

High Energy and High Power Li-Ion Batteries

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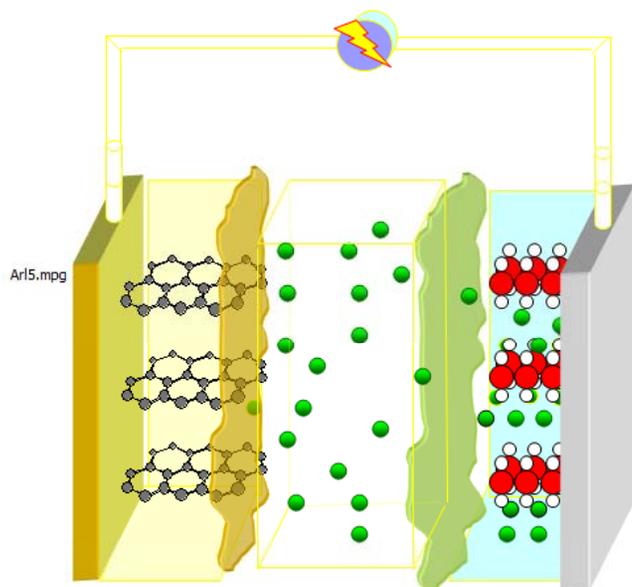
Objective:

Develop rechargeable batteries for achieving in 5 to 10 years

- Energy density: 400 Wh/kg; Power density: >16 kW/kg at 60 Wh/kg

State-of-the-Art (SOA) Li-ion Batteries:

- Energy density: 200 Wh/kg; Power density: 4 kW/kg at 60 Wh/kg
- Insertion types of cathode and anode for high rechargeability
- Protective solid electrolyte interphase (SEI) for long cycle and storage life



Materials Needs:

- For energy density: Higher voltage cathodes (>4.5 V) and higher charge capacity cathodes (> 300 mAh/g) and anodes (> 750 mAh/g)
- For power density: Functional electrolytes enabling fast Li⁺ transport across electrode-electrolyte interphases.

Challenges:

- The voltages of high voltage cathodes such as LiNi_{0.5}Mn_{1.5}O₄ (4.7 V) and LiCoPO₄ (4.8 V) are above the voltage stability range of the SOA electrolytes.
- Phase changes of these high voltage cathodes cause poor cycle life.
- Large capacity anodes suffer from large volume change and poor or no SEI protection, which result in poor cycle life.
- Charge-discharge rates of Li-ion batteries are limited by the large activation energy, 60-70 kJ/mol, for Li⁺ charge transfer across the graphite-electrolyte (SOA) interface.

Approaches:

- Modify LiNi_{0.5}Mn_{1.5}O₄ and LiCoPO₄ through studies of substitution chemistry for phase stability and high conduction.
- Explore new solvents and new additives enabling the formation of protective and conductive SEIs for high voltage cathode operations and faster kinetics.
- Interphasial chemistry studies through spectroscopic and electrochemical studies.
- Explore nanostructured Si anode materials for better performance.

Technical Gaps:

- Substitution chemistry through experiment alone lacks fundamental understanding of how electronic structures of the electrode materials are changed and improved.
- The SEIs formed at the electrolyte-electrode interfaces influence greatly the stability, life, kinetics of the cell operation. What roles do the electrode structure and surface chemistry, electrode potential, electrolyte composition, salt composition and additives play in SEI formation process, structure and properties?
- The chemistry occurs at the interface requires the understanding of the electronic structure of materials and the reactions happen at a time and length scale that is beyond the ab initio electronic structure.
- Fundamental understanding and predictive guide in materials development are needed.