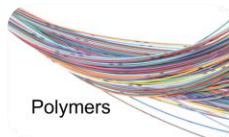
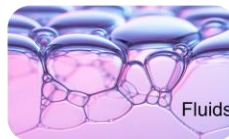




Battery Materials R&D

Advancing the Design of Batteries Through Atomic-Scale Modeling with MedeA[®]



Content

Overview

Echion Technologies and Materials Design (shown at AASC, 2022)

Uncovering New-Low-Li, High Capacity and Stable Electrolytes for Solid-State Batteries (SSB) (2022) (Early Access Article)

Electrochemical Stability (ES)

Calculation of Voltage Profile of Li_xNiO_2 (LNO)

Application example: Inverting Model (ICED-E, Model V0.0.0)

Li Transport Through Interphases

Application example: Inverting Model Conductivity and LAMMPS

Liquid electrolytes

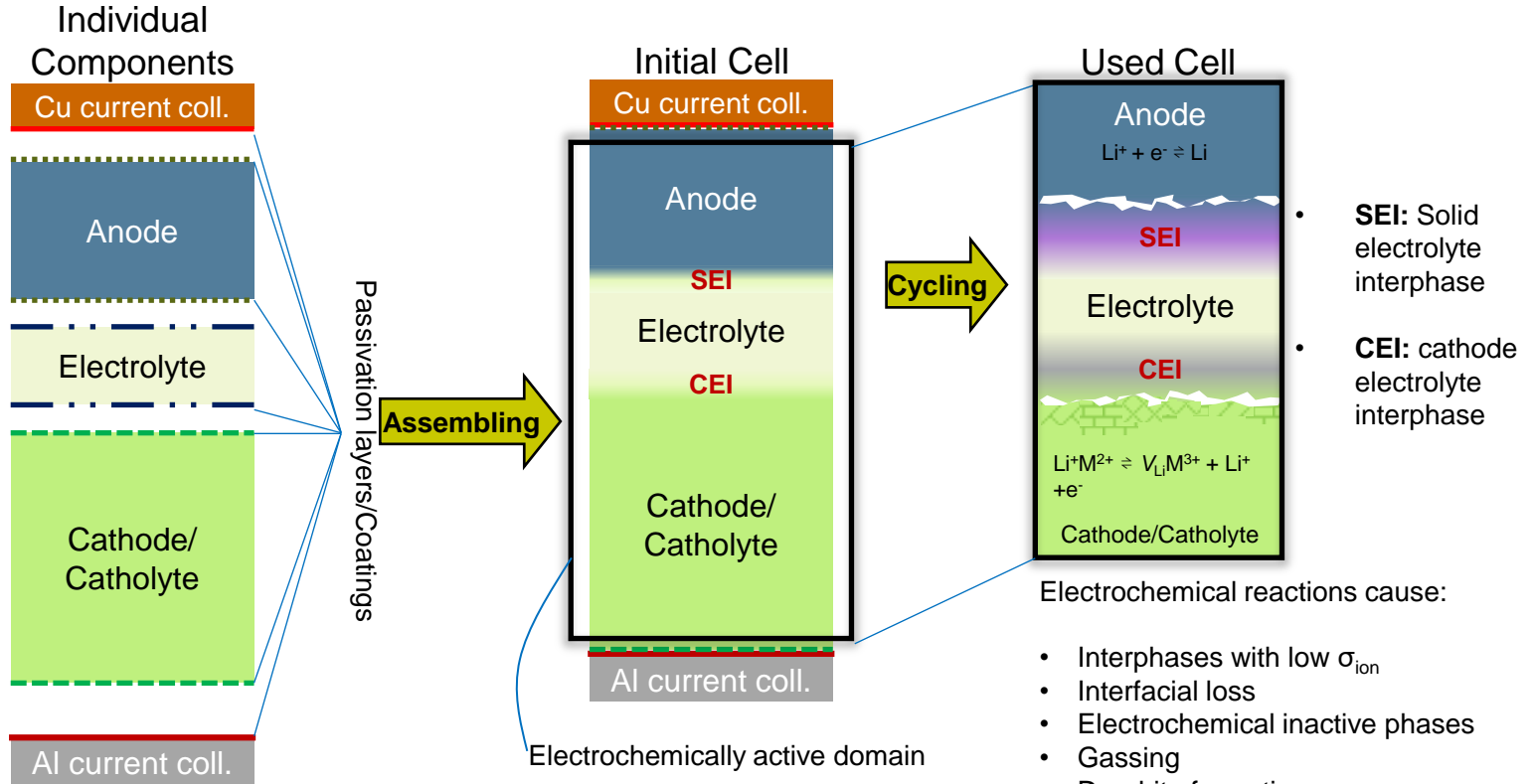
Capacity, ionic conductivity, viscosity

Organic Molecules on Inorganic Surfaces

Absorption of an PVDF oligomer on the $\text{Bi}(\text{Ti}_0.9\text{Nb}_{0.1})\text{O}_3$ surface

Overview

Battery Cells: Electrochemical Reactors



Passive components (binders, etc.) are omitted for clarity

Battery materials properties from atom-scale modeling/simulations

Materials Fabrication

- Free energies & phase diagrams: miscibility vs separation
- Elasticity: ductility, brittleness, hardness
- Permittivity Dielectric constants
- Piezoelectricity
- Diffusivity, viscosity
- Thermal conductivity
- Thermal expansion
- Heat capacity

Cycling Behavior, Fast Charging

- Conductivity: Ionic, Electrical, Thermal
- Electrochemical stability vs degradation
- Phase transformation of solids
- Volume change of particles
- Metal plating

Interfaces of Electrodes, Electrolytes, Coatings, Binders, etc.

- Interphase morphology
- Interfacial contact
- Current density
- Overpotentials
- Inter-diffusion & segregation
- Interfacial stabilities/delamination
- Potential profiles

Diagnostics & Analysis

- XPS (core level shifts)
- NMR (chemical shifts, field gradients, paramagnetic shifts)
- Powder diffraction patterns
- IR & Raman Spectra
- UV-Vis Spectra