ION TRANSPORT AND NANOSCALE STRUCTURE IN SODIUM FLOW BATTERIES

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PROJECT PROFILE

Topic: [Flow Batteries] | Vertical: [Materials and Systems Innovation]

Strategic Pathway: [Grow: Long-term expansion by enabling innovation, advancing new technologies, and building capacity for a future-ready electricity system

Project start and finish: FY26-FY27

PROBLEM

- Understanding enhanced ion transport at the atomic length scale through membrane in sodium (Na) flow battery (FB) can only be solved by molecular level simulations.
- Low-cost energy materials discovery requires large number of expensive experiments. High performance Computing (HPC) designs materials without materials cost.
- The Na-FB materials discovery currently based on trial-and-error, expensive experiments. HPC simulations will revolutionize the field by a-priori prediction and optimization of materials.

APPROACH

Describe the methodology used in your research.

- Developed molecular dynamics simulation based on experimental criteria. This approach will provide exact ion transport on Na surface.
- The simulations were developed on a Na substrate with or without carbon fiber (CF) and compared Na ion transport between them.
- We are leveraging ORNL's flagship supercomputer, Frontier at Oak Ridge Leadership Supercomputing Facility.

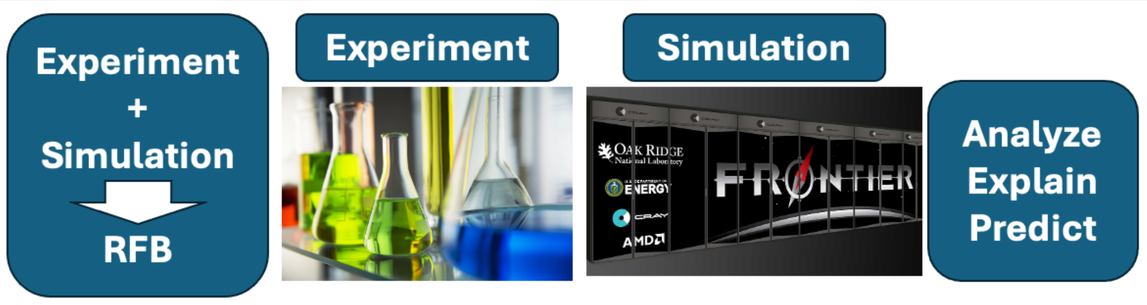

Fig. 1. Experiment and Simulation together develops materials for next generation battery storage, reducing R&D cost by performing in-silico materials discover for grid-scale energy storage materials.

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RESULTS

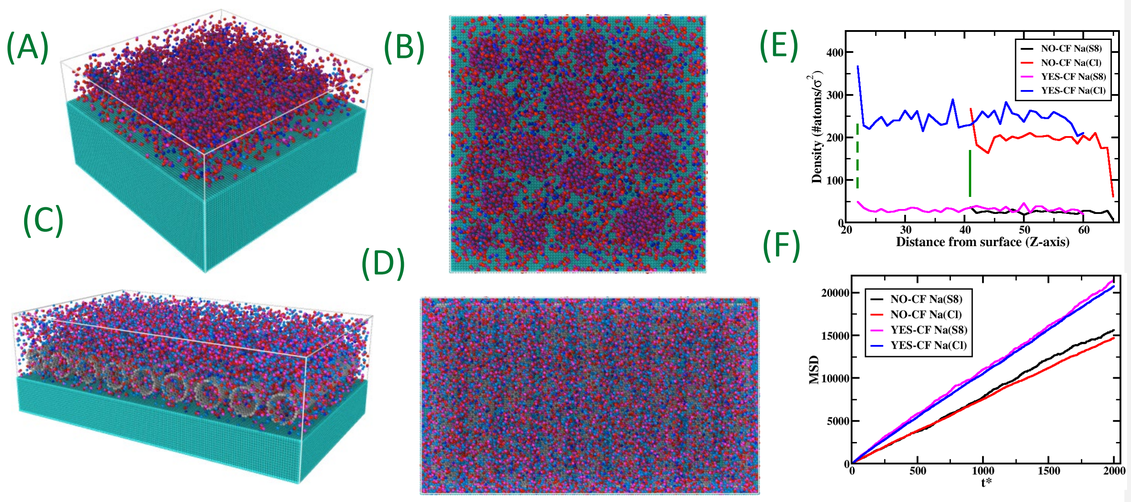

Fig. 2. MD simulation snapshots without (A) & (B) and with CF (C) & (D) on a sodium slab, (C) showing cluster formation without CF, cluster breaks down in (D) giving rise to free Na ions. (E) Higher Na Ion density and (F) faster Na dynamics as shown by mean square displacement (MSD) at the interface with CF. Results suggest that CF breaks down clusters enhancing ion transport.

CONCLUSIONS & IMPACT

- Without CF, Na ions form clusters with S-1 of sulfide that reduces ion transport. Figures 2 (A), (B) & (F).
- With CF, the interactions between CF and ions results in break-down of clusters thereby enhancing ion transport
- One high impact journal article published.
- Benefit the materials design community by predictively design materials thus, reducing cost of energy storage materials discovery.
- The data generated will be used for AI-model development for materials design.

FUTURE DIRECTIONS

- Perform MD simulations of NASICON and Vanadium RFB (VRFB) to reduce polysulfide transport and enhance Na diffusion.
- Extend HPC to solid-state battery (SSD) materials discovery.
- Develop huge *in-silico* dataset for future AI algorithm
- Final goal – integrate HPC to testbed to automate the materials design from grid-level feedback.

References

1. W. Wu, M. Goswami, C-T. Hsieh, C. Kim, Y, Li, N. Liu, G. Yang, "Cation Diffusive Carbon Interlayers Stabilize Na Metal and Double the Current in Na-S Redox-Flow Batteries for Grid-Scale Energy Storage", *Adv. Func. Mater*. **e31310**, (2026)

2. M. Goswami, G. Polyzos, M. Shahriar, G. Yang, " Correlation Between Ion Transport and Nanoscale Electrolyte Structure in Solid State and Sodium Metal Flow Batteries", MRS March Meeting, April 26-May 1, 2026

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