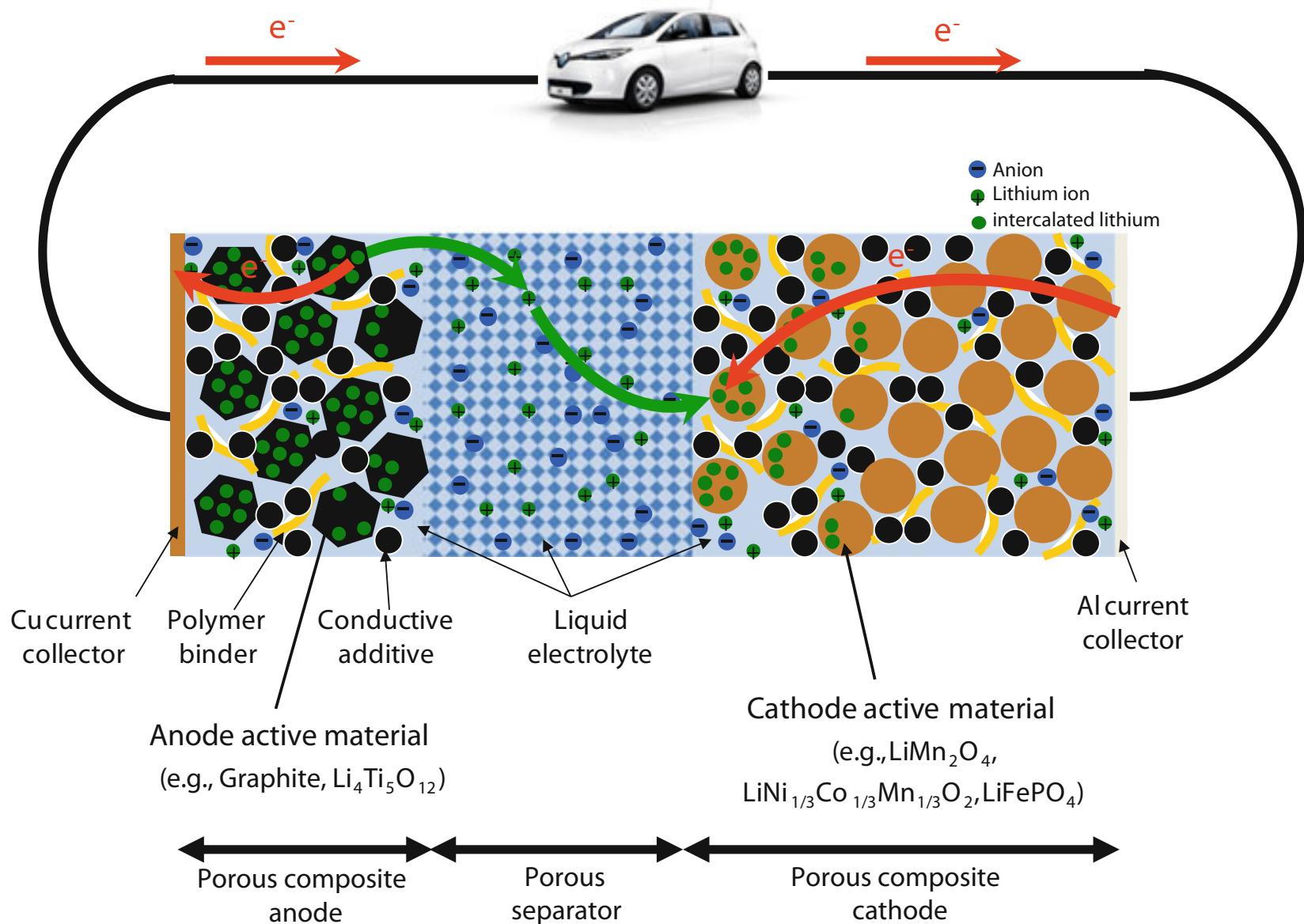


EAGER Kickoff Meeting: LIB Modeling Thrust

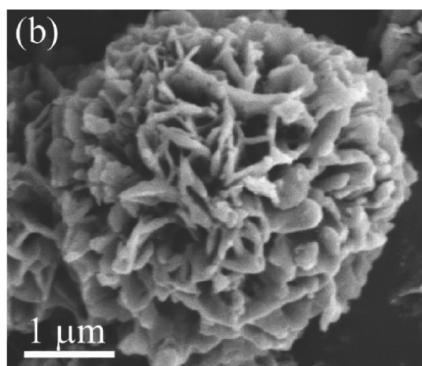
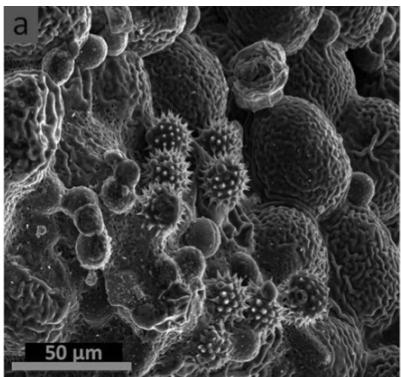
Abhas Deva, Luke Robinson, Alfonso Campos, and R. Edwin García
School of Materials Engineering
Purdue University



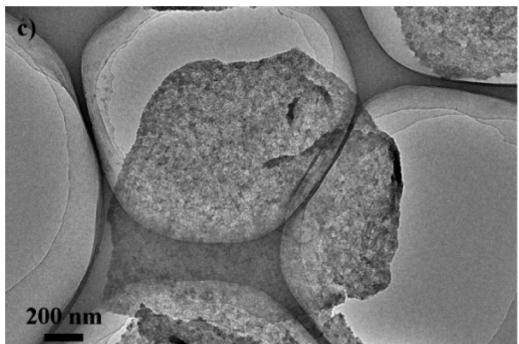
Introduction



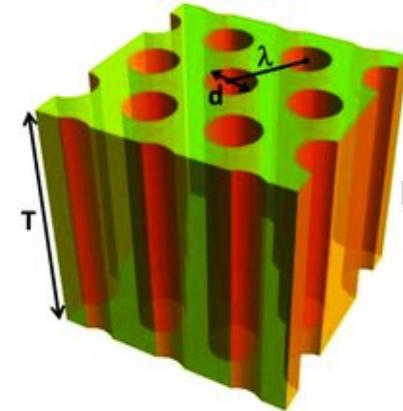
Current Strategies for Battery Design



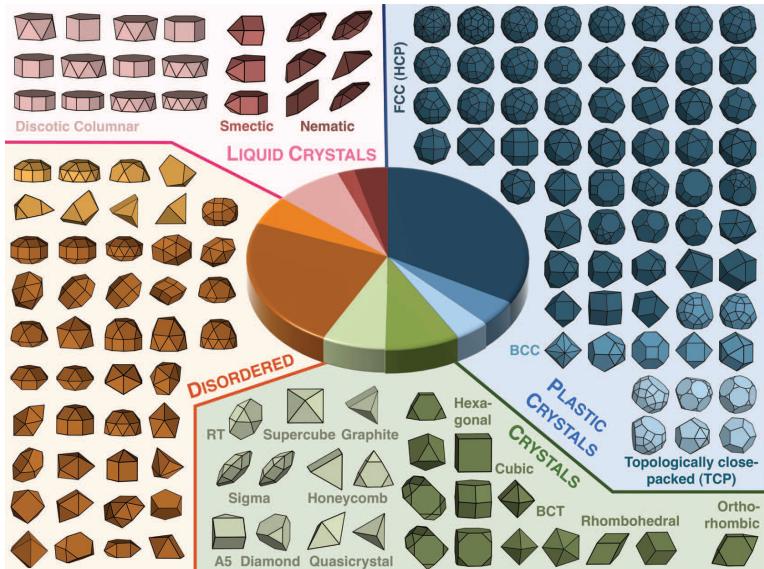
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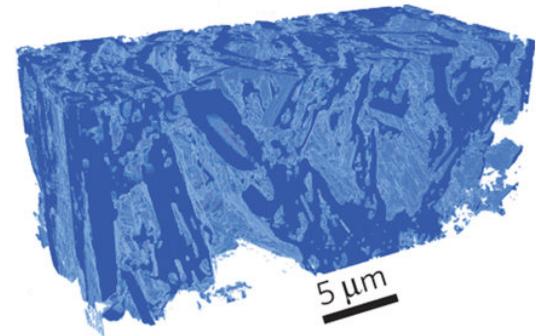
W. Li, D. Zhao et al. "General strategy to synthesize uniform mesoporous TiO₂/graphene/mesoporous TiO₂ sandwich-like nanosheets for highly reversible lithium storage." *Nano Letters* 15.3 (2015): 2186-2193.



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Battery Microstructure Descriptors

Porosity

$$\epsilon = 1 - \Omega_p$$

Tortuosity

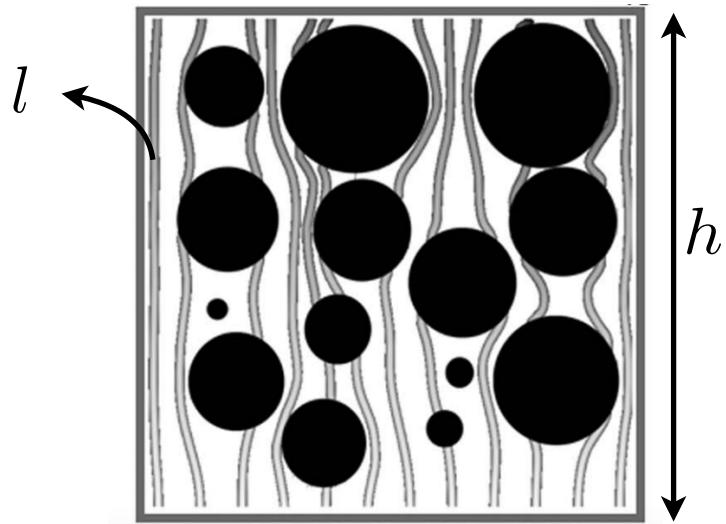
$$\tau = \frac{1}{\epsilon^\alpha}$$

Geometrical Interpretation

$$\tau = \frac{\langle l \rangle}{h}$$

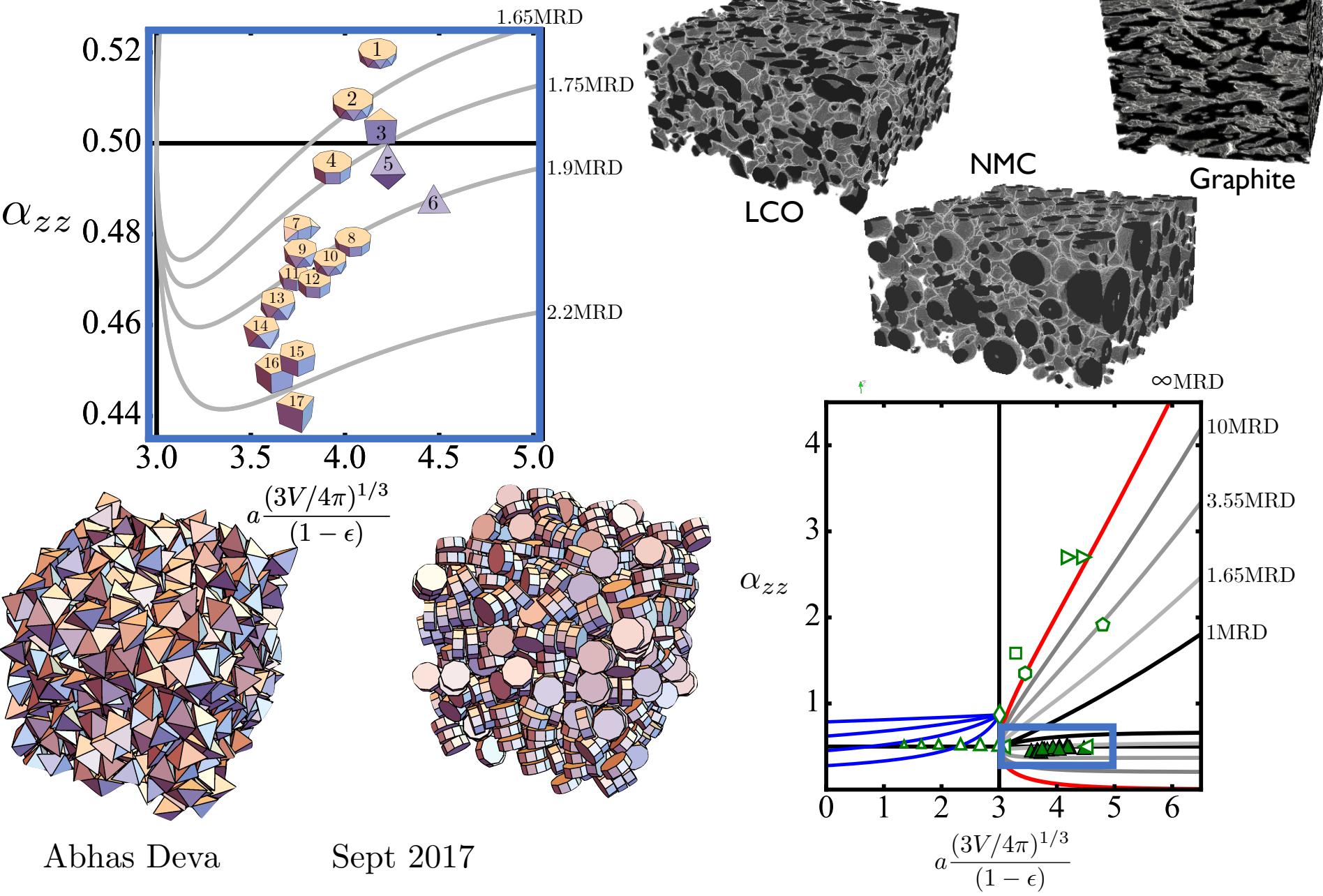
Reactive Area Density

$$a = \frac{3}{r}(1 - \epsilon)$$

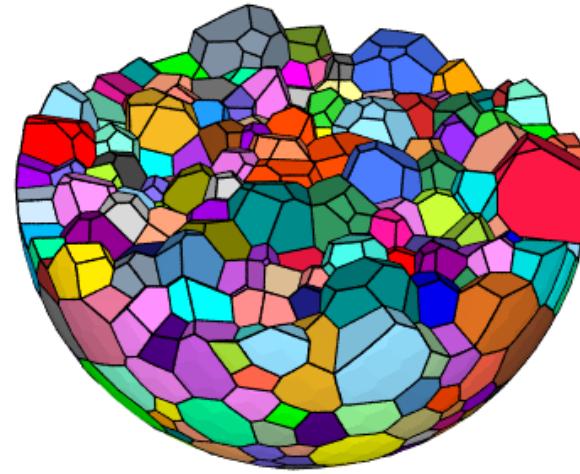
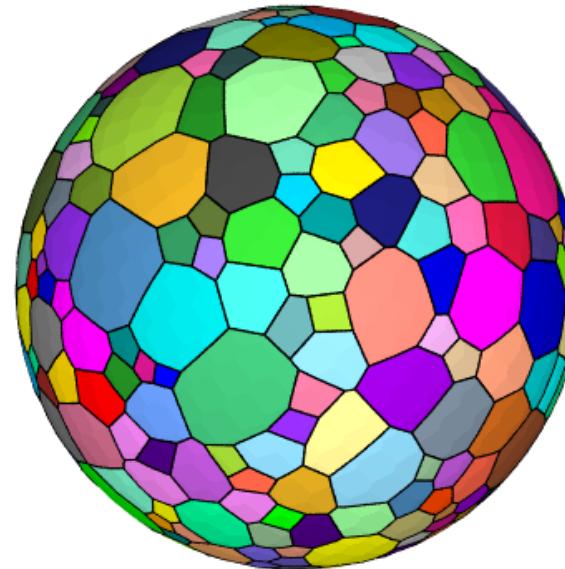
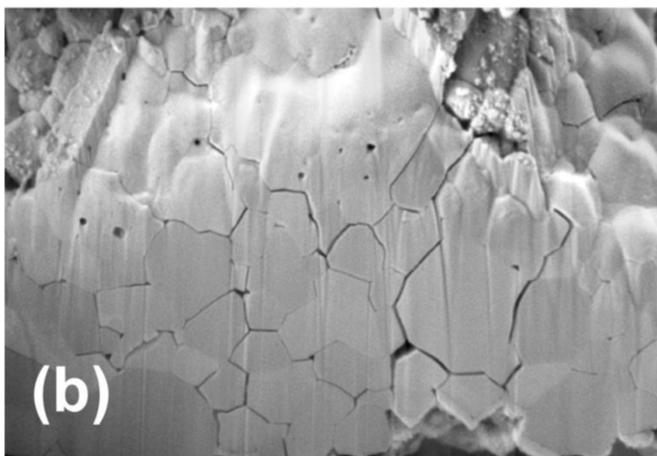
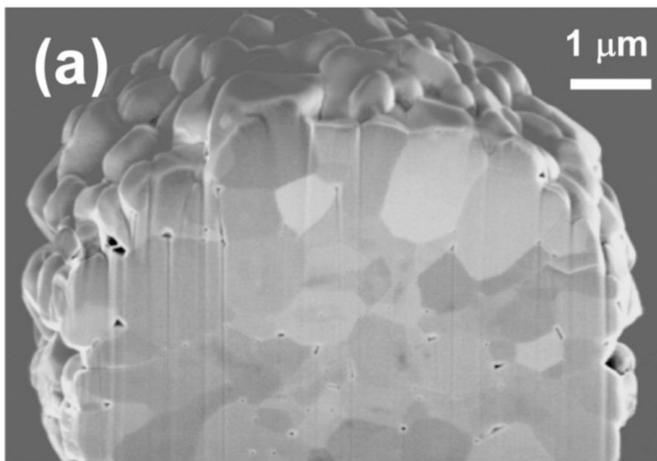


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Coarse-Graining of Properties of Porous Electrodes



The Internal (Meso) Structure of Particles



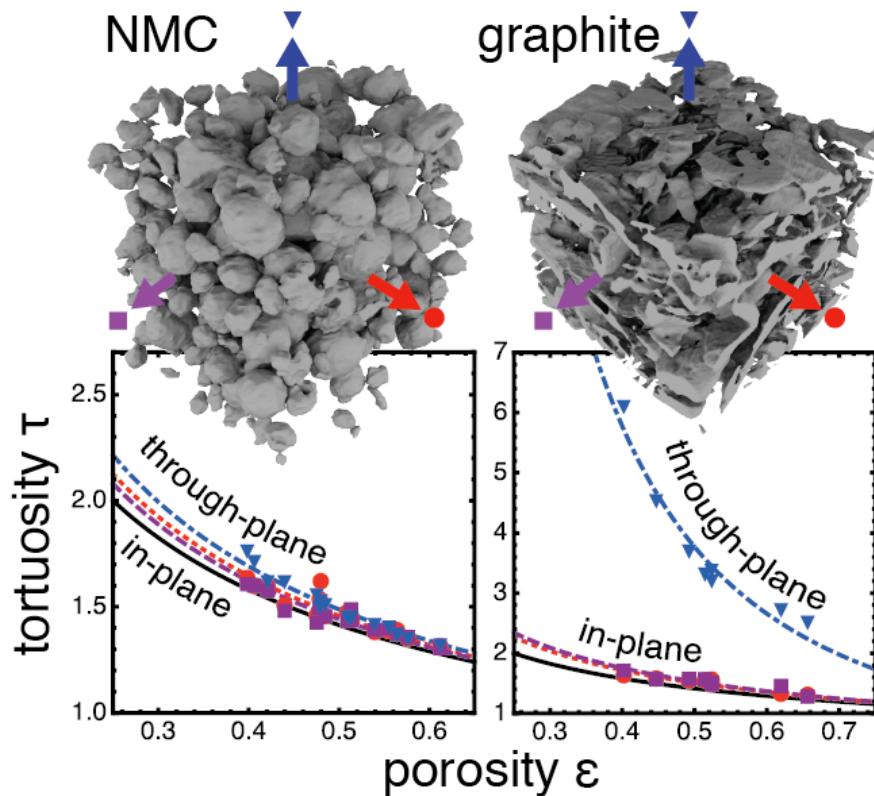
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Lithium-ion full cells." Journal of The
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Abhas Deva

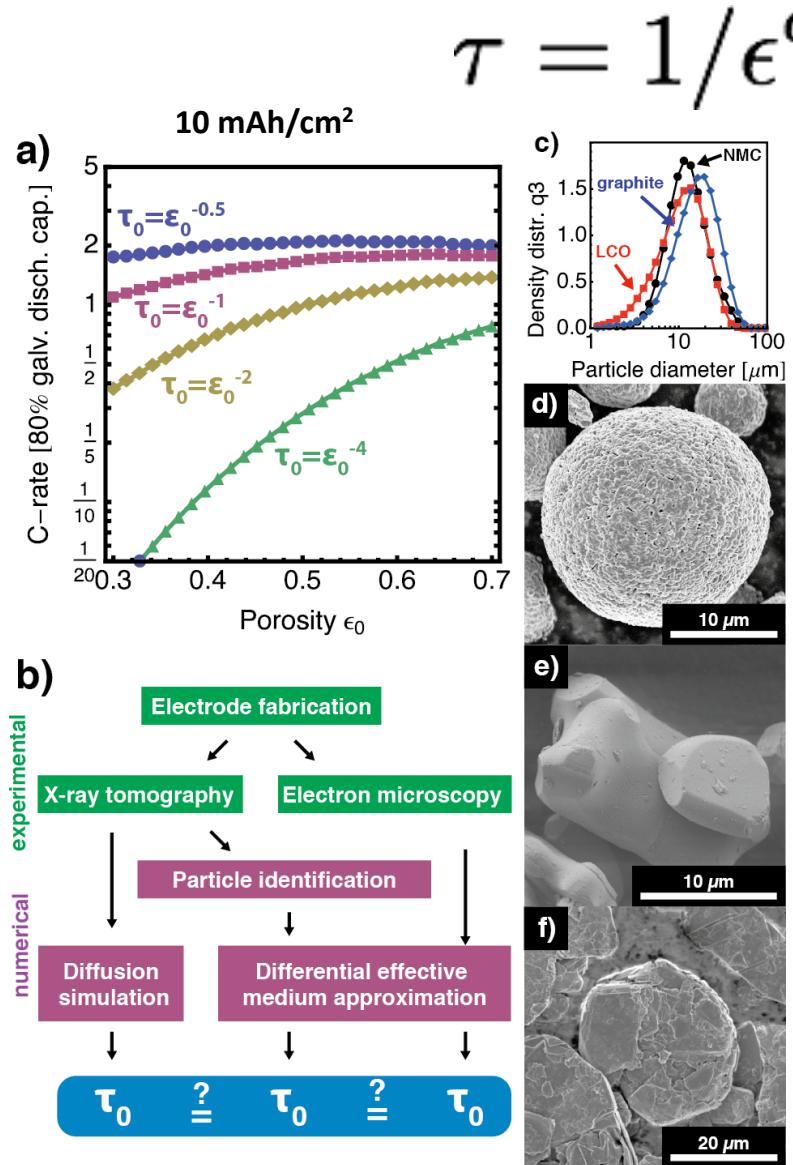
Sept 2017

Effect of Microstructure on Charge Utilization

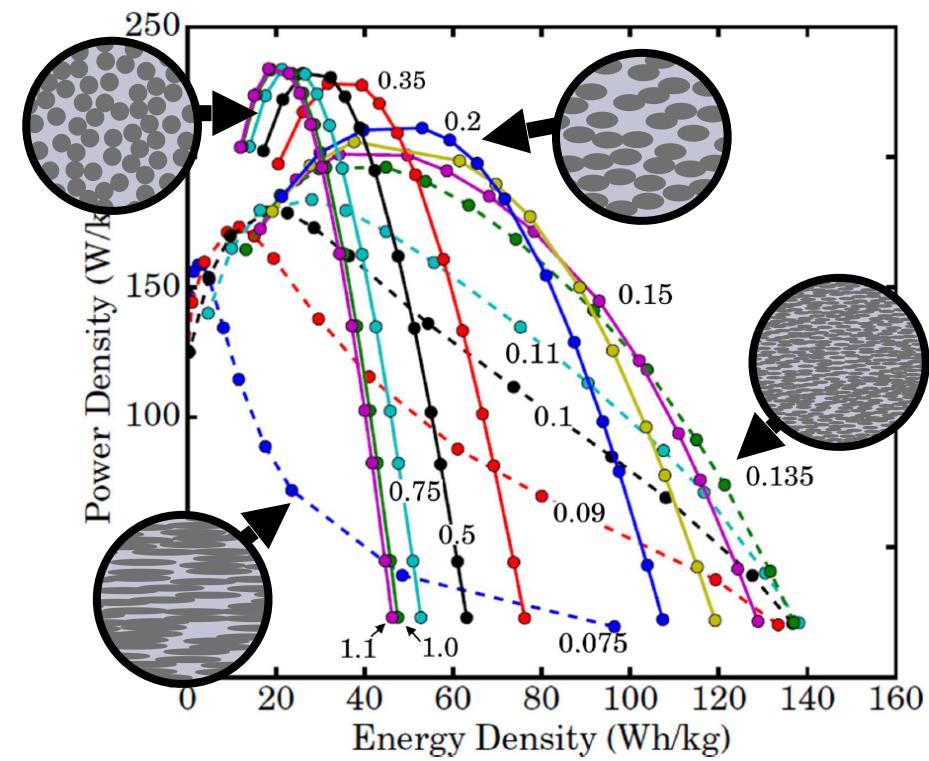
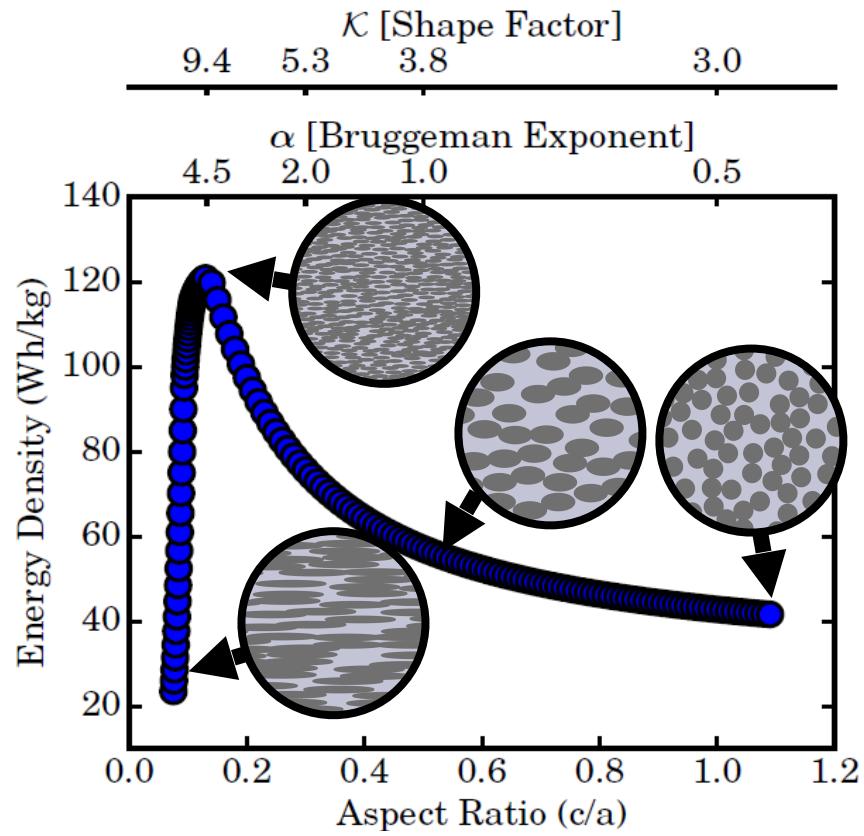
$$\tau = 1/\epsilon^\alpha$$



M Ebner, D-W Chung, RE García, and V Wood.
“Tortuosity Anisotropy in Lithium-Ion Battery
Electrodes.” *Advanced Energy Materials*. 2013. 4:
1301278. doi: 10.1002/aenm.201301278.

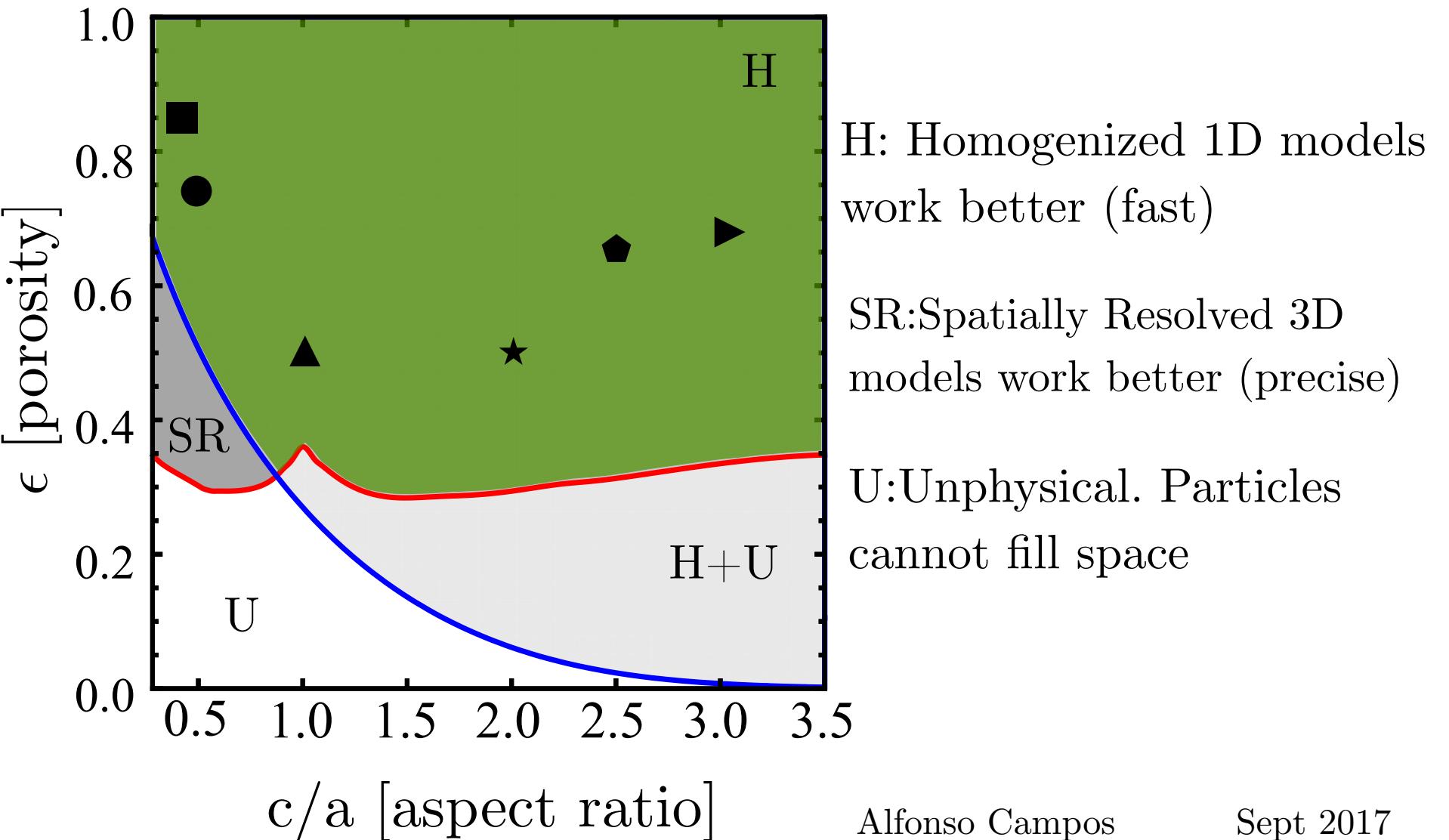


Effect of Microstructure Anisotropy on Power Density



(C₆ | LMO)

Rational and Guided Multi Scale Modeling of LIBs



Battery Modeling Data Flow

