Imperial College London

Optimising li-ion cell design for plug-in hybrid and battery electric vehicles

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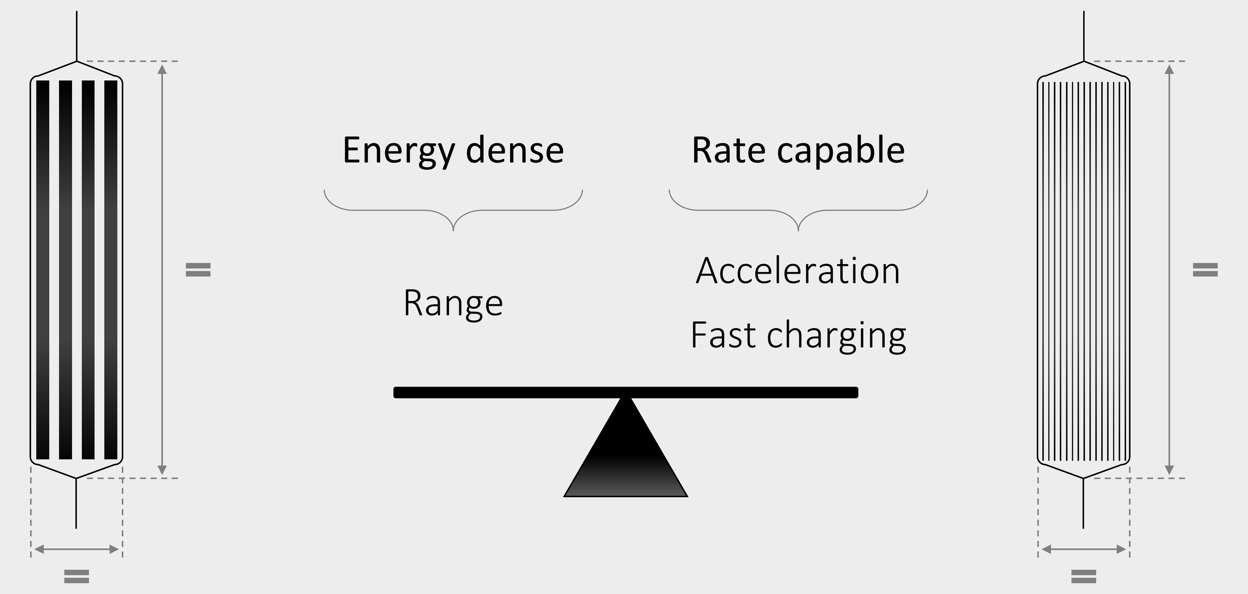

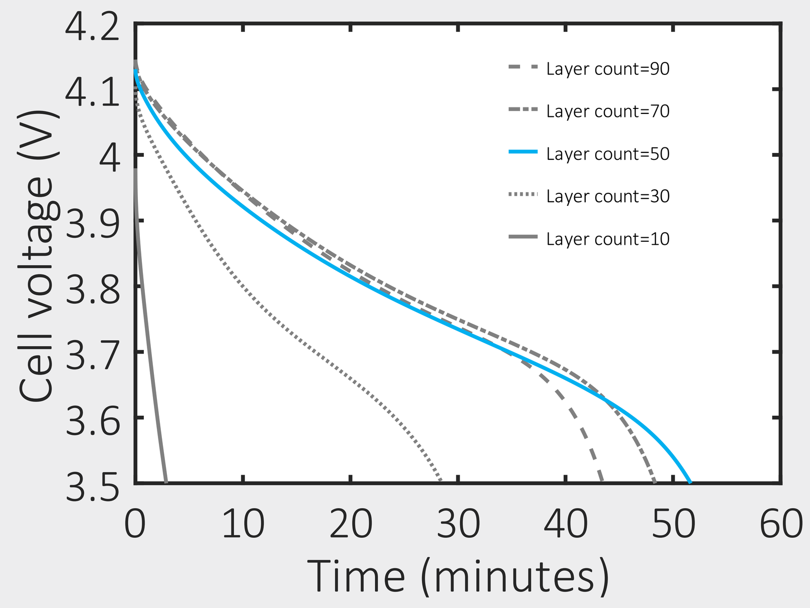

ENERGY & POWER BALANCE

- Conflicting requirements pose a layer optimisation problem
- Desire trading of energy & power in equally-dimensioned cells
- Layer reconfiguration trades fraction of active material mass with surface area available for redox reaction
- Maximum usable energy is available for neither the most rate capable nor most energy density layer configuration
- Empirical determination of optimal layer count is slow, costly & may not provide energy-density maximising result
- **We propose a rapid & inexpensive model-based alternative**

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LAYER OPTIMISATION

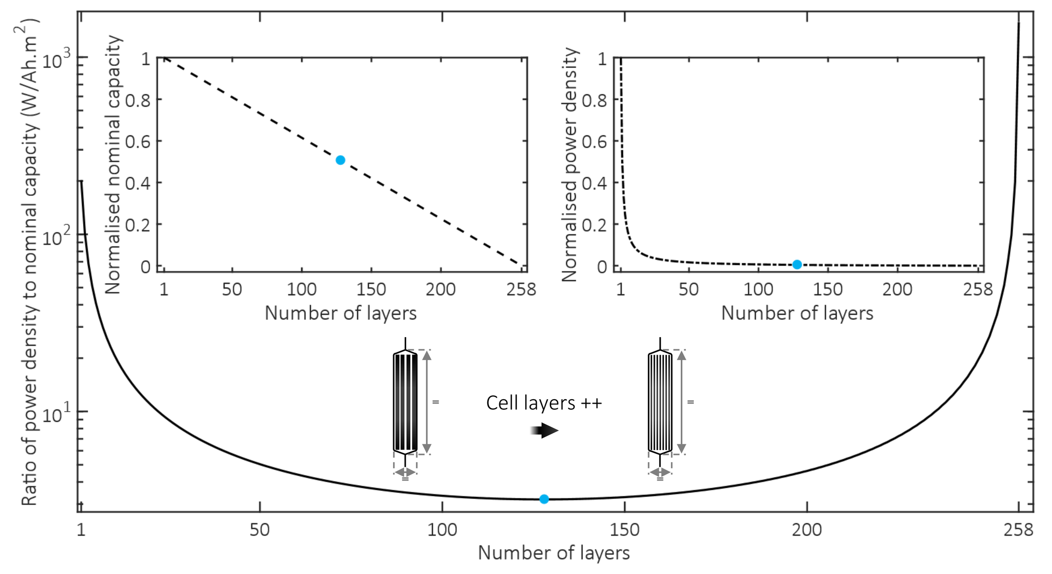
- Stack thickness & active & inactive material quantities are recalculated for each new layer count (n) using derived expressions
- The optimal (i.e. range-maximising) layer configuration is the minimum number of layers that meets EV acceleration and fast charging targets
- Initially, we gain a lot of rate capability for little energy density loss since power density per layer decreases faster than cell nominal capacity
- At higher layer counts it becomes increasingly expensive, in terms of energy density sacrificed, to accommodate higher powers
- **Efficient designs employ < half the maximum possible number of layers**

$$L_{stack} = \sum_j L_j(n) + L_{Al}(n) + L_{Cu}(n) \quad \ldots\forall\, n \in \mathbb{N},\ j \in \{pos, sep, neg\}$$

$$L_j(n) = nl_j$$

$$L_{Al}(n) = \begin{cases} \left(\frac{n}{2}\right) l_{Al}, & \text{if } n \text{ is even} \\ \left(\frac{n+1}{2}\right) l_{Al}, & \text{if } n \text{ is odd} \end{cases}$$

$$L_{Cu}(n) = \begin{cases} \left(\frac{n+2}{2}\right) l_{Cu}, & \text{if } n \text{ is even} \\ \left(\frac{n+1}{2}\right) l_{Cu}, & \text{if } n \text{ is odd} \end{cases}$$



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1 Define vehicle

xEV platform	PHEV
Powertrain	(series)
Module & cell configuration	8S1P (mod.) 12S1P (cells)
xEV mass (w/o cells)	1,654 kg (inc. ICE)
Fast charge SOC range	30 - 80 %

2 Define criteria

Fast charging	*Acceleration*
$T(t) < T_{max}$	$T(t_f) < T_{max}$
$V(t) < V_{max}$	$V(t_f) > V_{min}$
$z(t) \geq z^*$	$z(t_f) > z_{min}$
$C_s^*(t) < C_{s_{sat}}$	
$t < t_{max}$	

$$l_{ce} = \frac{L_{stack} - [0.5(n+1)]l_{cu} - [0.5n]l_{al}}{n} - l_{sep}$$

$$l_{ratio} = \frac{l_{neg}}{l_{pos}} = \frac{\varepsilon_{pos}}{\varepsilon_{neg}}$$

$$l_{neg} = l_{ce} - l_{pos}$$

$$l_{pos} = \frac{l_{ce}}{l_{ratio} + 1}$$

Li-PLATING PROTECTED FAST CHARGE

- Specify desired xEV configuration & define performance criteria
- Cells undergo simulated vehicle acceleration & fast charging
- Charge time is minimised with a constant power strategy
- **Design for highest powers & impose Li concentration limit, $C_{s_{sat}}$**
- **Cell designs exhibit Li-plating protection & max. energy density**
- Individual domain thicknesses are recomputed using stack thickness & a fixed, capacity-balanced, electrode thickness ratio

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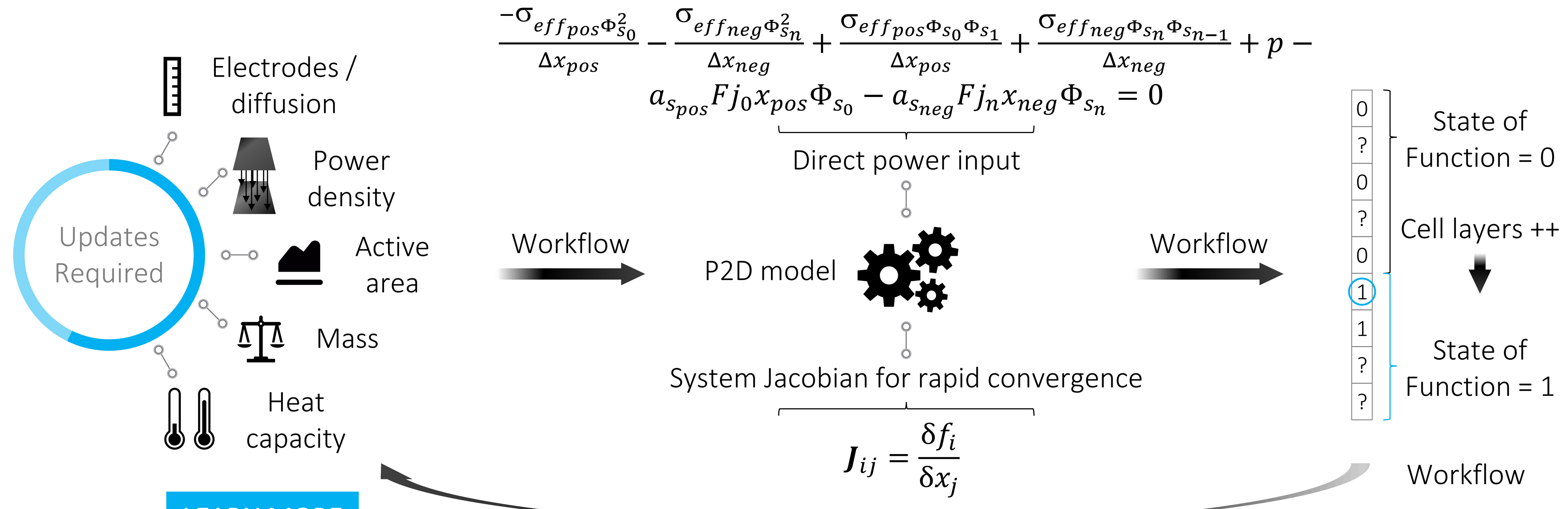
P2D SIMULATION

- Custom, efficient **binary search screens layer configurations**
- Open-source electrochemical **P2D model directly accepts power input**, solves for current & converges rapidly owing to Jacobian generated using algorithmic differentiation
- Each new layer configuration requires model updates
- Vector of layer State-of-Functions is produced; lowest layer count with a unity SoF is the optimal



$$\frac{-\sigma_{eff\,pos}\Phi_{s_0}^2}{\Delta x_{pos}} - \frac{\sigma_{eff\,neg}\Phi_{s_n}^2}{\Delta x_{neg}} + \frac{\sigma_{eff\,pos}\Phi_{s_0}\Phi_{s_1}}{\Delta x_{pos}} + \frac{\sigma_{eff\,neg}\Phi_{s_n}\Phi_{s_{n-1}}}{\Delta x_{neg}} + p - a_{s_{pos}} F j_0 x_{pos} \Phi_{s_0} - a_{s_{neg}} F j_n x_{neg} \Phi_{s_n} = 0$$

$$J_{ij} = \frac{\delta f_i}{\delta x_j}$$

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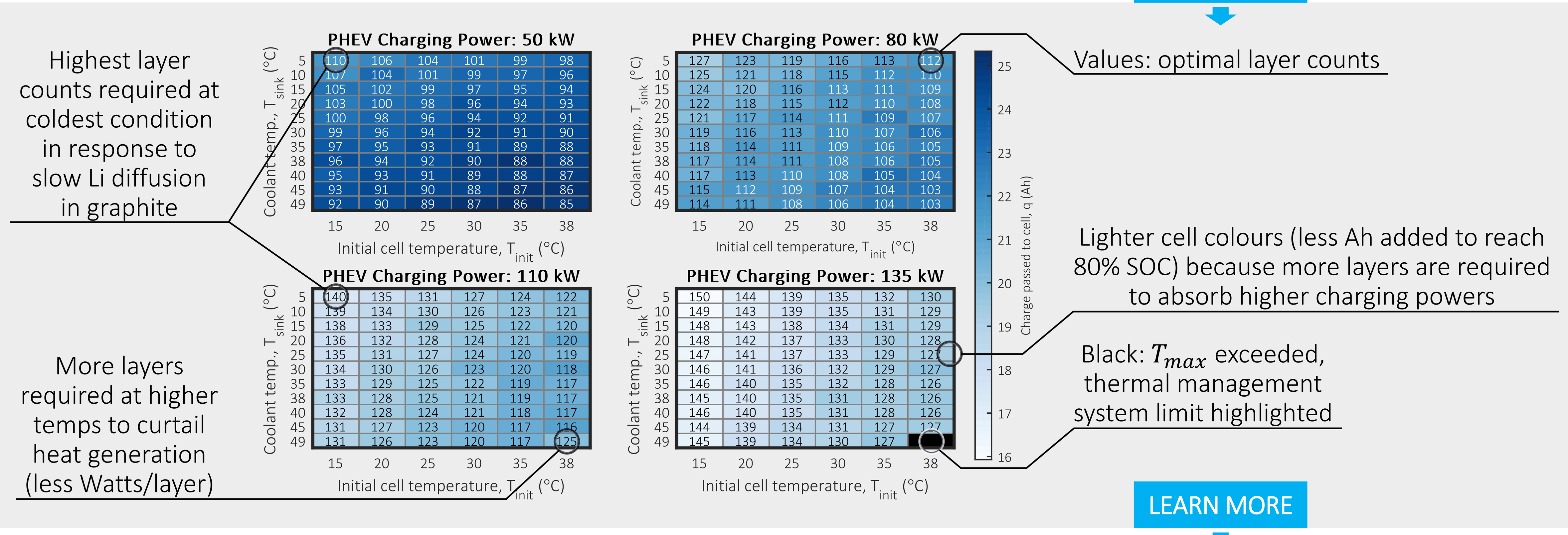

TAILORED CELL DESIGN MAPS

- Repeat for new coolant (ambient) & cell temperatures to generate cell design maps precisely tailored to vehicle fast charge targets
- Values in coloured cells are optimal layer configurations/counts
- Map colour is usable capacity; charge added, 30 – 80 % SOC window
- Black colours indicate unsuitable cell materials & thermal management system for specified temperatures & design targets
- Faster & lower cost than iterative, empirical cell development
- **Method can offer xEV range extension over empirical cell designs by producing energy-density optimised layer configurations**

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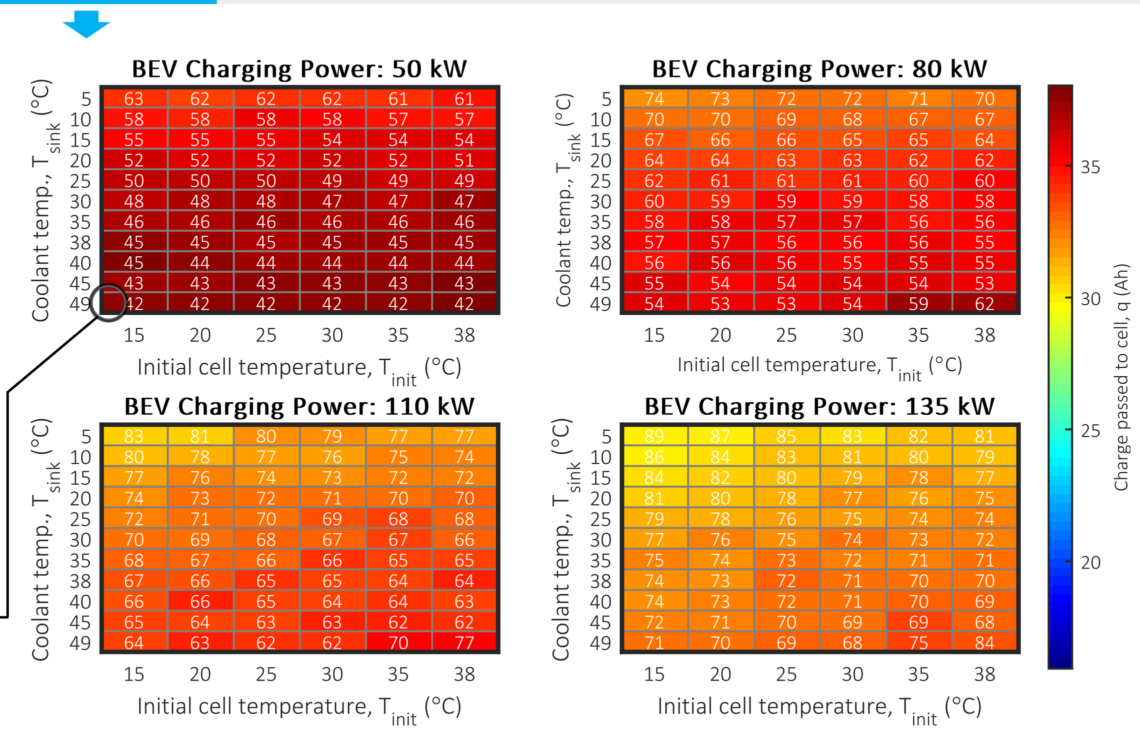
COMMON MODULE DESIGN FOR EV PACKS

- New layer configurations generated for a different vehicle platform, **using a cell with identical external dimensions**
- Produces energy-density maximising designs for this new vehicle.. ..and **enables common battery pack module design across both/many platforms, lowering R&D costs & time to market for automotive OEMs**

Cell colour: 8S3P BEV pack layout provides more nominal capacity, lowering the E-rate during charge.

With less power-per-cell-layer, we need fewer layers & can design more energy dense cells vs. PHEV configuration



1 Define another vehicle

xEV platform	BEV
Powertrain	(all-electric)
Module & cell configuration	8S3P (mod.) 12S1P (cells)
xEV mass (w/o cells)	1,687 kg
Fast charge SOC range	20 - 80 %

See the paper: Ian D. Campbell, Krishnakumar Gopalakrishnan, Monica Marinescu, Marcello Torchio, Gregory J. Offer, Davide Raimondo. *Optimising lithium-ion cell design for plug-in hybrid and battery electric vehicles* Journal of Energy Storage 22 (2019), pp. 228–238. DOI: https://doi.org/10.1016/j.est.2019.01.006.