Multiscale Modeling of Electrochemical Capacitors: From Atomic Scale to System-Level

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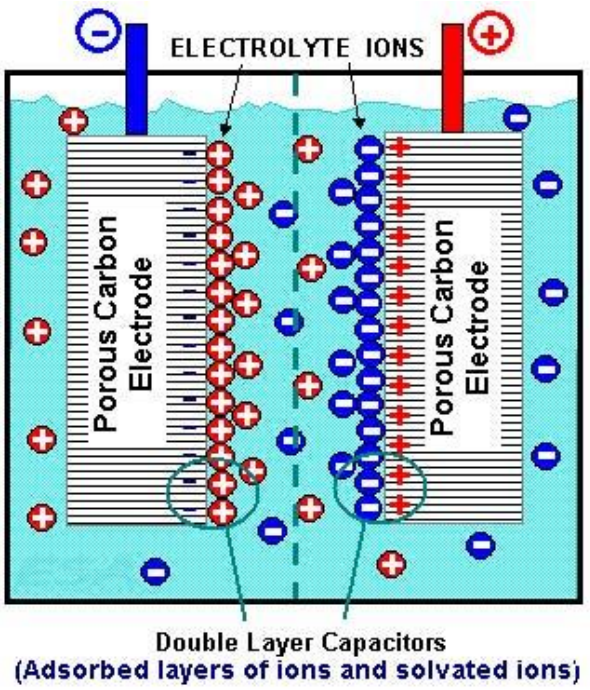
Outline

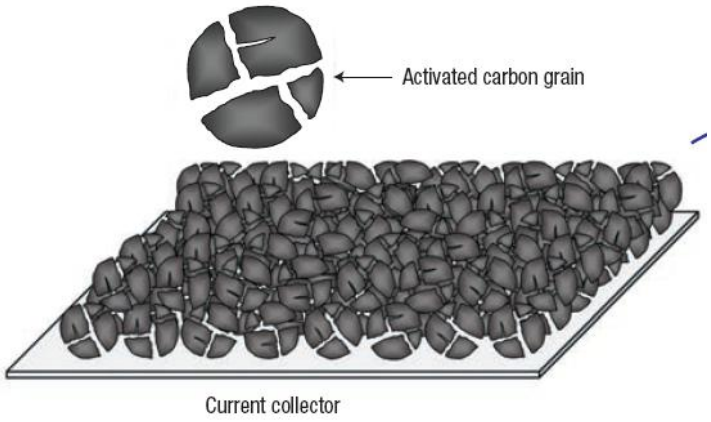
- Basic concepts of supercapacitor
- Numerical modeling
  - Why modeling?
  - Modeling at different scales
  - Our capability
- Project: virtual prototyping of supercapacitors

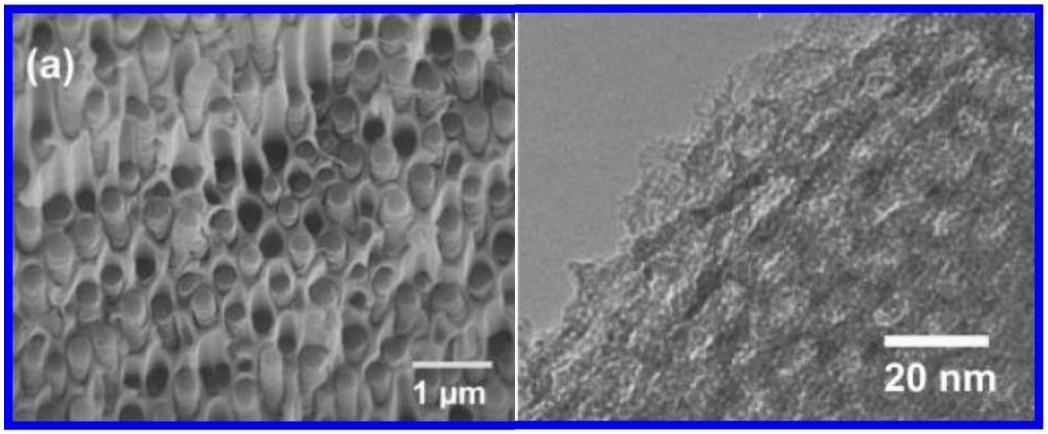
Basic Concepts

- **Supercapacitor**: electrical energy storage device based on the electrical double layers
- **Key performance parameters**
  - energy density $\propto c\, A\, V^2$
  - power density
- **Components and design issues**
  - electrode
    - large specific area desired (~2000m^2/g)
    - pore wettability
    - kinetic pore accessibility
  - electrolyte
    - high specific capacitance
    - wide electrochemical window
    - high conductivity
  - separator



Emerging hierarchical materials design





- Hierarchical porous materials with both nano- and meso-pores
  - address the competing demands from large surface area vs. good kinetic pore accessibility
  - to achieve a balance between energy density and power density

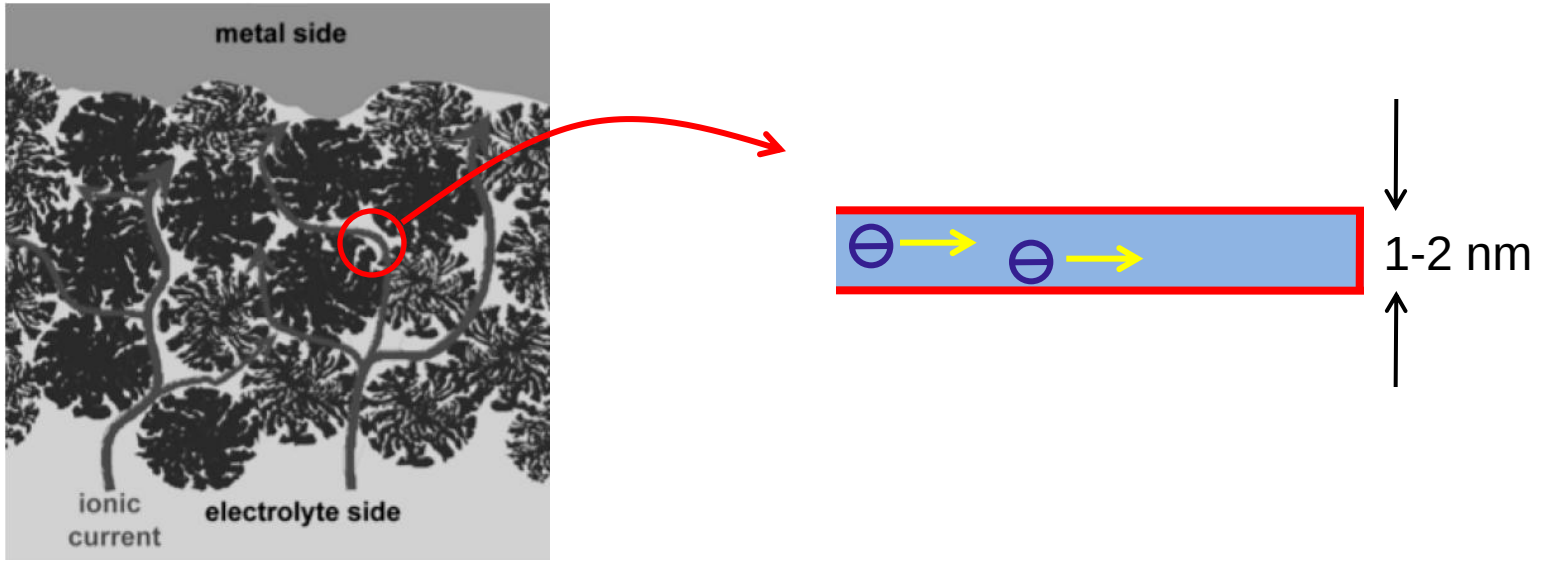
Materials issues related to superCap performance

- Given an electrode-electrolyte pair, what are the
  - specific capacitance in mesopores
  - specific capacitance in nanopores
    - typically decreases with pore size, but increase is also observed
  - wettability of the nano/meso-pores by electrolytes

❖ dictates the maximum energy density of the supercapacitor
❖ primarily an interfacial and electrochemistry problem

Transport phenomena related to superCap performance

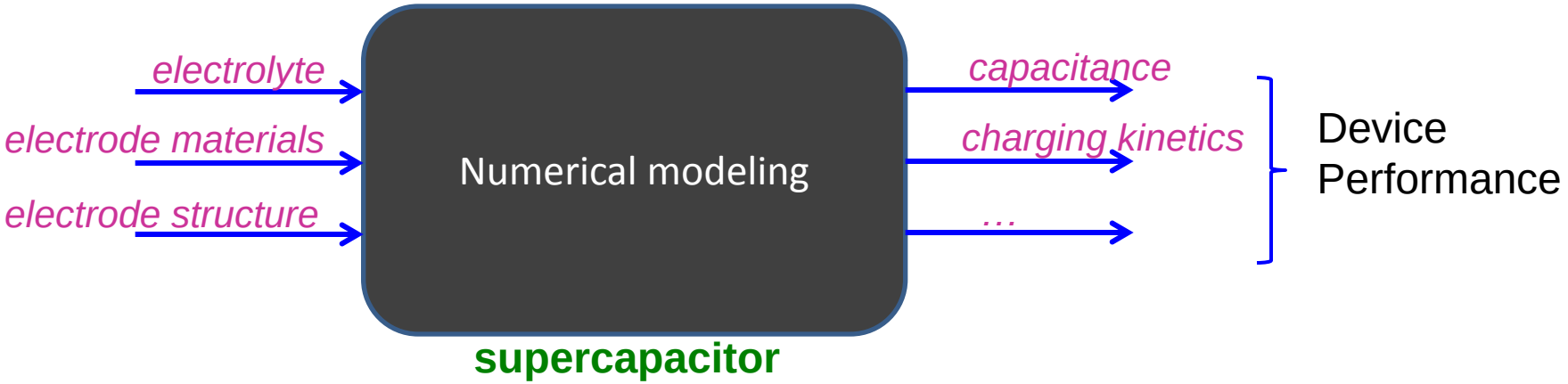
- Charging of a porous electrode
  - charging dynamics in mesopores
  - ion dynamics in nanopores



- ❖ dictates the charging/discharging kinetics and **effective capacitance**
- ❖ governed by the Nernst-Planck equations

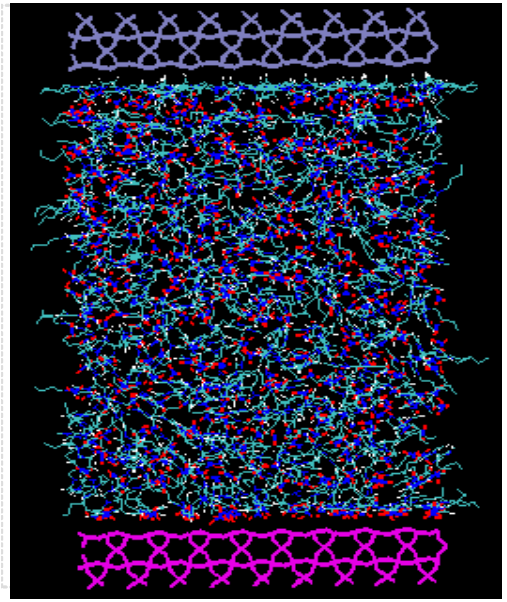
Why numerical modeling?

- A tool to understand the working of superCap
- A tool for design optimization
  - help explore design parameter space effectively
  - help handle the conflicting requirements from different aspects of performance

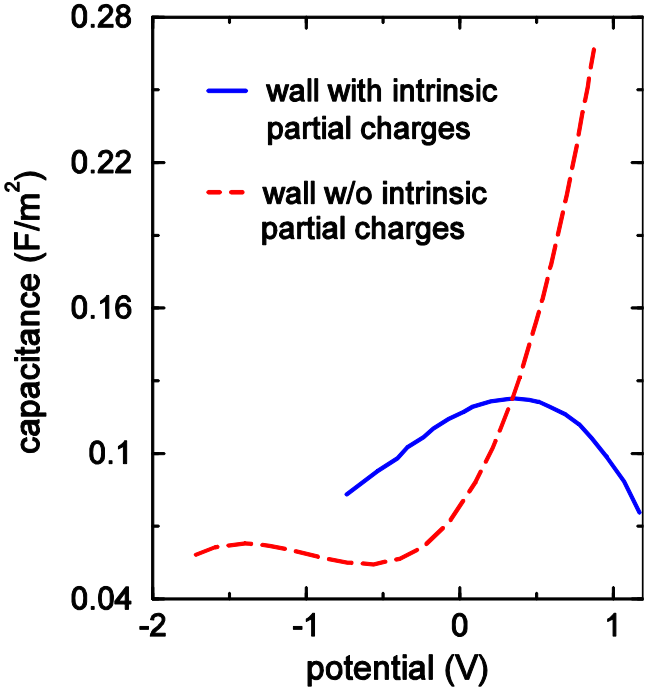


Our modeling capability – materials engineering

- Materials chemistry modeling to understand the specific capacitance of an electrode-electrolyte pair



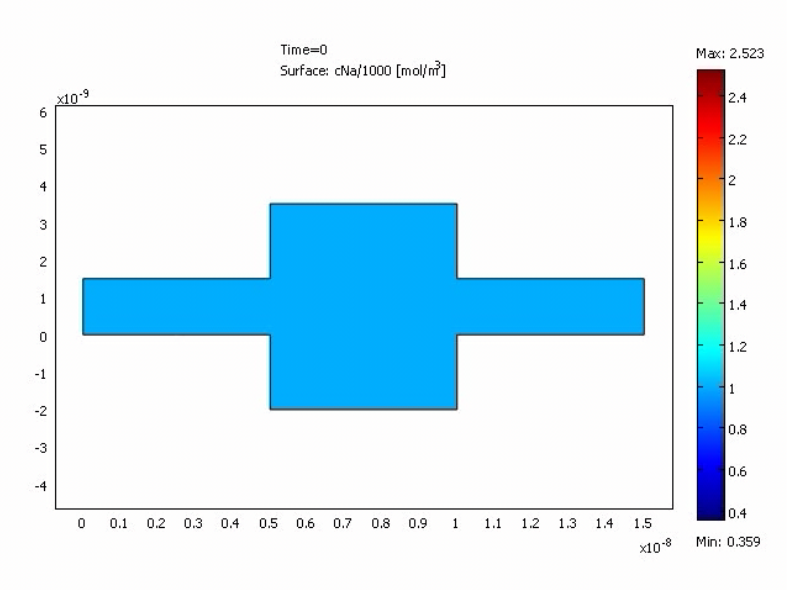
[BMIM][NO_3] between electrodes

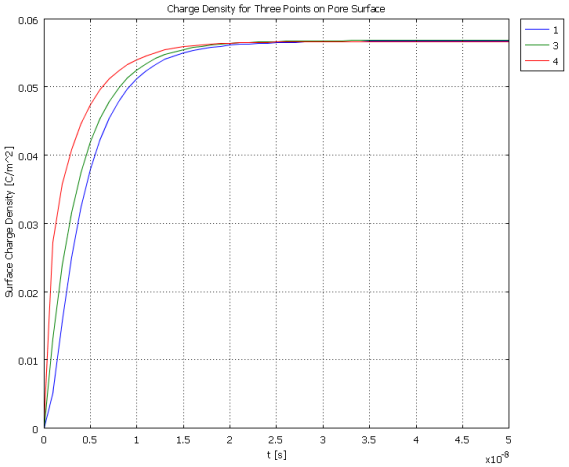


differential specific capacitance of an ionic liquid near a planar electrode

Our modeling capability – transport phenomena

- Pore scale modeling of charging kinetics



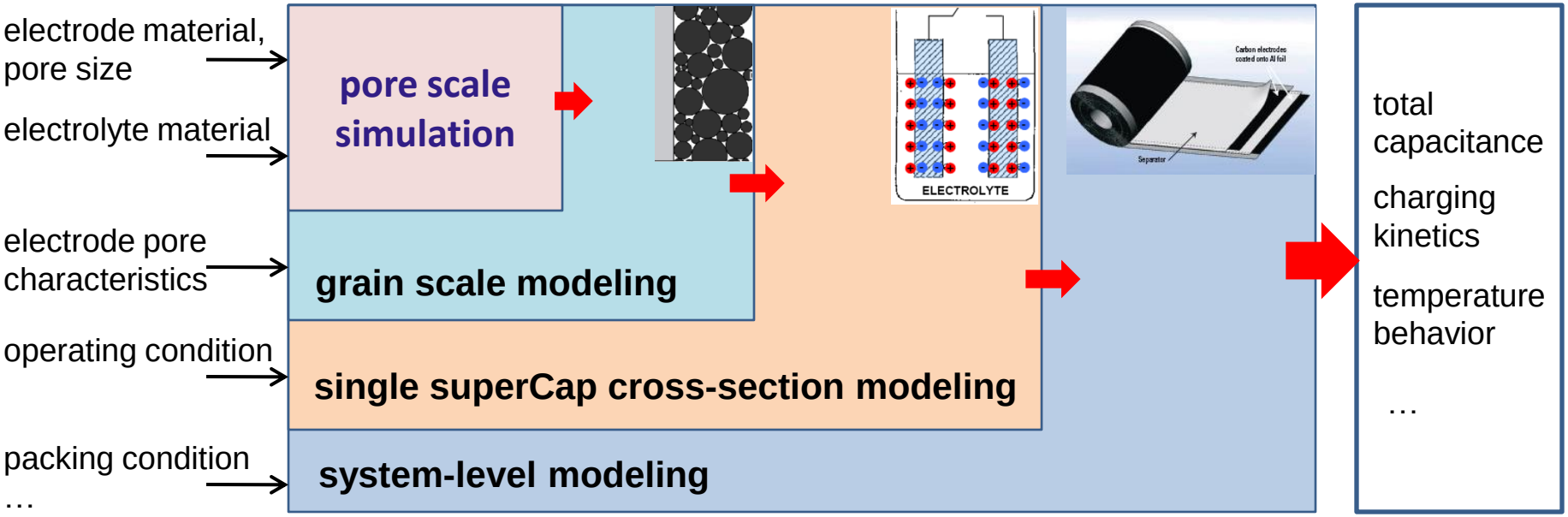


- System level modeling
  - feed pore scale results into system-level models

Proposed project

Ultimate goal:

to develop user-friendly software for virtual prototyping of a superCap based on hierarchical nanomaterials



One-year plan

- Develop a cross-section scale and system-level modeling package capable of handling capacitance design at the device level
  - charging kinetics
  - discharging kinetics
  - temperature behavior
  - thermal management