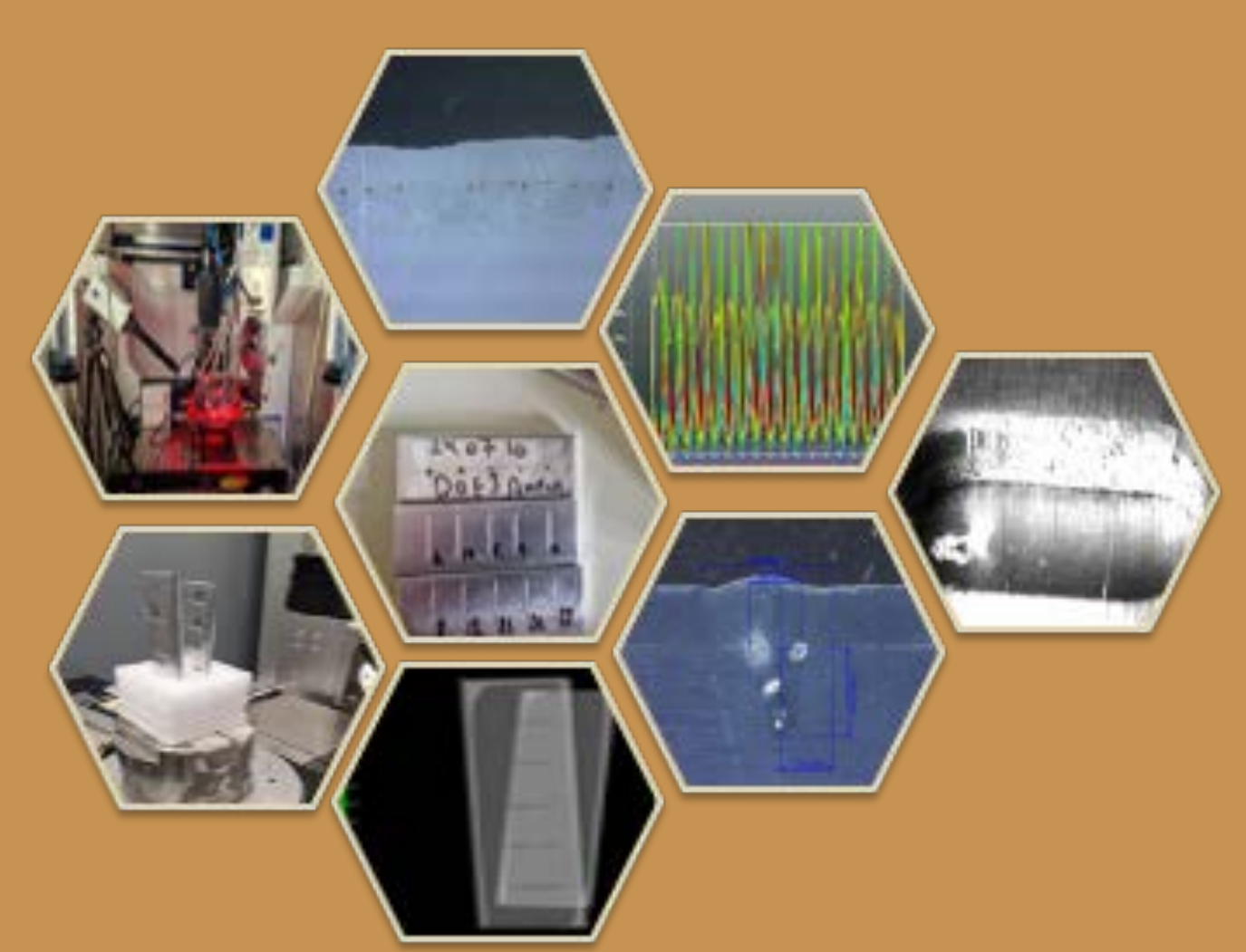# LaserBATMAN

Multi-scale simulation of laser welding for optimal battery pack manufacturing

Operational efficiency

- Operating closer to limits
- Higher returns on batteries
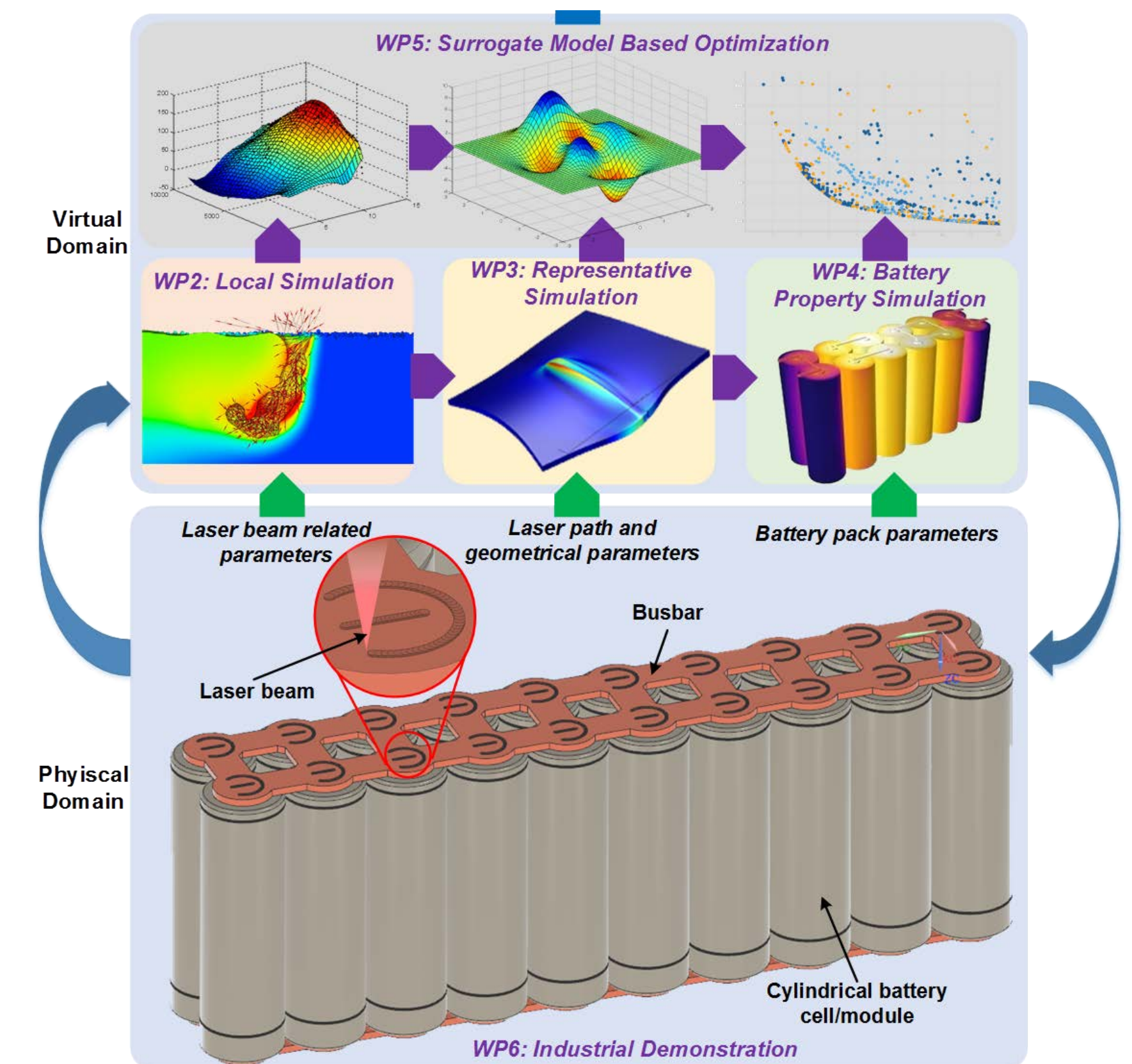- Minimizing overcapacity

Safe operating condition

- Predicting failure rates
- Predicting capacity loss over time
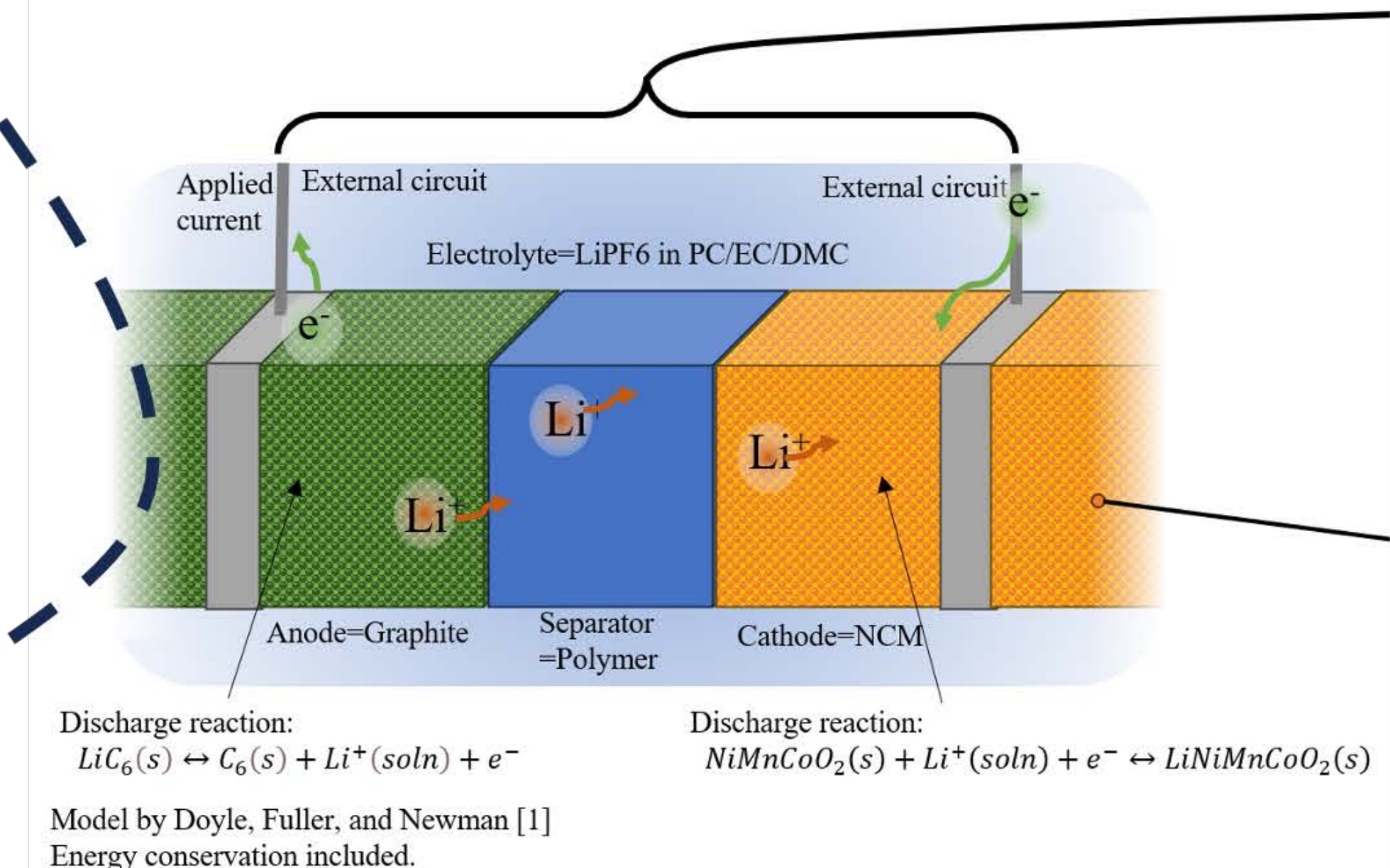- Calculating running temperatures to keep clear of thermal runaway
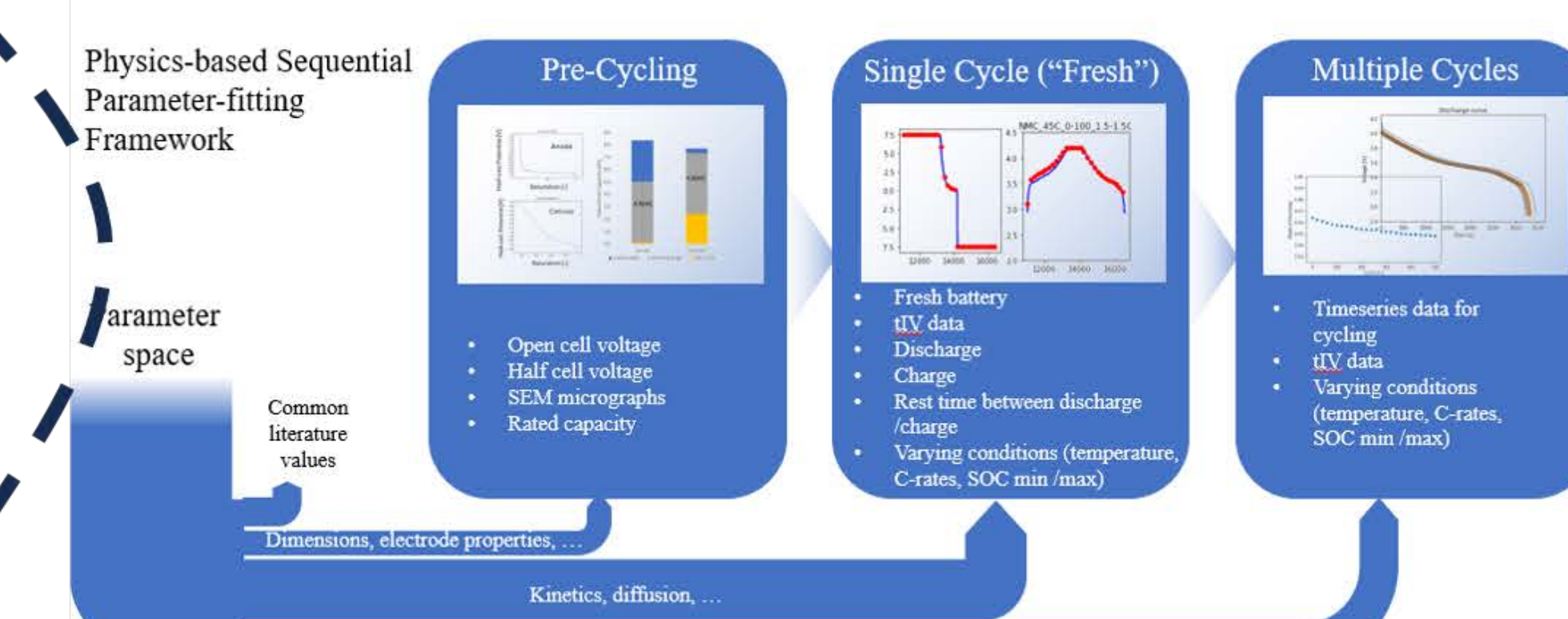

Longer lifetime

- Optimizing performance for longer battery lifetime
- Keeps the batteries in the electric cars / battery parks longer, and out of the landfill
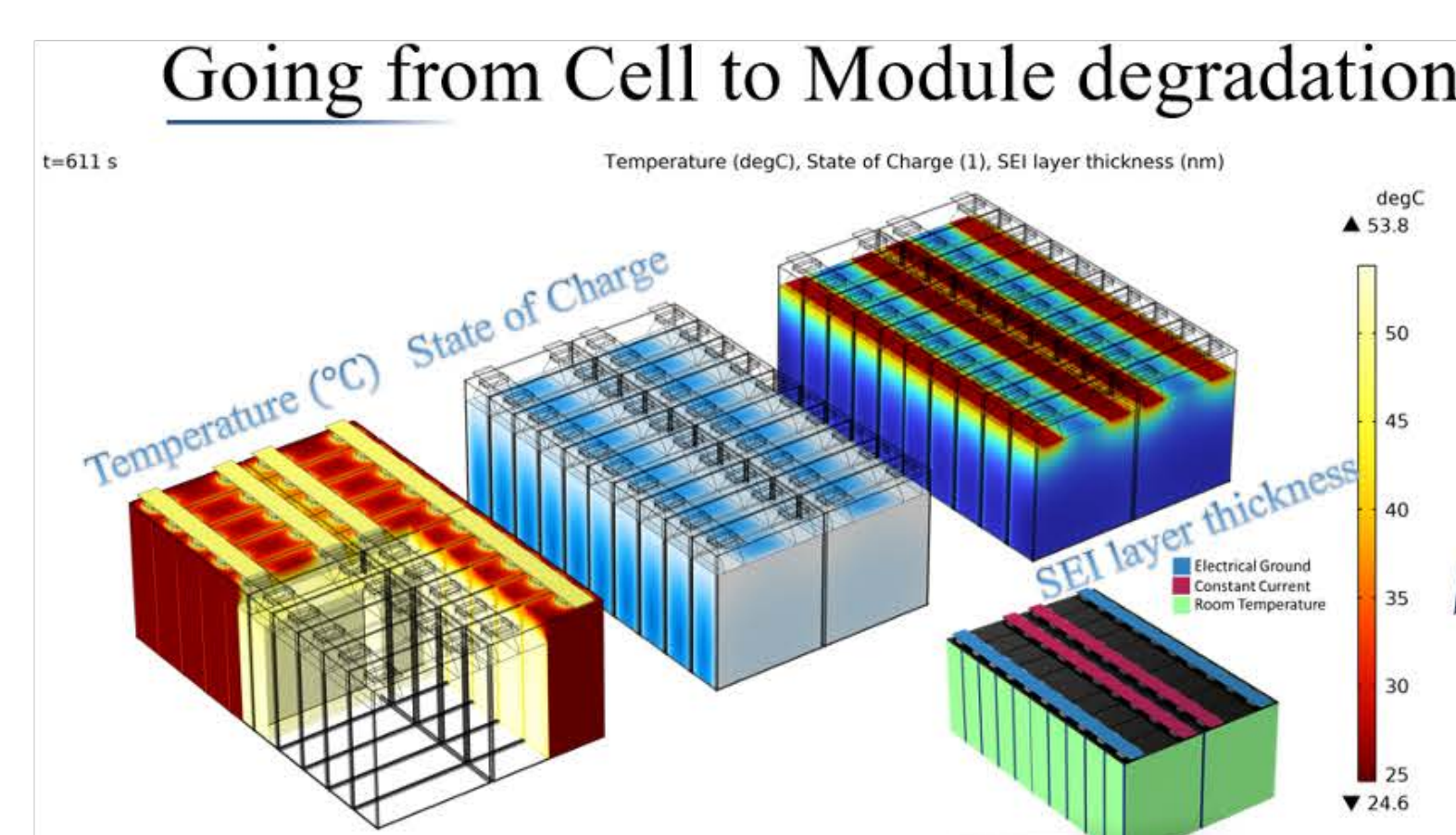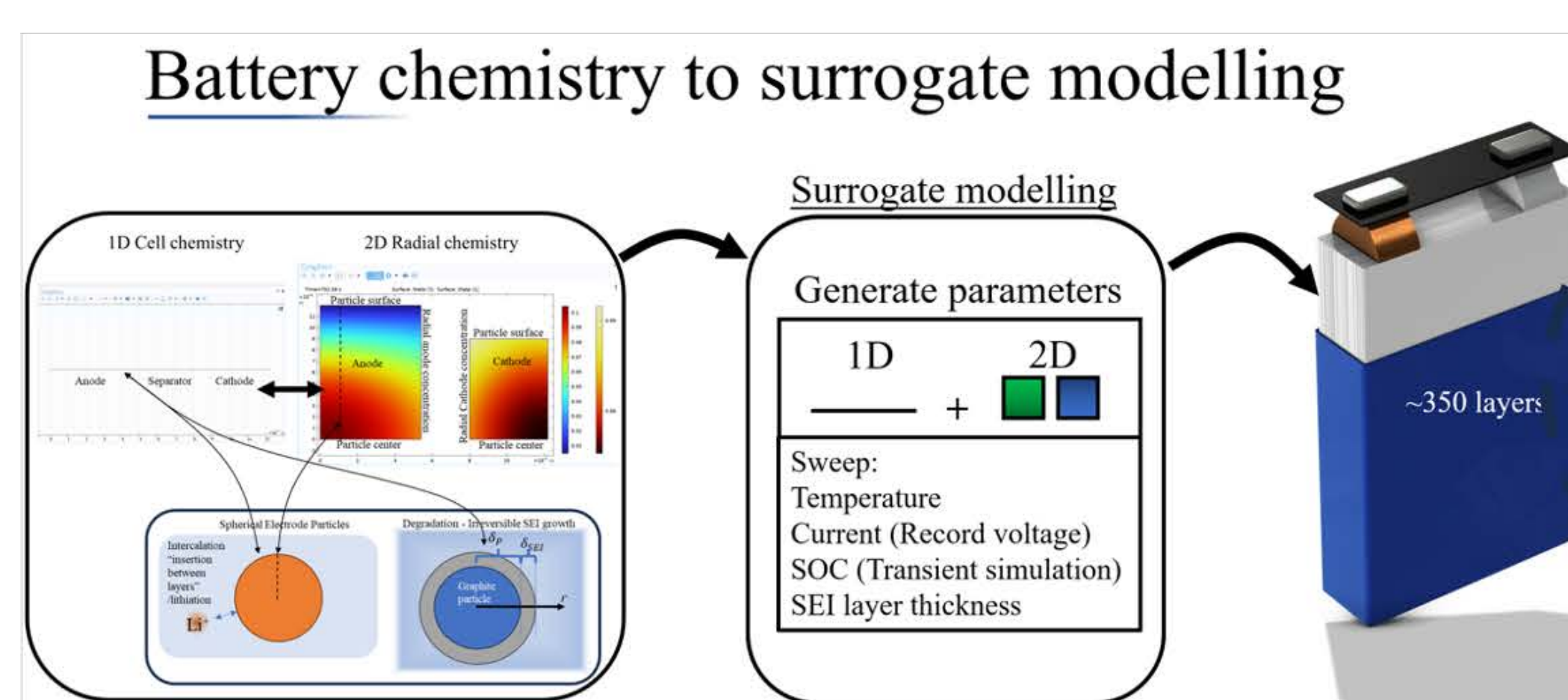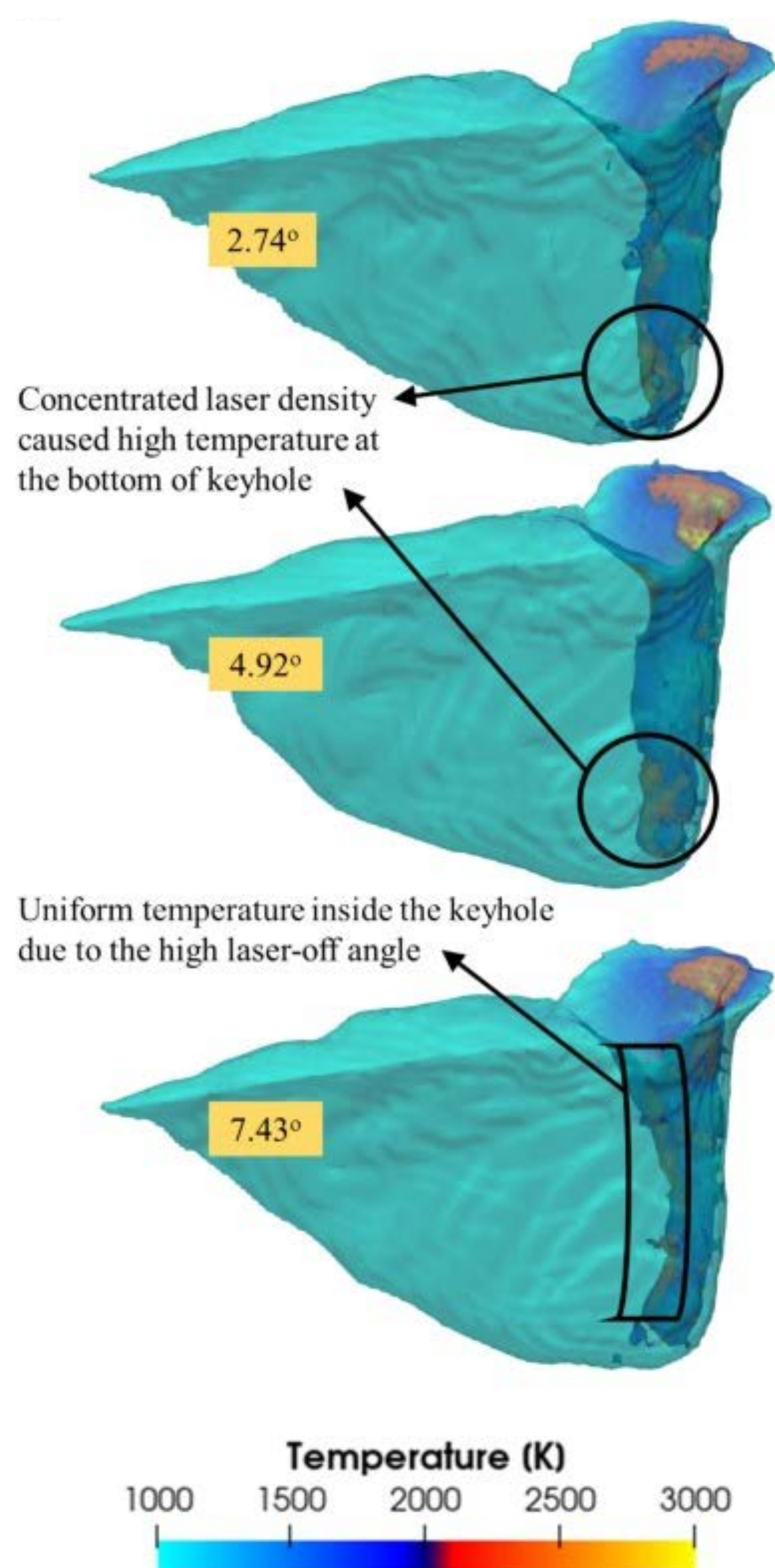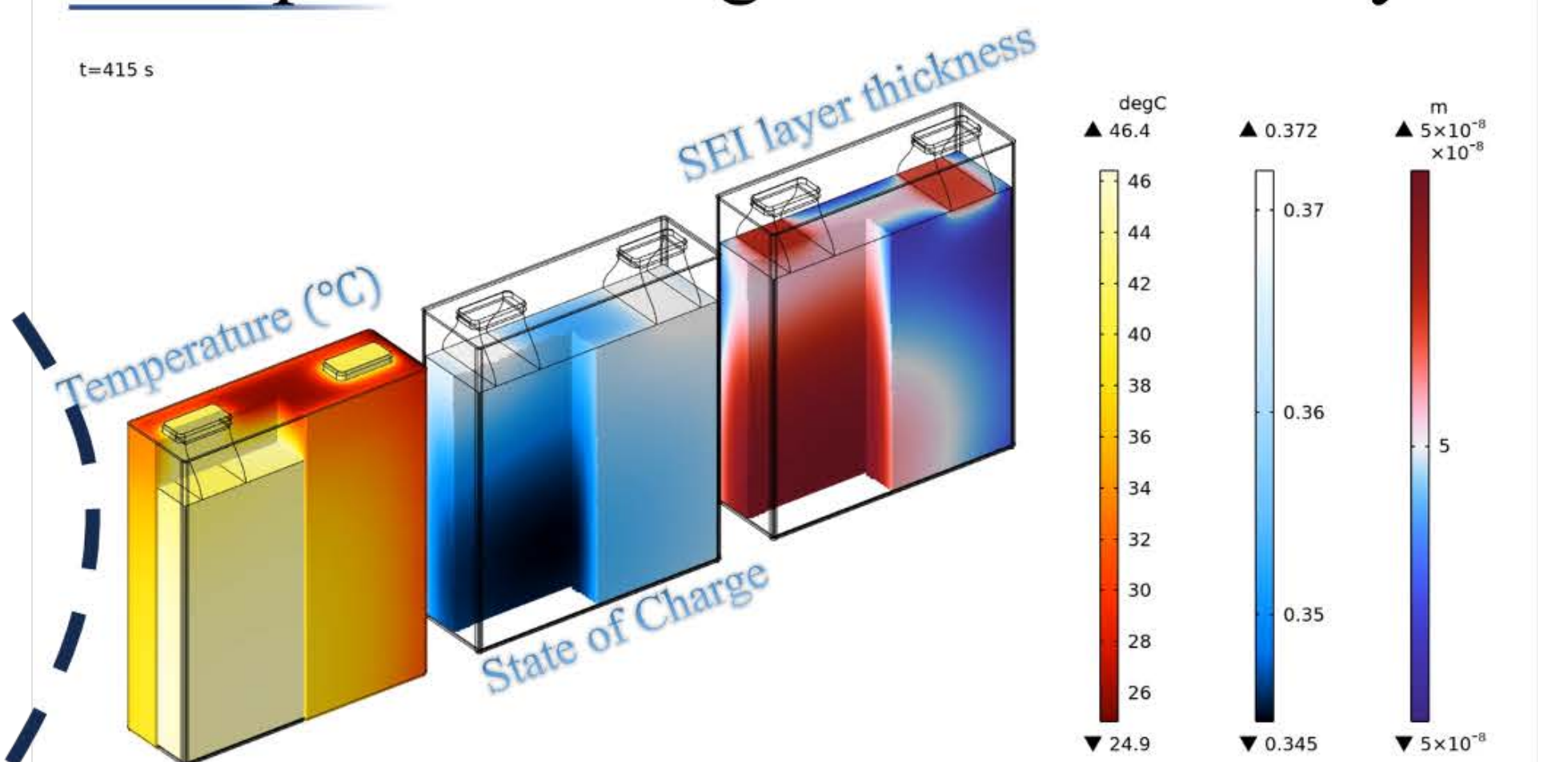

WP5: Surrogate Model Based Optimization

Virtual Domain

WP2: Local Simulation | WP3: Representative Simulation | WP4: Battery Property Simulation

Laser beam related parameters | Laser path and geometrical parameters | Battery pack parameters

Laser beam | Busbar | Cylindrical battery cell/module

Phyiscal Domain

WP6: Industrial Demonstration

Concentrated laser density caused high temperature at the bottom of keyhole

2.74°

4.92°

Uniform temperature inside the keyhole due to the high laser-off angle

7.43°

Temperature (K)

1000   1500   2000   2500   3000

Battery chemistry

Applied current — External circuit — External circuit

Electrolyte=LiPF6 in PC/EC/DMC

Anode=Graphite | Separator ~Polymer | Cathode=NCM

Discharge reaction:
$LiC_6(s) \leftrightarrow C_6(s) + Li^+(soln) + e^-$

Discharge reaction:
$NiMnCoO_2(s) + Li^+(soln) + e^- \leftrightarrow LiNiMnCoO_2(s)$

Model by Doyle, Fuller, and Newman [1]
Energy conservation included.

Battery Degradation – SEI Layer

Solvent (EC)

Anode particle

Solvent diffusion through SEI layer

$$\frac{\partial c_{EC,P}}{\partial t} = \frac{\partial}{\partial r}\left[\varepsilon D_{EC}\frac{\partial c_{EC,P}}{\partial r}\right] - \frac{d\delta_{SEI}}{dt}\frac{\partial c_{EC,P}}{\partial r}$$

$$\frac{d\delta_{SEI}}{dt} = \frac{i_s}{2F}\frac{M_{SEI}}{\rho_{SEI}}$$

Reaction on particle surface

SEI Layer formation $2EC + 2e^- + 2Li^+$

$$i_s = -Fk_f c_{EC} \exp\left[-\frac{\beta F}{RT}\left(\phi_{S,n} - \frac{\delta}{\kappa_{SEI}}i_{tot}\right)\right]$$

Model Summary

√ LLI
√ T, I, SOC
% LAM
% Li+ transport resistance
% Anode porosity

Intercalation $LiC_6(s) \leftrightarrow C_6(s) + Li^+(s$

$$i_{int} = i_{int,0} \cdot 2\sinh\left[\frac{0.5F}{RT}\left(\phi_{S,n} - \phi_{E,n} - U_{0,n}\right)\right]$$

Total $i_{tot} = i_s + i_{int}$

Mass balance in particle surface:

Lithium: $\left(-D_{eff,s}r^2\frac{\partial c_{S,p}}{\partial r}\right)|_{r=R_{P,n}} = \delta_{P,n}^2 \frac{i_{int,n}}{F}$

Solvent: $\left(-D_{EC}\frac{\mu_{EC}}{\partial r} + c_{EC}\right)|_{r=\delta_{P,n}} = i_s/F$

Battery chemistry Parameter Setup

Physics-based Sequential Parameter-fitting Framework

Parameter space

Pre-Cycling | Single Cycle ("Fresh") | Multiple Cycles

Common literature values

Dimensions, electrode properties,   Kinetics, diffusion, ...

Battery chemistry to surrogate modelling

1D Cell chemistry | 2D Radial chemistry

Surrogate modelling

Generate parameters

1D + 2D

~350 layers

Sweep:
Temperature
Current (Record voltage)
SOC (Transient simulation)
SEI layer thickness

Example of the degradation of one cycle

t=415 s

Temperature (°C)

SEI layer thickness

State of Charge

Going from Cell to Module degradation

t=611 s

Temperature (degC), State of Charge (1), SEI layer thickness (nm)

Temperature (°C)

State of Charge

SEI layer thickness