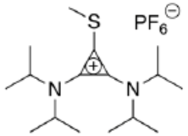
CP+PIMs membrane prevents Crossover
Hendricks et al 2018



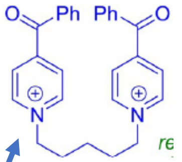
MLR predicts CP solubility
Robinson et al 2019

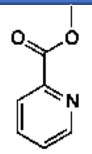


Tune CP for high voltage operation
First 3.2 V battery
Yan et al 2019



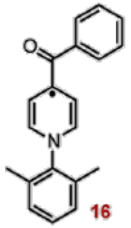

Iterative design prevents crossover, degradation
Shrestha et al 2020

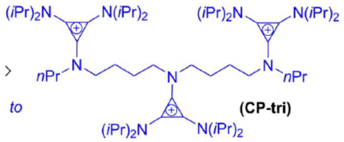


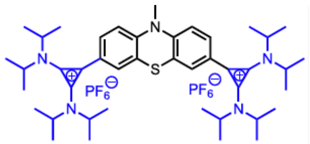


Pyridinium (Py) Anolyte
Sevov et al 2015

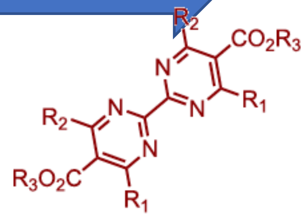
Multivariant Linear Regression (MLR) predicts Py solubility
Sevov et al 2017



High voltage, two-electron, high solubility Py dimer
Yan et al 2021



MLR predicts Bipyrimidine for two electron transfer, reduce degradation due to rotational strain
Griffin et al 2021

>130 papers, top 20 → 2800 citations

# *Multivalent-Ion Material Design* .

## High-Voltage Cathodes for Ca-Ion Batteries at Room Temperature

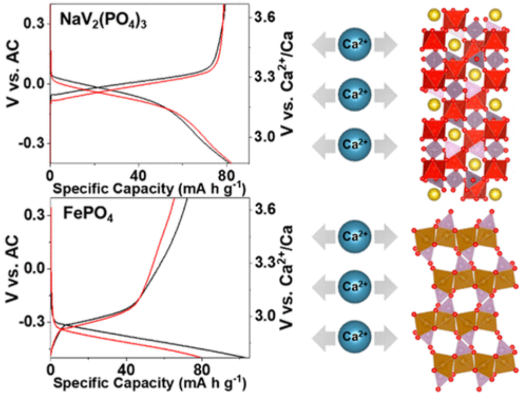
$Ca^{2+}$: high voltage, salts non-toxic, abundant, widely available

Cathodes and electrolytes not same as for Mg or Zn

$NaV_2(PO_4)_3$ reversibly intercalate 0.6 mol of $Ca^{2+}$ near 3.2 V

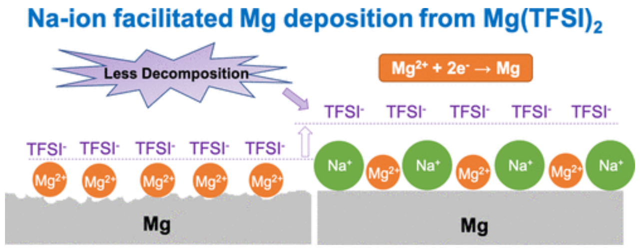
$FePO_4$ reversibly intercalates 0.2 mol of $Ca^{2+}$ near 2.9 V

*First high voltage cathode demonstration*




Kim et al, ACS Energy Lett 5, 3203 (2020)

## Enabling Mg Anodes by Electrolyte Design

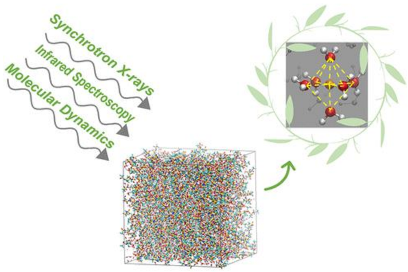



Larger size and lower charge of $Na^+$ compared to $Mg^{2+}$ excludes $TFSI^-$ from the interfacial double layer and prevents its breakdown to form a passivating layer.

MD, DFT simulations and XPS, SEM, EDX characterization confirm this mechanism.
A new route to operational Mg anodes

Wen et al, ACS Appl. Mater. Interfaces 13, 52461 (2021)

## Strong Zn-$H_2O$ Solvation in High Concentration TFSI Electrolyte

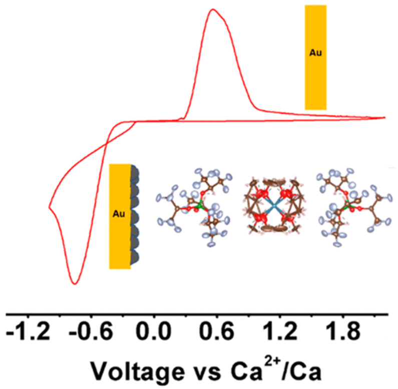



Even in 20m LiTFSI:1m ZnTFSI water-in-salt electrolyte, $Zn^{2+}$ contains only 6 $H_2O$ in its first solvation shell, TFSI is absent.

This contradicts previous understanding that $H_2O$ is completely excluded from the first solvation shell of Zn in WISE electrolytes, allowing Zn batteries using WISE electrolytes to operate without dendrite growth or water consumption.

Zhang et al, *ACS Energy Lett* 6, 3458 (2021)

## New High Voltage Electrolyte for Ca-ion Batteries




Reversible plating and stripping of Ca from solutions of $Ca(B(Ohfip)_4)_2$ in DME at 25C with an anodic stability of >4.1 V.

Combined with high voltage cathodes (above left) this accelerates progress to $Ca^{2+}$ full battery demonstration.

Shyamsunder et al, ACS Energy Lett 4, 2271 (2019)

>200 Papers, 12 Highly Cited, 2 Hot, 7 Reviews, 11,000 Citations

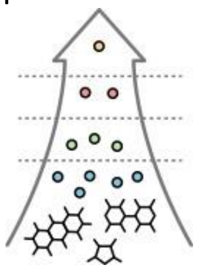
**JCESR has built a foundation for revealing the atomic and molecular origins of material performance and building on these insights to design better materials**

# Artificial Intelligence for Materials Discovery

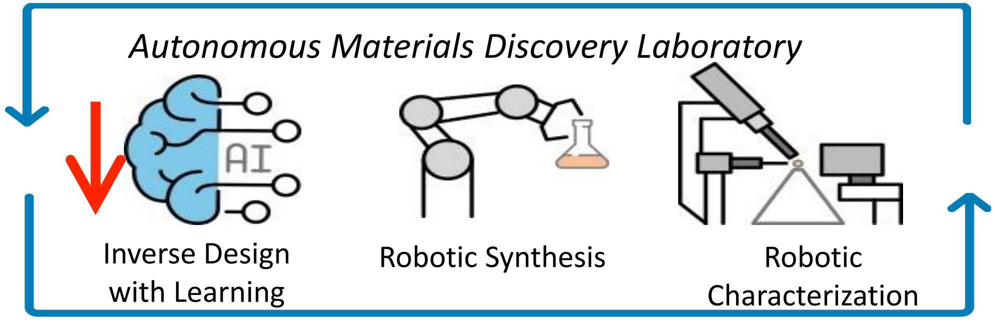
Performance: *Stability* *Voltage* *Fast Charging* *Multi-Electron Transfer* . . .

Direct Design

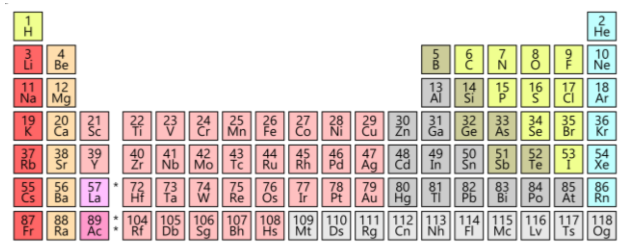
Human Imagination



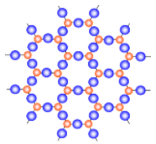
Computational Screening

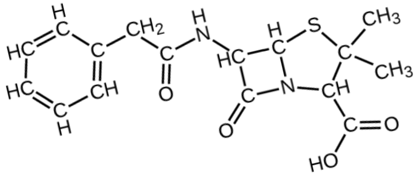



Materials:



composition





structure

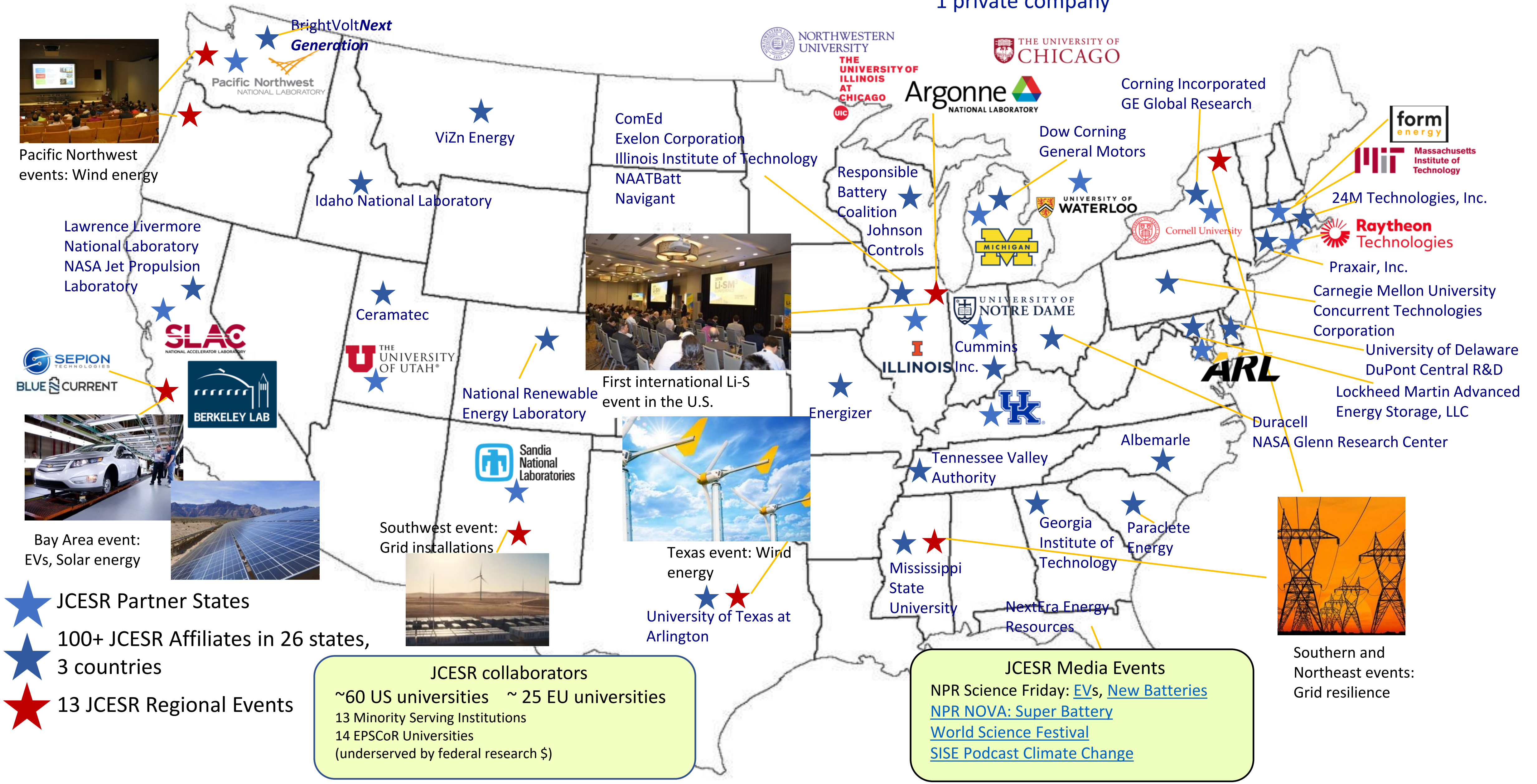
Qu, et al, The Electrolyte Genome Project . . ., Computational Mater Sci 103, 56 (2015)
Ward et al, *Materials Genomics Screens For. . .*, ACS Cent Sci 3,399 (2017)
Narayanan et al, *Accurate quantum chemical energies for 133 000 organic molecules*, Chem Sci 10, 7449 (2019)
Ward_Machine Learning Prediction of Accurate Atomization . . . , MRS Communications 9, 891 (2019)
Nisbet et al, *Machine-Learning-Assisted Synthesis of Polar Racemates,* JACS 142, 7555 (2020)
Crabtree, *Self-Driving Laboratories Coming of Age,* Joule 4, 2537 (2020)
Xie et al, *Incorporating Electronic Information into Machine Learning . . . ,* J Chem Theory Comput 16, 4256 (2020)
Dandu et al, *Quantum-Chemically Informed Machine Learning-Prediction of Energies of Organic Molecules with 10 to 14 Non-hydrogen Atoms,* J Phys Chem A 124, 5804 (2020)
Ward et al, *Graph-Based Approaches for Predicting Solvation Energy . . .*, J Phys Chem A 125, 5990 (2021)
Szymanski et al, *Toward autonomous design and synthesis . . ,* Mater Horiz 8, 2169 (2021)
Wen et al, *BonDNet-a graph neural network for the prediction of . . . ,* Chem Sci 12, 1858 (2021)
Ward et al, *Graph-Based Approaches for Predicting Solvation Energy . . . ,* J Phys Chem A125, 5990 (2021)
Spotte-Smith et al, *Quantum chemical calculations of lithium-ion battery electrolyte and interphase species,* Scientific Data 8, 203 (2021)
Agarwal et al, *Discovery of Energy Storage Molecular Materials Using Quantum Chemistry-Guided Multiobjective Bayesian Optimization,* Chem Mater 33, 8133 (2021)
Wen et al, *Improving machine learning performance on small chemical reaction data with unsupervised contrastive pretraining,* Chem Sci 13, 1446 (2022)

# JCESR: Next Generation Energy Storage

19 partners
6 national labs
12 universities
1 private company

~180 researchers
Including grad students,
postdocs and senior scientists

JCESR




JCESR collaborators
~60 US universities ~ 25 EU universities
13 Minority Serving Institutions
14 EPSCoR Universities
(underserved by federal research $)

JCESR Media Events
NPR Science Friday: EVs, New Batteries
NPR NOVA: Super Battery
World Science Festival
SISE Podcast Climate Change

# JCESR Alums at a Glance

**JCESR has 229 alumni to date**

- 85 grad students and 144 postdocs

**In the private sector they work across diverse industries**

- Automotive (Tesla, Volkswagen)
- Financial Services (Northwestern Mutual)
- Management Consulting (Exponent)
- Manufacturing (Apple, Dow, DuPont, Intel, Samsung)
- Oil and Gas (Aspen Aerogels)
- Pharmaceutical (Amgen, TC Scientific)

**Includes 7 startups**

- Aspen Aerogels—aerogel insulation products
- Form Energy—multi-day energy storage systems**
- FLO Materials—recyclable polymers
- Lyten—Li-S batteries for EVs
- Sepion Technologies—size-selective PIM polymer membranes**
- Sila Nanotechnologies—silicon-based anodes
- Wildcat Discovery Technologies—advanced battery materials

**Based on JCESR data to date; 2 percent "Other"   **JCESR startup*

## *Where Are They Now?**

**41%** industry  **44%** academia  **13%** National Laboratories

**Fik Brushett**
Associate Professor
Chemical Engineering
MIT

**Kimberly See**
Assistant Professor
Chemistry
CALTECH

**Krista Hawthorne**
Section Manager
Pyroprocess Engineering
ARGONNE

**Billy Woodford**
Co-founder & CTO
FORM ENERGY

**Artem Baskin**
Senior Researcher
GENERAL MOTORS

**Sang-Dong Han**
Research Scientist
NREL

This human capital is one of our most impactful and enduring contributions to the energy storage community. Our alums have disseminated JCESR's culture of thought leadership and innovation far and wide.

# *Community Outreach*

*JCESR has led and hosted a wide spectrum of outreach events to engage with the diverse energy storage ecosystem.*

## Mentorship Events for Pipeline Development

- 2015-2016: Events for high schoolers
- JCESR-Case Western Reserve University virtual event for graduate students; *Organizers:* JCESR, Rohan Akolkar (CWRU, BEES EFRC) and Grant Goodrich (CWRU, Great Lakes Energy Institute), April 13, 2021
- "Careers after grad school in the energy sciences," JCESR-UIC virtual event for graduate students and undergraduates; April 21, 2022

## Scientific Workshops to Accelerate Innovation and Invite Collaboration

- Artificial Intelligence for Energy Storage: *Translating Innovation*, Aug. 17, 2020
- Artificial Intelligence for Energy Storage 2: *Materials Discovery*, Oct. 29, 2020
- Enabling Solid Electrolyte Batteries: *Can solids replace liquids?* Dec. 17, 2020
- Artificial Intelligence for Energy Storage 3: *Materials Synthesis*, Mar. 4, 2021
- Designer Interfaces: *Always to blame?* Mar. 23, 2021
- Enabling Solid Electrolyte Batteries 2: *Anodeless Design*, May 6, 2021
- Designer Interfaces 2: *Chemomechanical Properties*, Feb. 17, 2022

## Conference Organization to Lead and Foster Scientific Discussion

- MRS, ACS, and ECS symposiums
- Li-SM$^3$, MagBatt, and Beyond Li-ion conferences

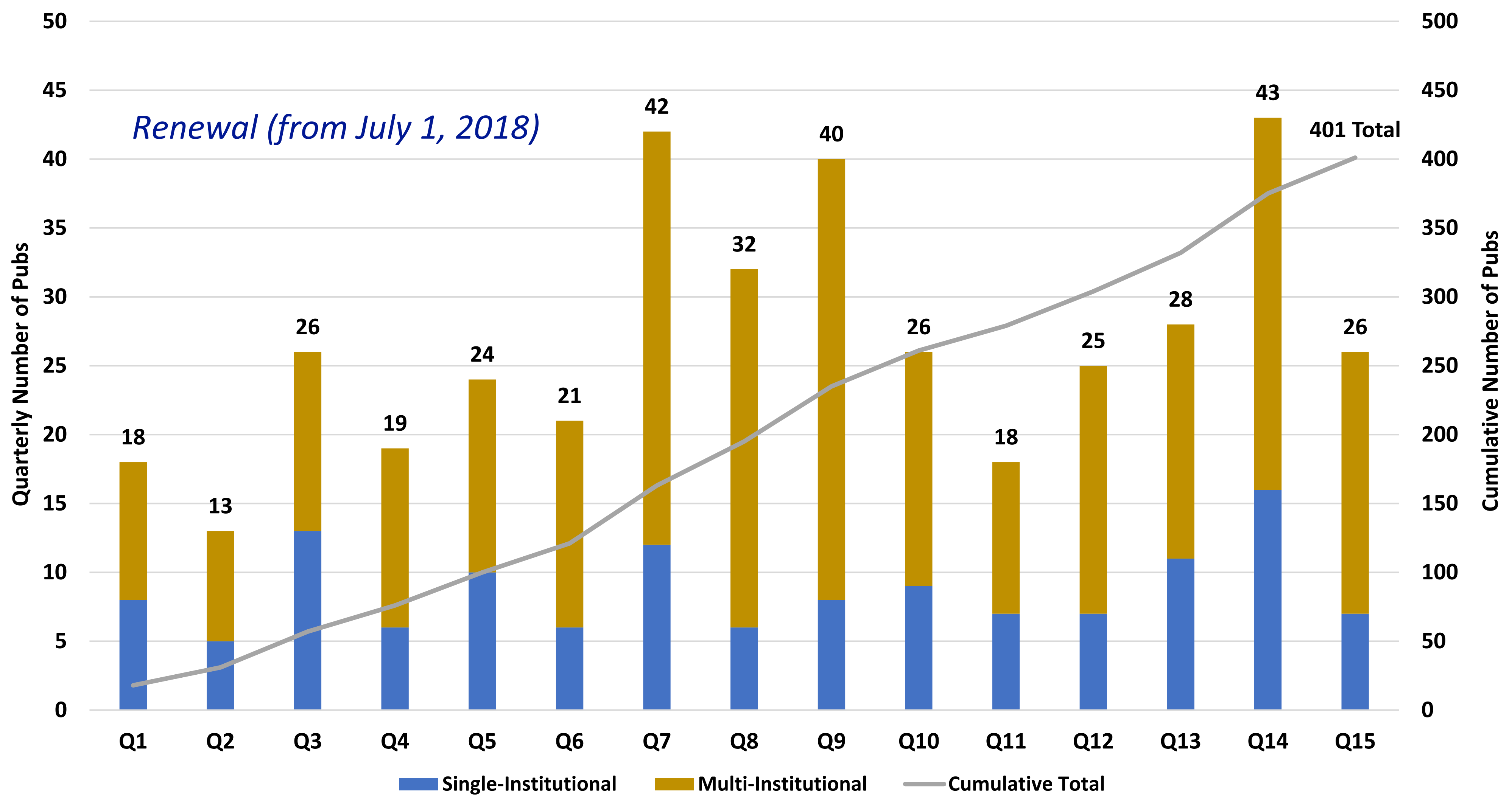
## Industrial Outreach to Routinely Connect with Value Chain

- 2014-2020: Regional Events throughout US to understand local energy storage needs by bringing together industries, utilities, government, and academia; Affiliate events to showcase JCESR's connections to technology
- Summer 2022: Regional event with our industrial partner, RTRC, to explore the fundamental electrochemical and system challenges regarding energy storage for electric aviation
- Summer 2022: JCESR Industry Day to showcase JCESR legacies and their translation to current and future technology

In JCESR, external and external integration efforts are largely led by our Research Integration Leads and the management team at ANL.

Diversity, equity, and inclusion are stridently sought in the selection of initiatives, speakers, and attendees.

# *Publications and Patents* *(as of 3/31/2022)*




*From launch (Dec 2012), ISI Web of Science*

774 Publications, 56 Highly Cited, 5 Hot, 53 Review Articles, 43, 400 Citations, H-Index = 103

User Facilities Acknowledged: ALS: 55 APS: 84 ALCF: 9 NERSC: 85

Patent activity since launch

82 total invention disclosures

57 active patents

# Many-Day Discharge Storage

JCESR


*Energy Storage Gap*

Stabilize the renewable grid against up to 10 consecutive days of cloudy or calm weather

*Li-ion ~ 4-6 hrs*

*2017*

*JCESR spins out Form Energy*

$360M funding

*Eni Next LLC, MIT The Engine, Breakthrough Energy Ventures, Capricorn Investment Group, Macquarie Capital, . . .*


Yet-Ming Chiang
Co-founder
JCESR Member

Liang Su
Employee #1
JCESR Alum
*(not pictured)*

Billy Woodford
CTO
JCESR Alum

GREAT RIVER ENERGY™

Fe-O battery discharging at full power for four days

*Inexpensive, earth-abundant, domestically sourced*

Georgia Power

*Partnering with Great River Energy to deploy 1.5 MW/150 MWh of multi-day energy storage in Cambridge, Minnesota in 2023*

*Collaborating with Georgia Power to place up to 15MW/1500MWh of energy storage in the utility's service area*


**Air-Breathing Aqueous Sulfur Flow Battery for Ultralow-Cost Long-Duration Electrical Storage**
Zheng Li, et al, Joule 1, 306 (2017)

**Lowering the Bar on Battery Cost**
Yet-Ming Chiang, Liang Su, Mengshuan Sam Pan, and Zheng Li, Joule 1, 212 (2017)

**Demonstrating Near-Carbon-Free Electricity Generation from Renewables and Storage**
M Ferrara, Y-M Chiang, J M Deutch, Joule 3, 2585 (2019)

**The iron-energy nexus: A new paradigm for long-duration energy storage at scale and clean steelmaking**
Woodford et al, One Earth 212, March 18, 2022

*Thank You!*