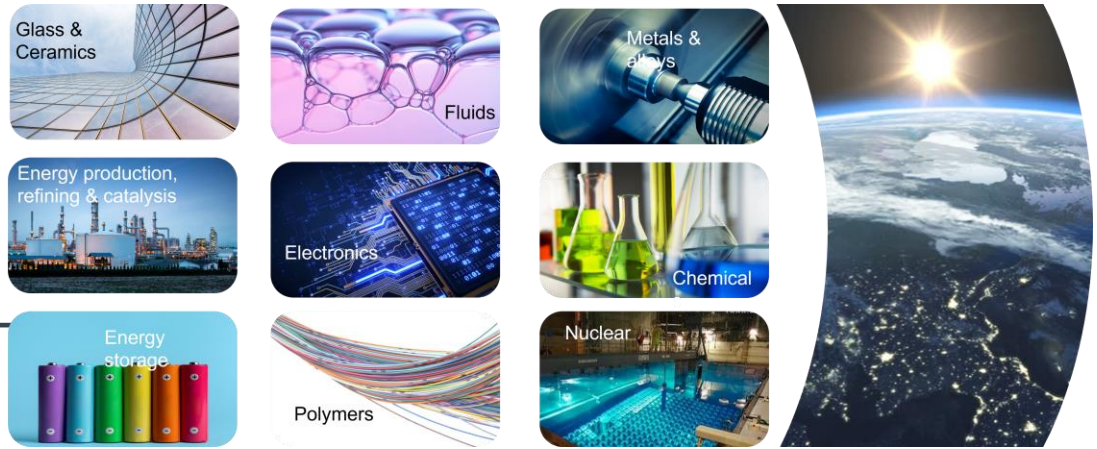
materials design

Battery Materials R&D

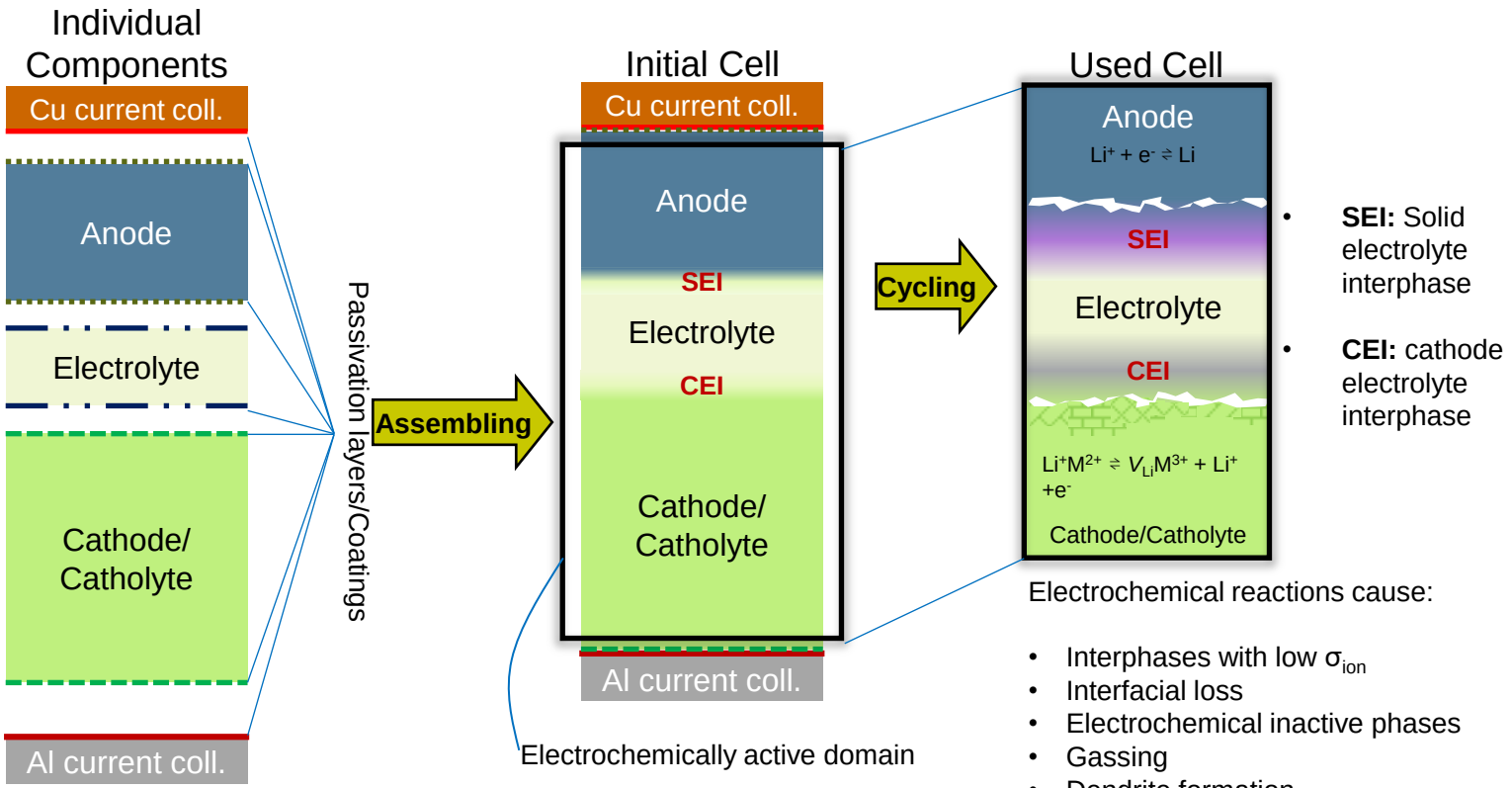
Advancing the Design of Batteries Through Atomic-Scale Modeling with MedeA®



Content

Overview

Battery Cells: Electrochemical Reactors



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

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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

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