

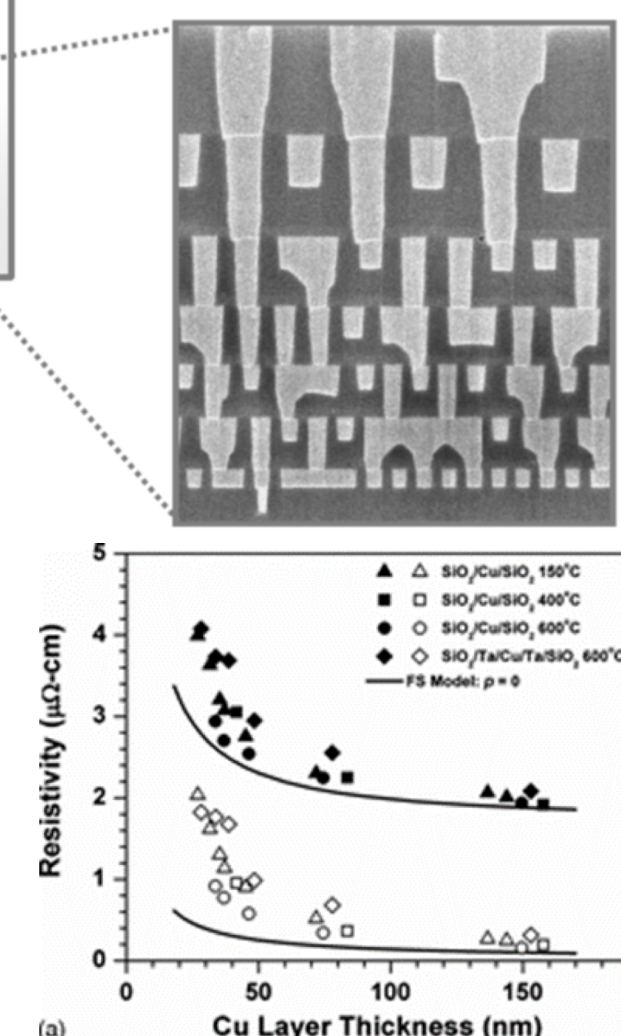
## Investigation of New Interconnect Metals

- Cobalt will be investigated as a replacement for copper in IC chip interconnects
- Electrodeposition of single crystal interconnects will result in ballistic conductance

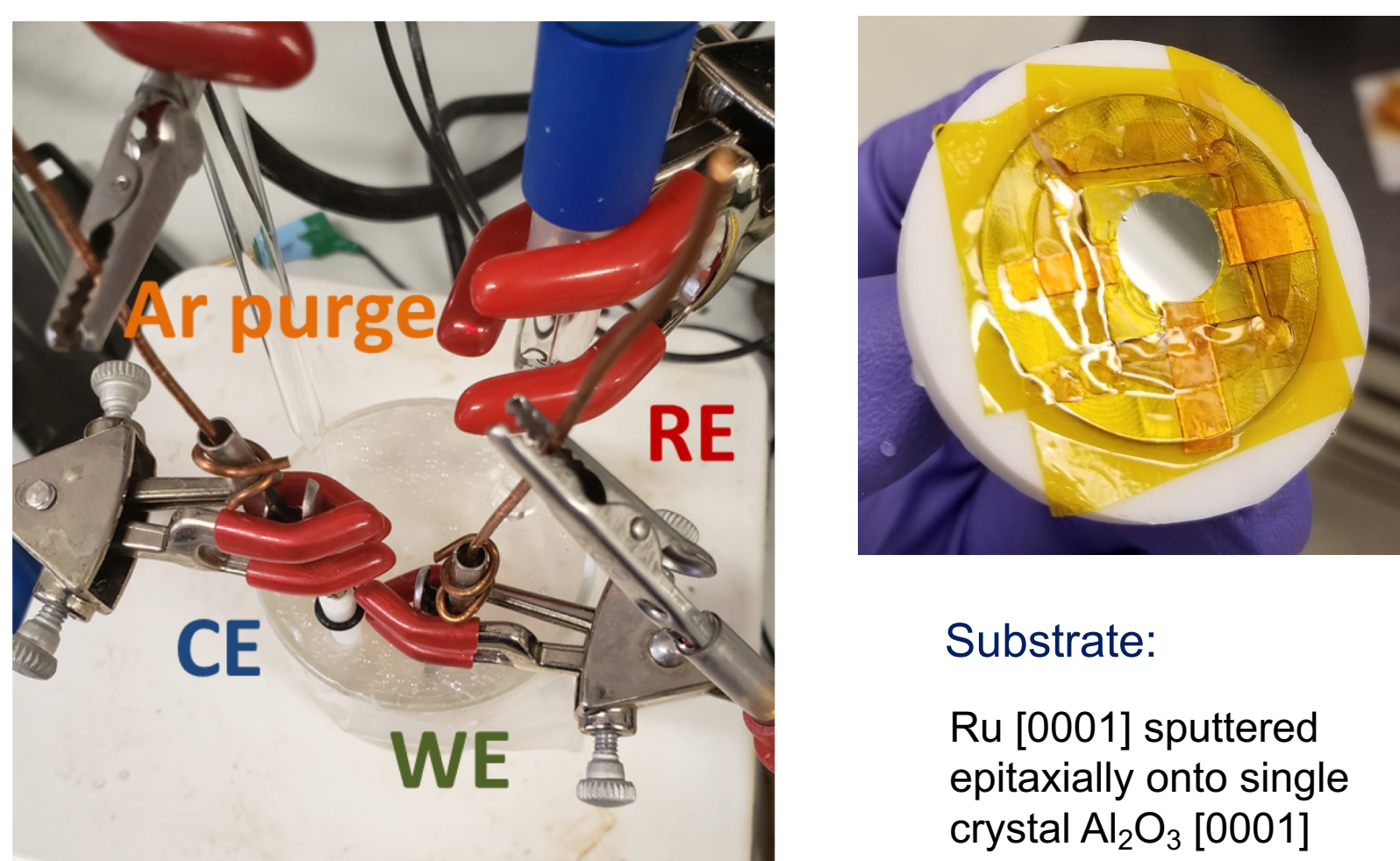
### Issues at the Nano-scale: Resistivity

- IC chips are at the core of all sophisticated electronic devices
- Moore's Law is driving interconnect scaling
- Interconnects will make up 79% of total semiconductor operating power at 10 nm node

Images used with permission from Kailash Venkatraman and Dr. Rohan Akolkar of CWRU

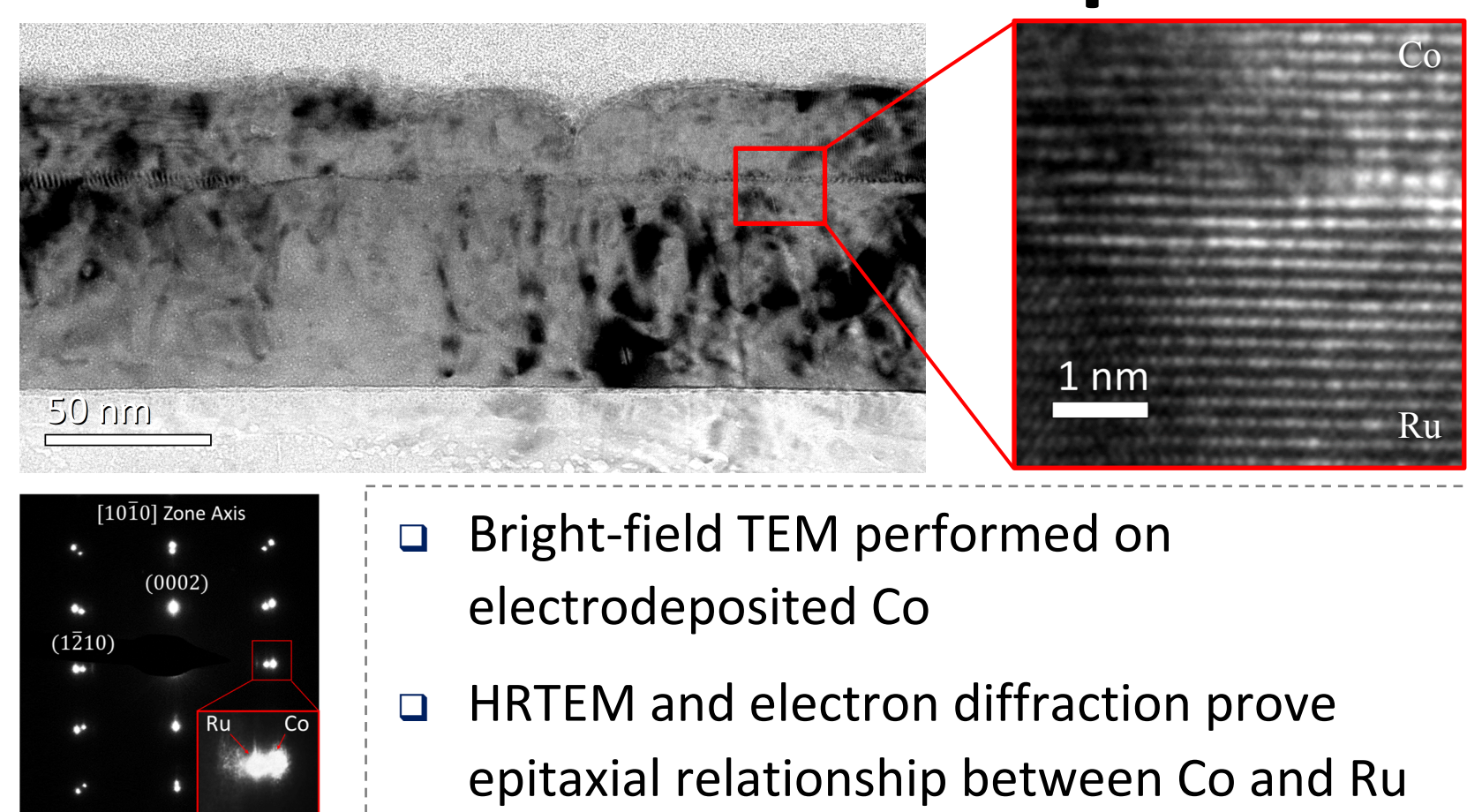


### Set-up for Co Electrodeposition



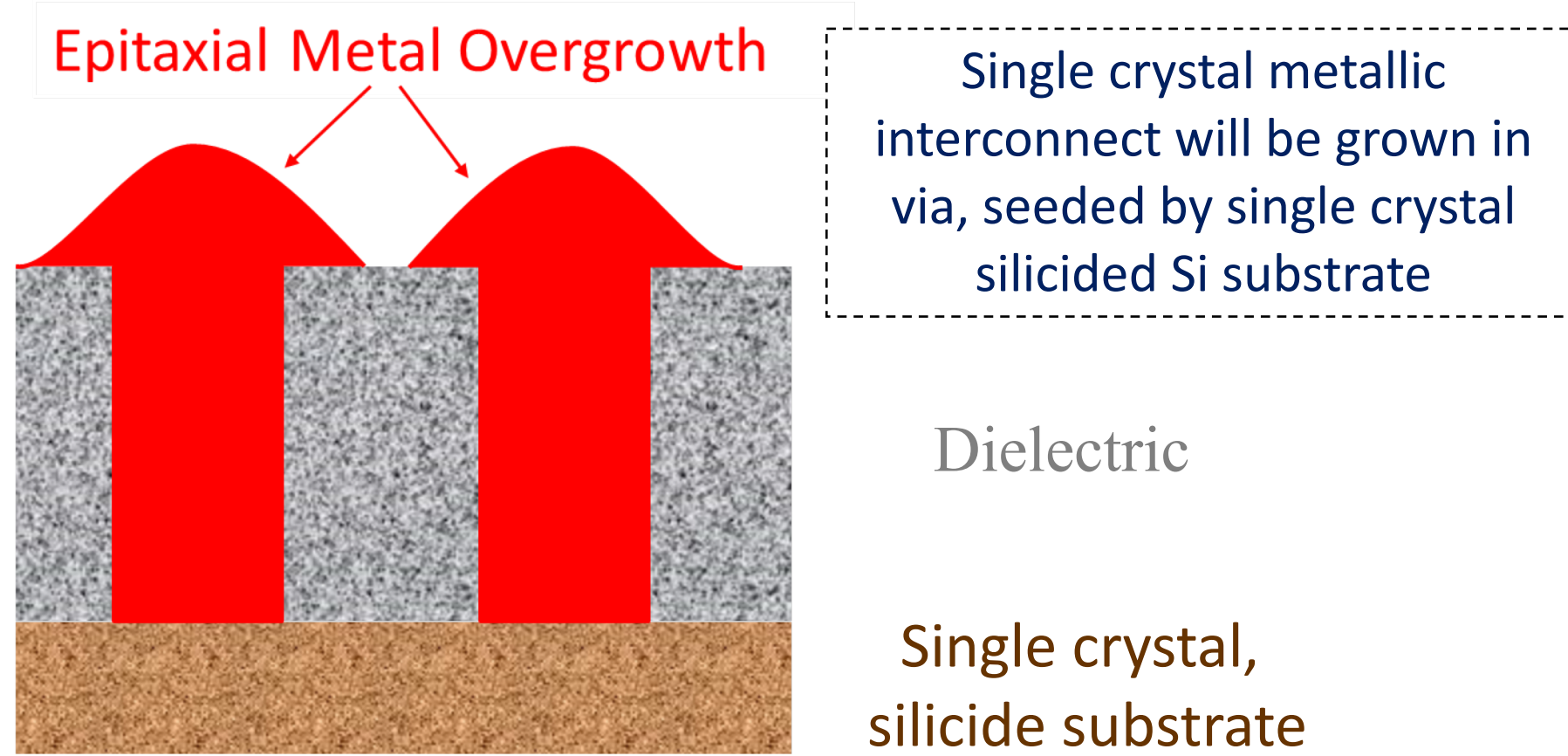
Substrate:  
Ru [0001] sputtered epitaxially onto single crystal  $Al_2O_3$  [0001]

### Cross-sectional TEM of Epitaxial Co



- Bright-field TEM performed on electrodeposited Co
- HRTEM and electron diffraction prove epitaxial relationship between Co and Ru

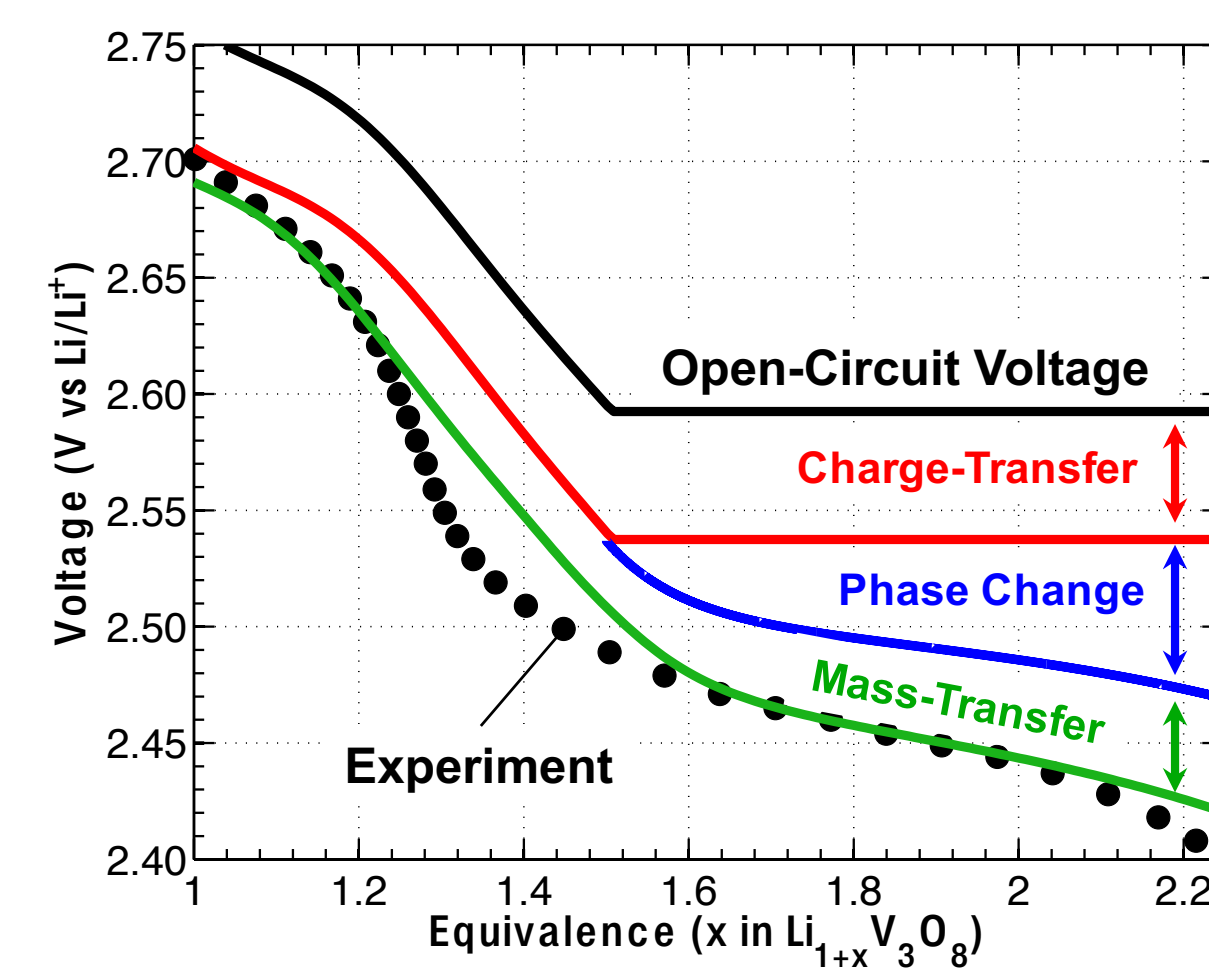
### Electrodeposition on Patterned Substrates



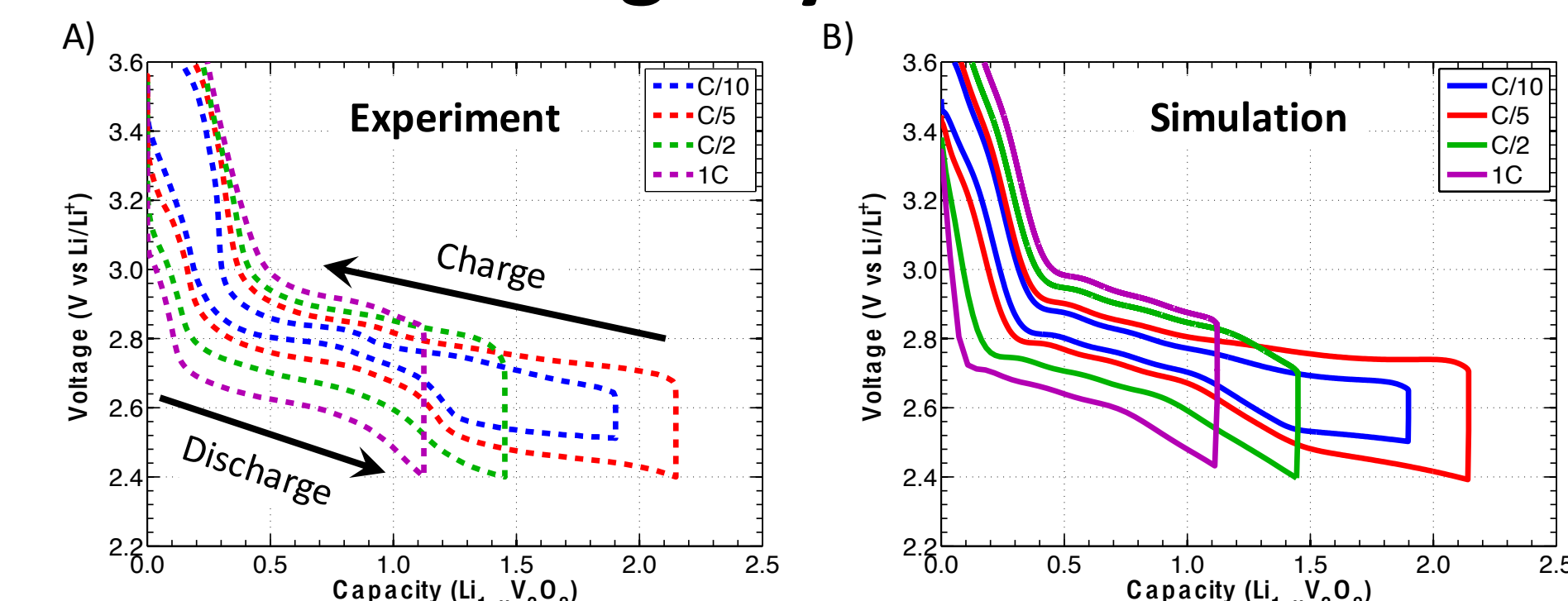
Dielectric  
Single crystal, silicide substrate

## Developing and Testing Physical Models

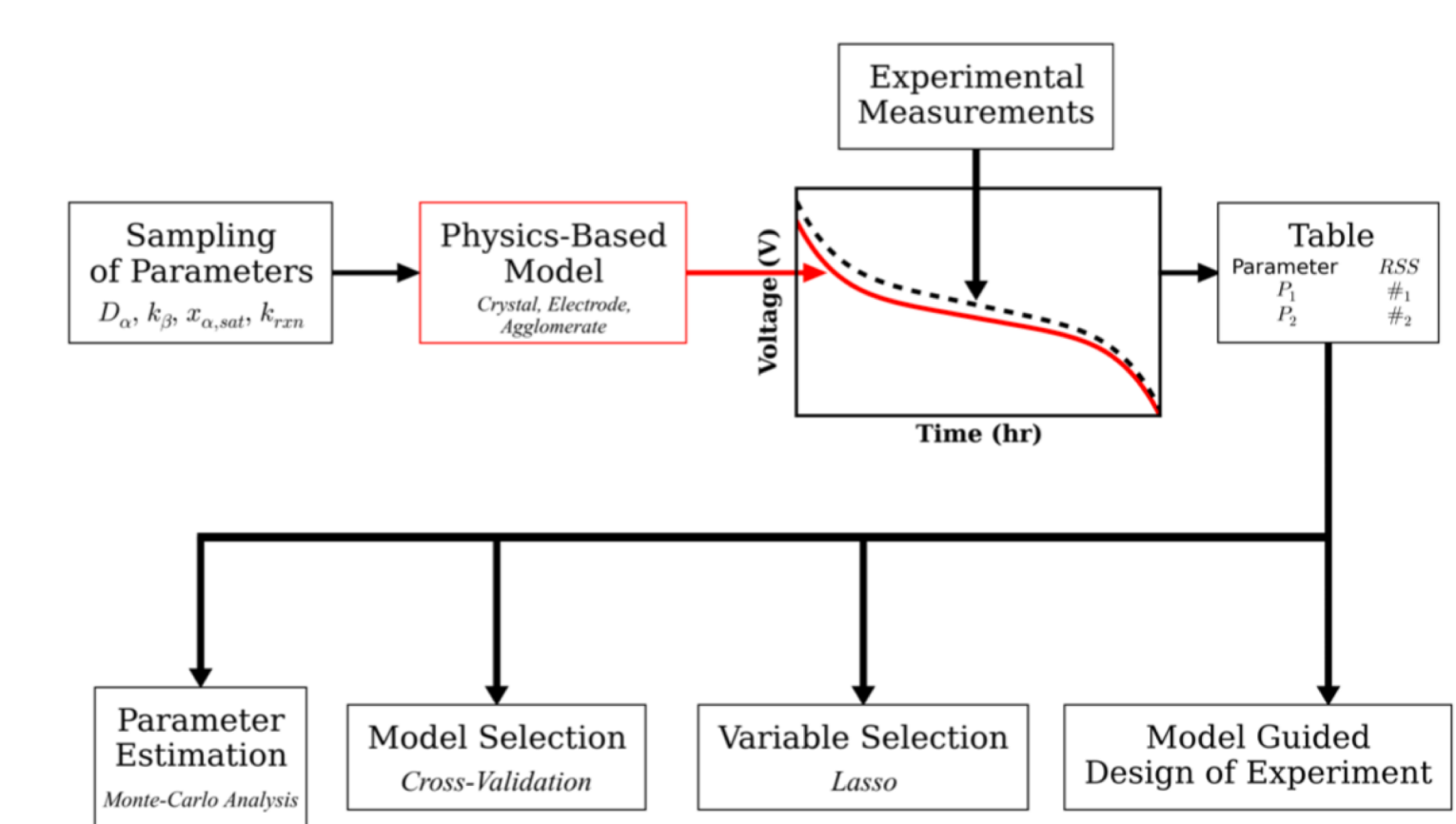
### Understanding Limiting Processes



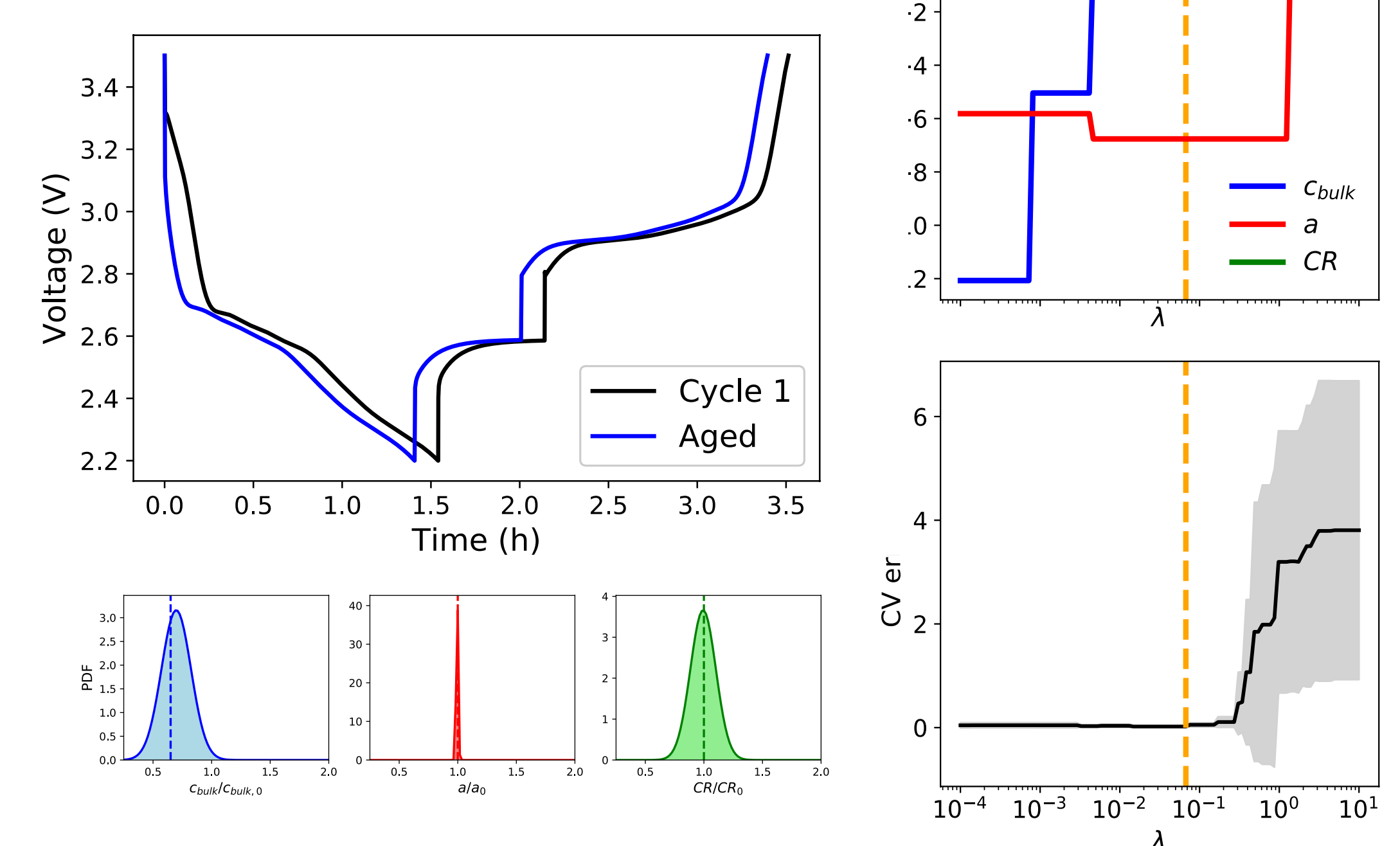
### Building Physical Models



### Algorithmic Model Development



### Modeling Cathode Aging



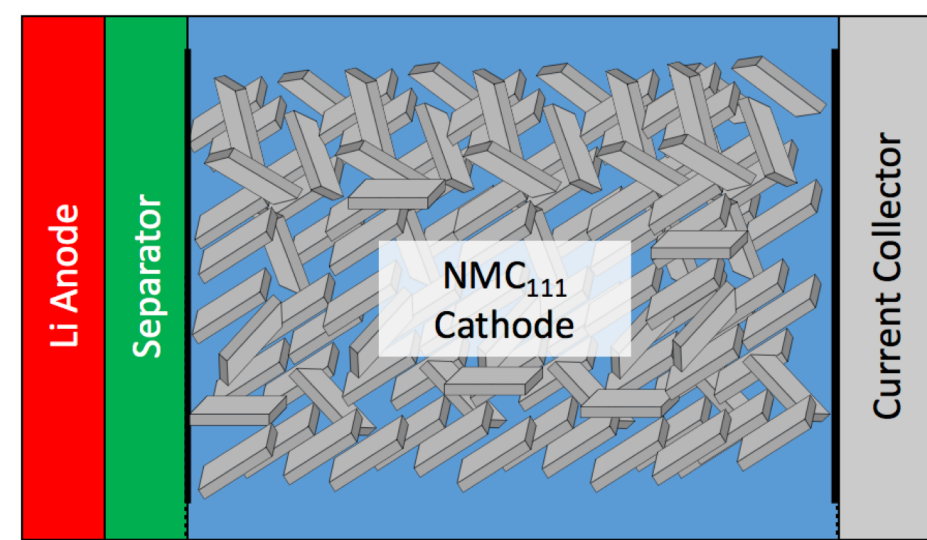
## Simulation for State-of-art Battery

## Characterization of Membranes

### Experimental Set-up

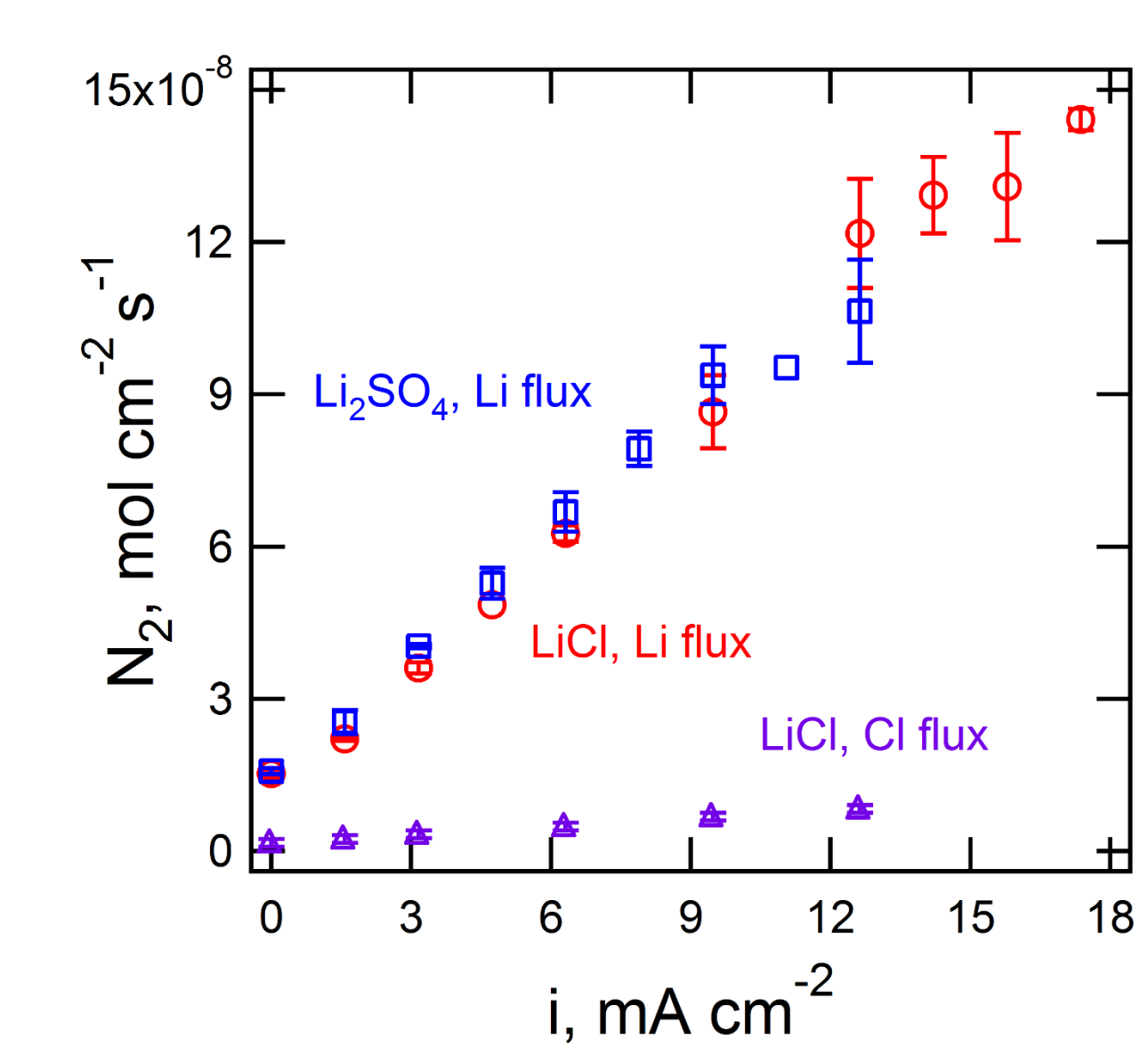
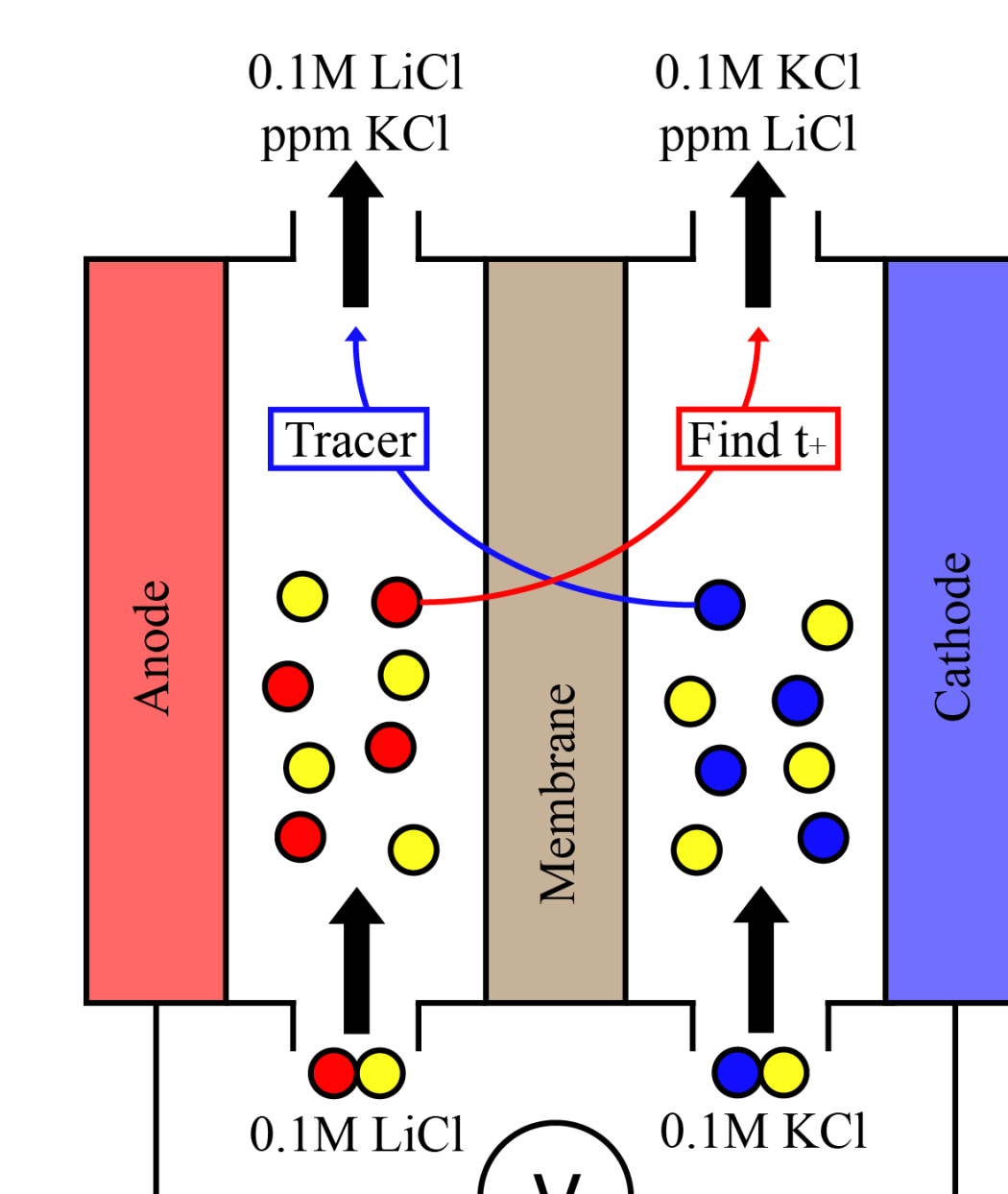
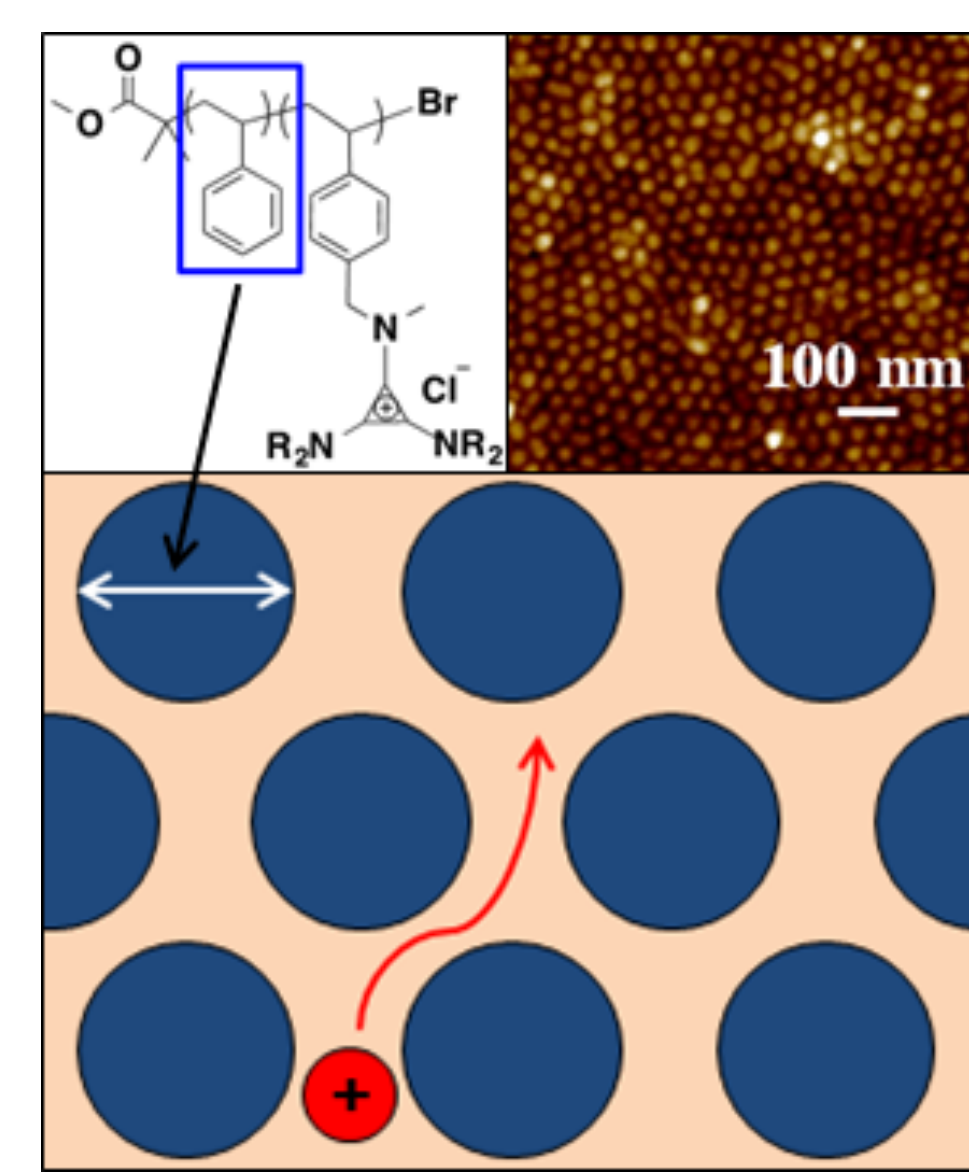
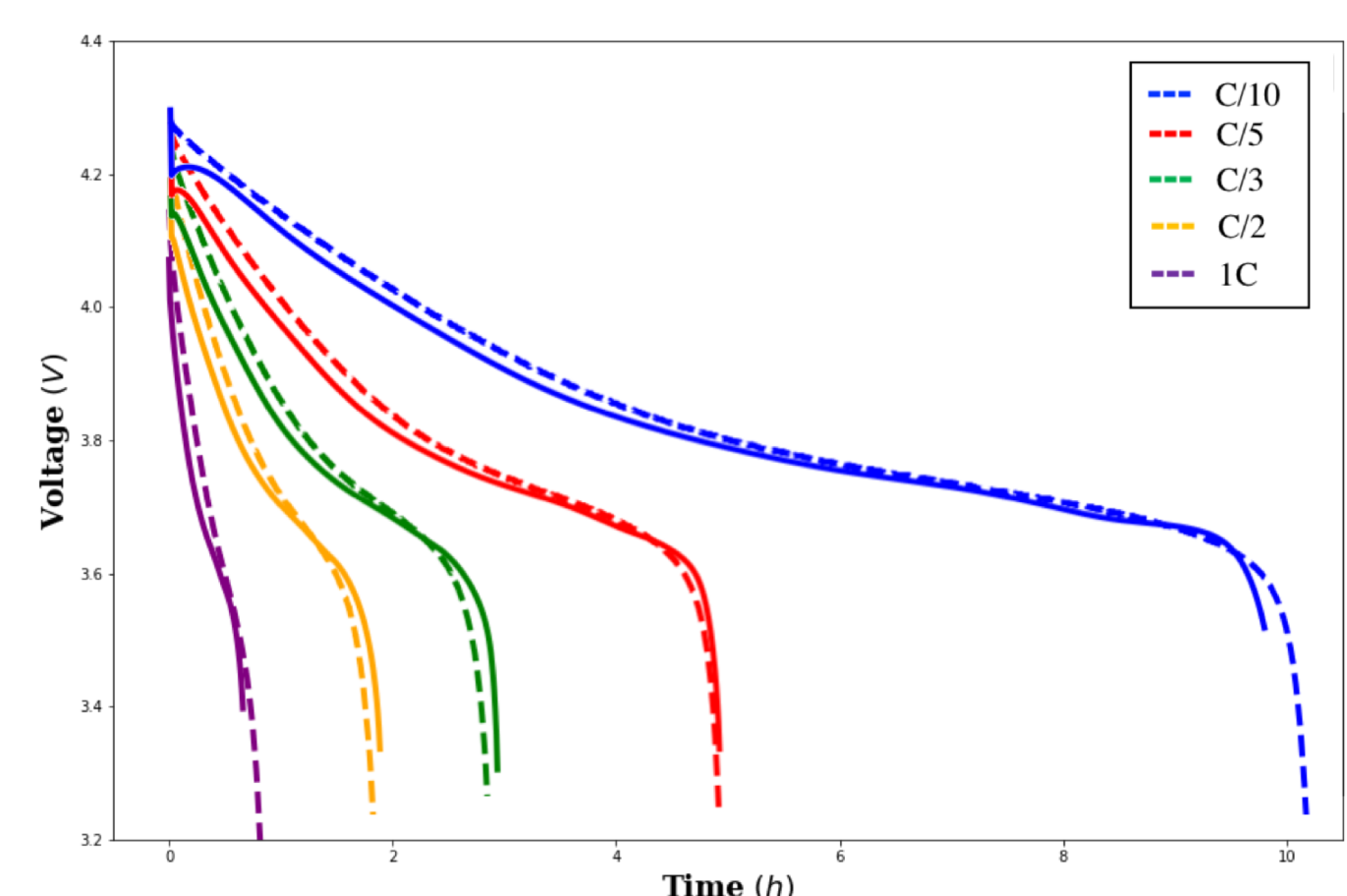


### Model Configuration

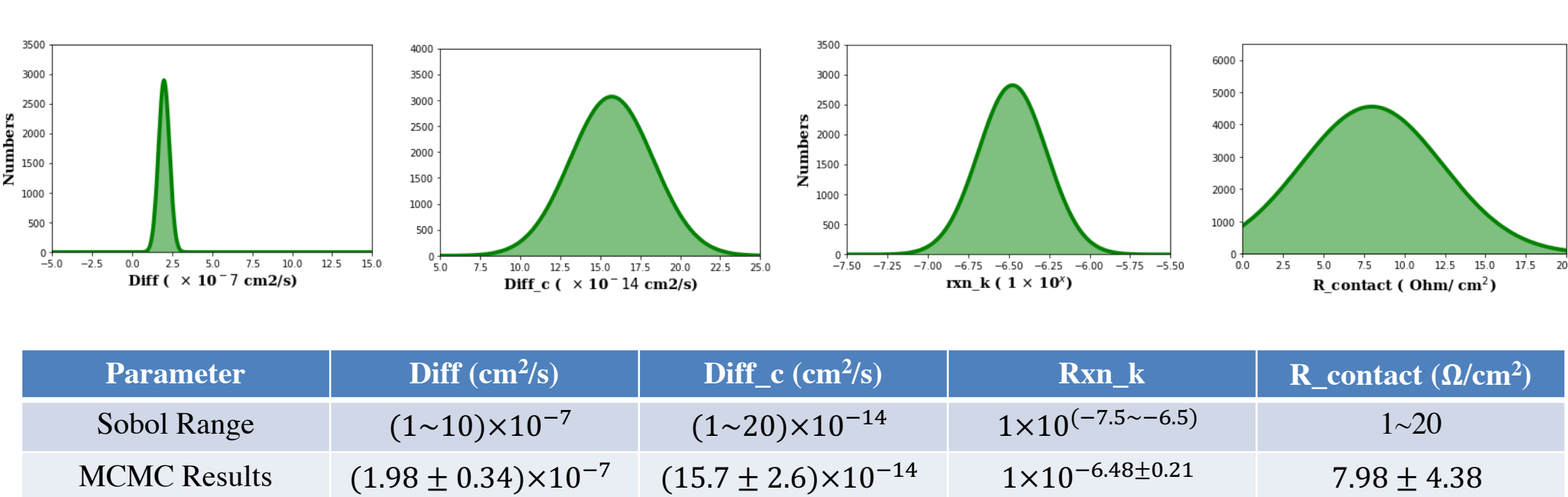


$$\begin{aligned}
 & \text{Li Anode: } \begin{cases} 1. \frac{\partial C_s}{\partial t} = -F N_s \\ 2. \nabla^2 \phi_s = 0 \\ 3. \nabla^2 \psi_s = 0 \\ 4. \frac{\partial C_s}{\partial t} = 0 \end{cases} \\
 & \text{Separator: } \begin{cases} 1. N_{s,e} = N_{s,w} \\ 2. i_{s,e} = i_{s,w} \\ 3. i_{s,e} = i_{s,w} \\ 4. (1-\epsilon) \frac{\partial C_s}{\partial t} = -\frac{a i_{rxn}}{F} \end{cases} \\
 & \text{Cathode: } \begin{cases} 1. N_s = 0 \\ 2. i_s = i_{applied} \\ 3. i_s = 0 \\ 4. (1-\epsilon) \frac{\partial C_s}{\partial t} = -\frac{a i_{rxn}}{F} \end{cases}
 \end{aligned}$$

### Simulation Result Compared with Experiment Data



### Parameter Estimation Using Data Science Technique



Parameter	Diff ( $cm^2/s$ )	Diff_c ( $cm^2/s$ )	Rxn_k	R_contact ( $\Omega/cm^2$ )
Sobol Range	$(1\sim 10)\times 10^{-7}$	$(1\sim 20)\times 10^{-14}$	$1\times 10^{(-7.5\sim -6.5)}$	1~20
MCMC Results	$(1.98 \pm 0.34)\times 10^{-7}$	$(15.7 \pm 2.6)\times 10^{-14}$	$1\times 10^{-6.48 \pm 0.21}$	$7.98 \pm 4.38$

