

Project Profile

Topic: Next Generation, Large Scale Energy

Storage

Vertical: Materials and Systems Innovation

Strategic Pathway: Grow

Project start and finish: FY24 - FY27

Problem

Background

- Energy storage is needed across all time scales, from fast grid services to seasonal storage
- Batteries enable distributed energy resources to support a reliable, resilient, affordable, and flexible grid
- Data centers, AI technology, and advanced manufacturing increase the need for dependable infrastructure
- Diversifying battery chemistries reduce foreign supply-chain dependence and energy security
- AI-based batteries leverage low-cost domestic materials and U.S. manufacturing/recycling infrastructure

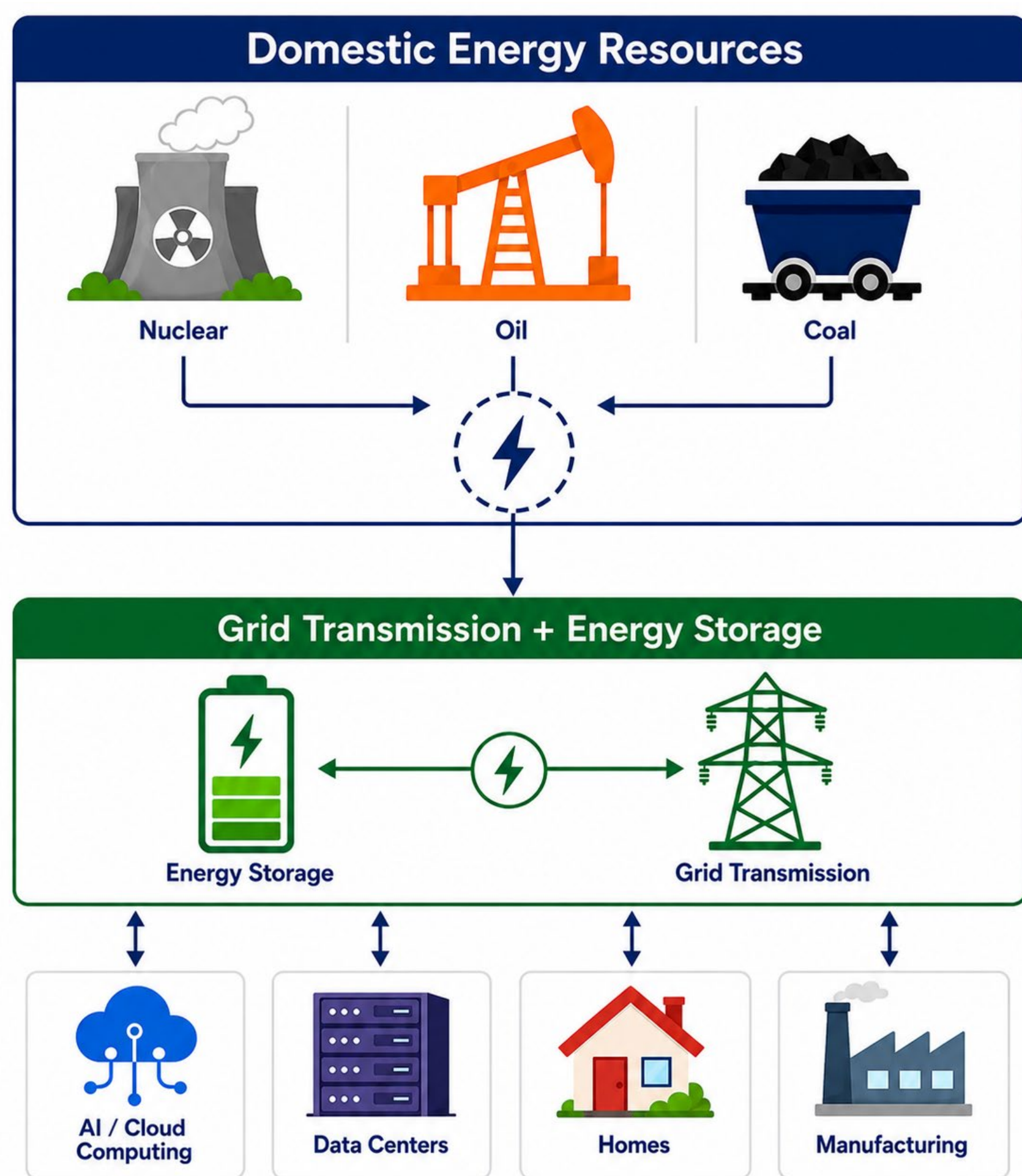


Fig. 1. Schematic diagram showing how energy storage connects domestic energy generation, grid transmission, and end-use demand in a distributed energy system

Limitations on State-of-Art Commercialized Battery Technologies

- Li-ion batteries rely on flammable electrolytes and critical materials, creating safety and domestic supply-chain concerns, respectively
- Redox flow batteries provide long-duration storage, but require large system footprints and costly active materials
- ZEBRA batteries (Na-NiCl₂) use chemically stable molten salt chemistry but require high temperature (~250 °C) and subject to supply-chain volatility

Approach

- Develop moderate-temperature Al-based molten salt electrolyte chemistry for all-duration grid storage
- Demonstrate a safe and cost-effective pathway toward durable grid storage

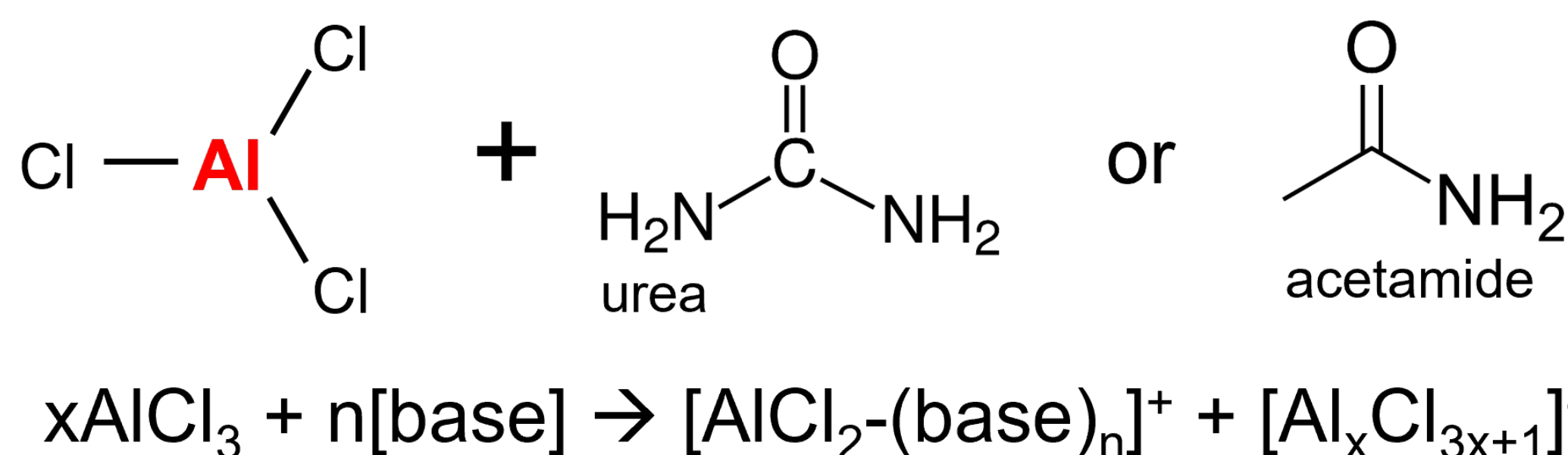


Fig. 2. Molecular structures of the Al-based electrolyte constituents and representative reaction scheme to form chloroaluminate anions and AlCl₂-base cationic complexes

Conclusions & Impact

- Al-based molten-salt electrolytes provide a pathway to diversify grid-storage chemistries using low-cost, domestically abundant materials
- Coupling spectroscopy and modeling enables the design of safer, lower-cost, and more reliable batteries

Results: Electrochemistry

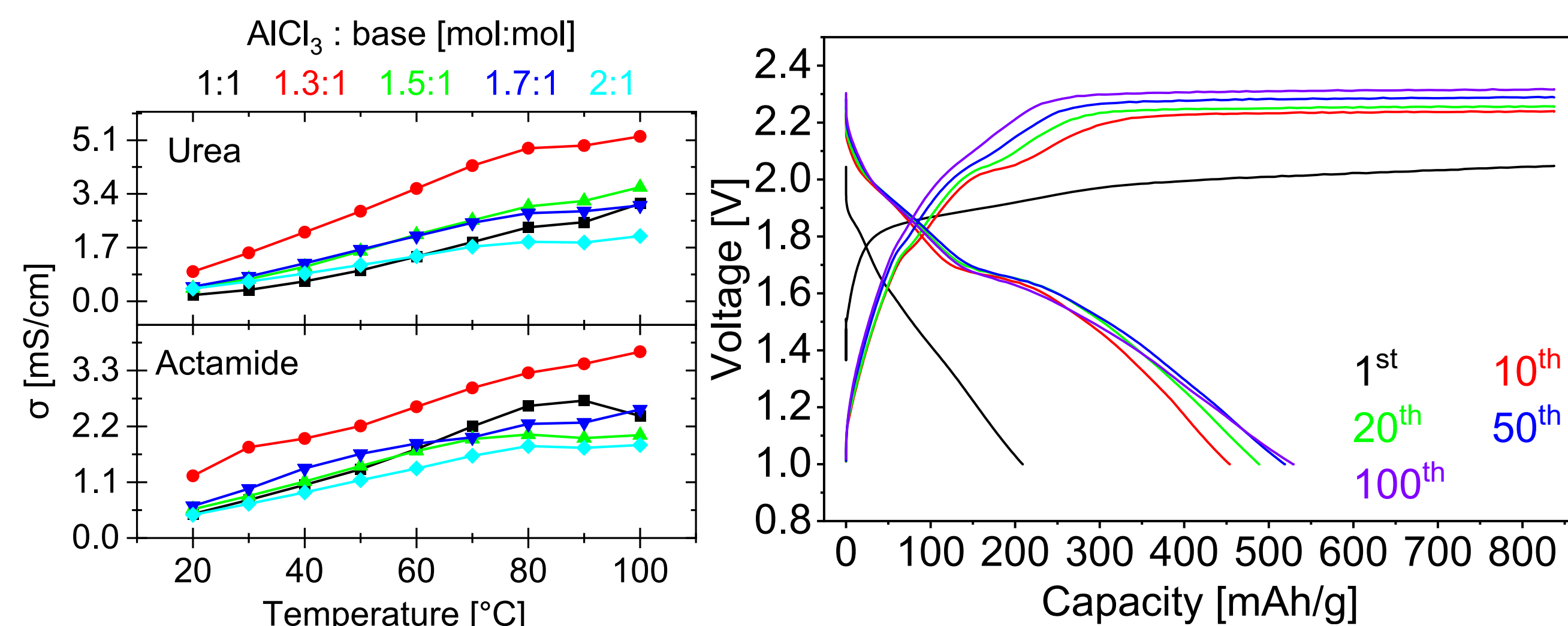


Fig. 3. (left) Ionic conductivity of two Al-based molten-salt electrolyte candidates (right) Prototype molten-salt Al-S cells using AlCl₃:urea = 1.3:1 electrolyte and sulfur oxidation pathways in development

- Moderate-temperature Al-based molten-salt batteries show promise for all-duration grid storage

Results: Advanced Characterization

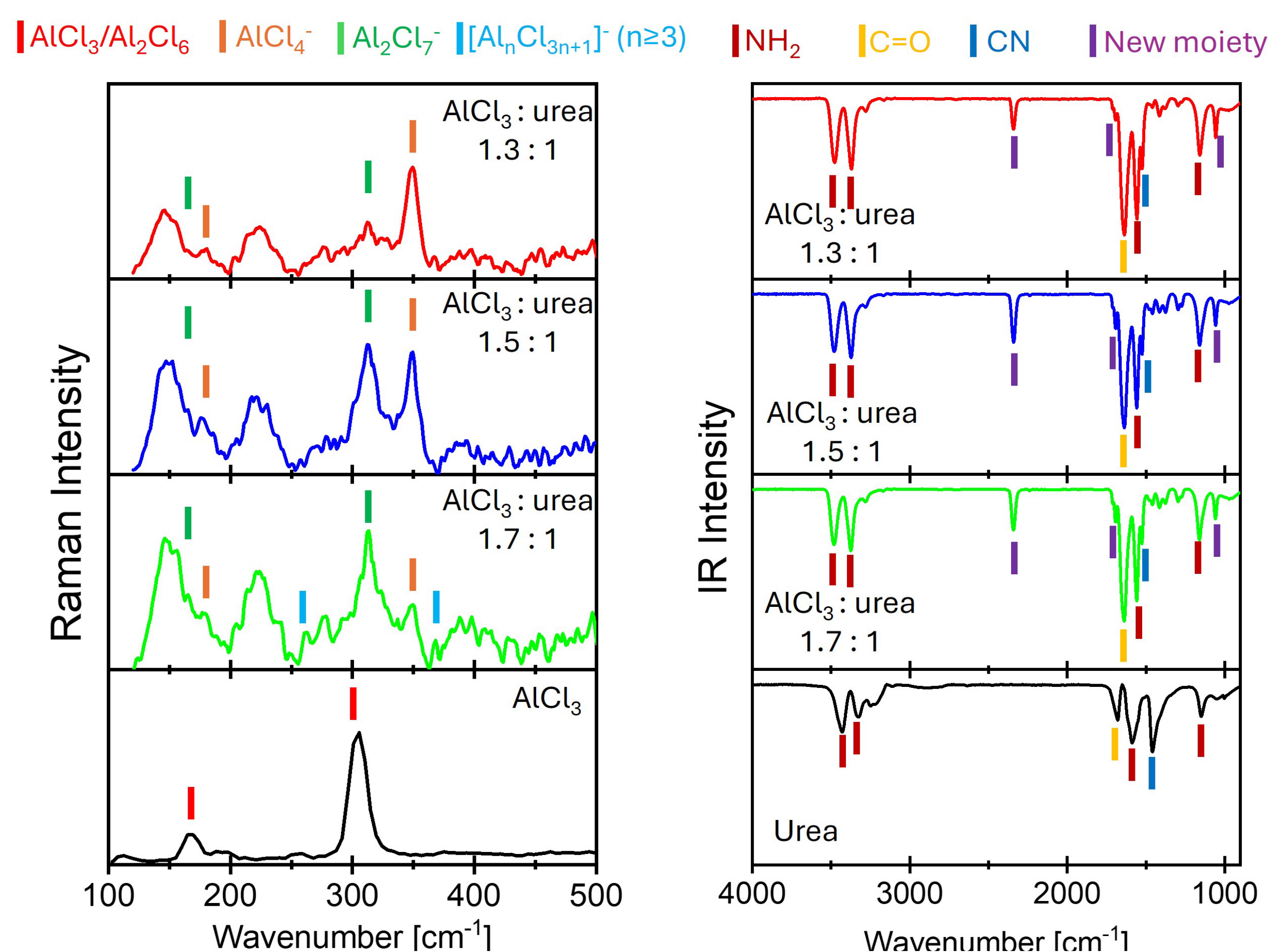


Fig. 4. Raman (left) and FTIR (right) spectra of AlCl₃-urea electrolytes identifying chloroaluminate transport species, AlCl₃-urea interactions, and possible AlCl₃-urea-derived species

- Electrolyte speciation and molecular interactions were identified using Raman and FTIR methods

Results: Computational Modeling

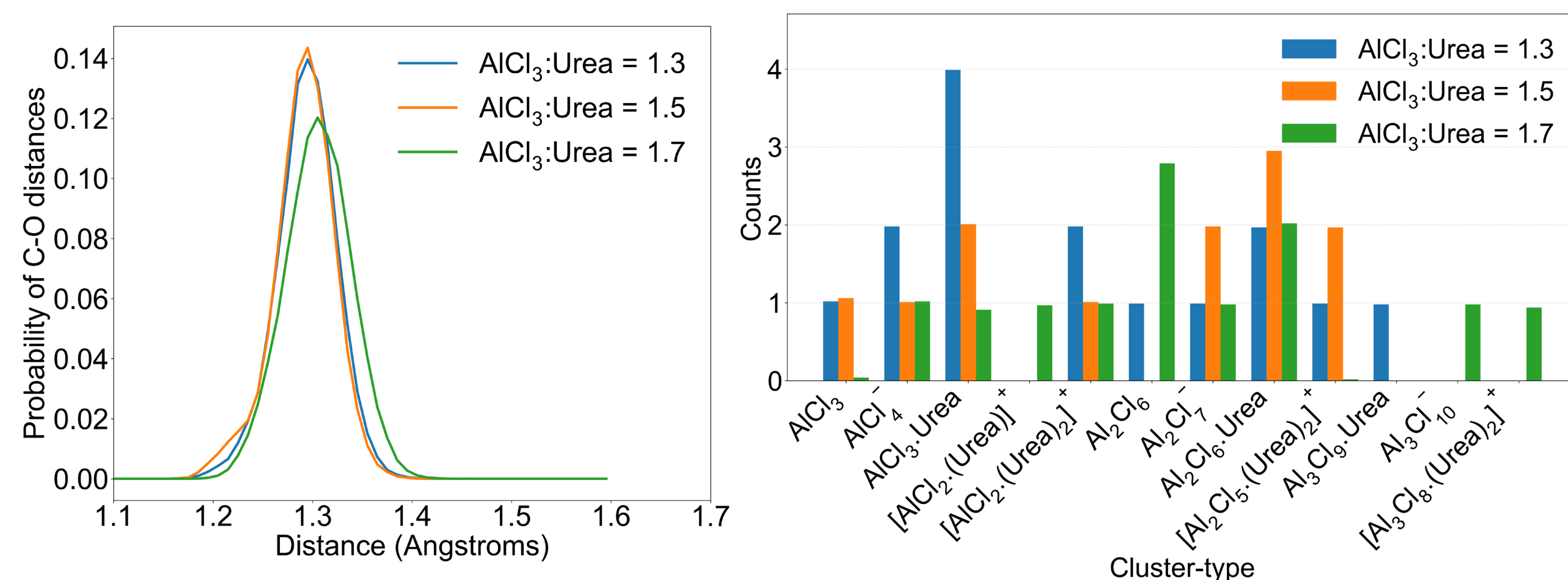


Fig. 5. AIMD analysis of AlCl₃-urea electrolytes showing carbonyl-related distance distributions, AlCl_x speciation, and composition-dependent cluster formation

- Computational modeling and advanced characterization jointly reveal electrolyte speciation and coordination

Future Directions

- Improve cycling stability and reversibility toward durable Al-based energy storage devices for all-duration grid storage
- Advance Al-based molten-salt chemistry using low-cost, domestically abundant materials
- Scale electrolyte and cell designs toward safer, more cost-effective all-duration storage