Engineering Porous Electrodes for Redox Flow Batteries

Antoni Forner-Cuenca

Associate Professor
Department of Chemical Engineering and Chemistry
Eindhoven University of Technology

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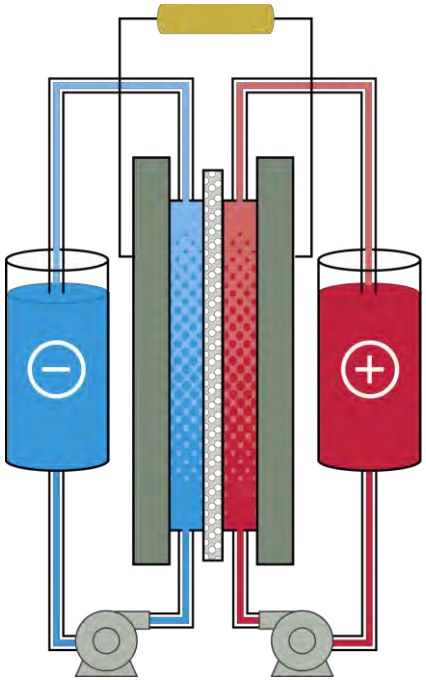
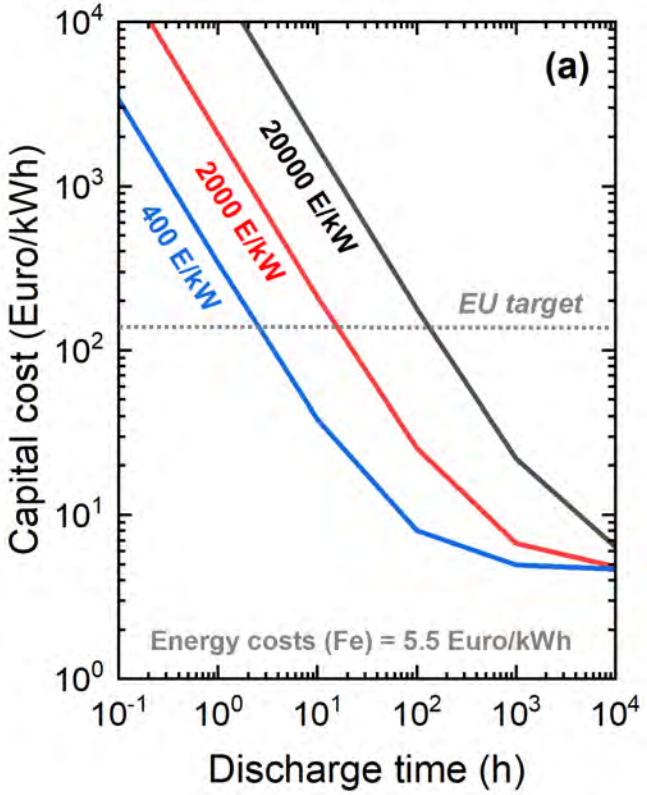
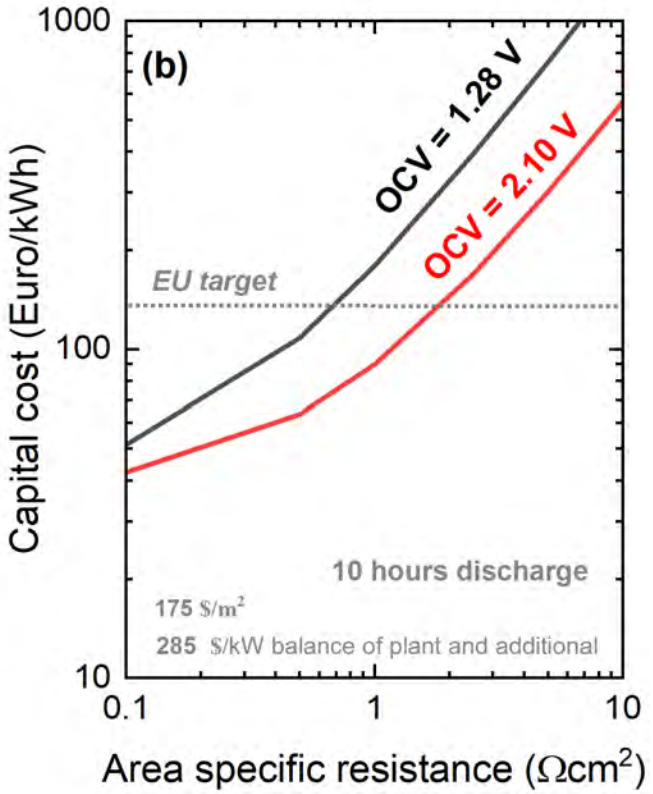
CIC energiGUNE, Vitoria-Gasteiz (ES) | 16th May 2023

How does increasing power density and reducing materials costs affect the economics?



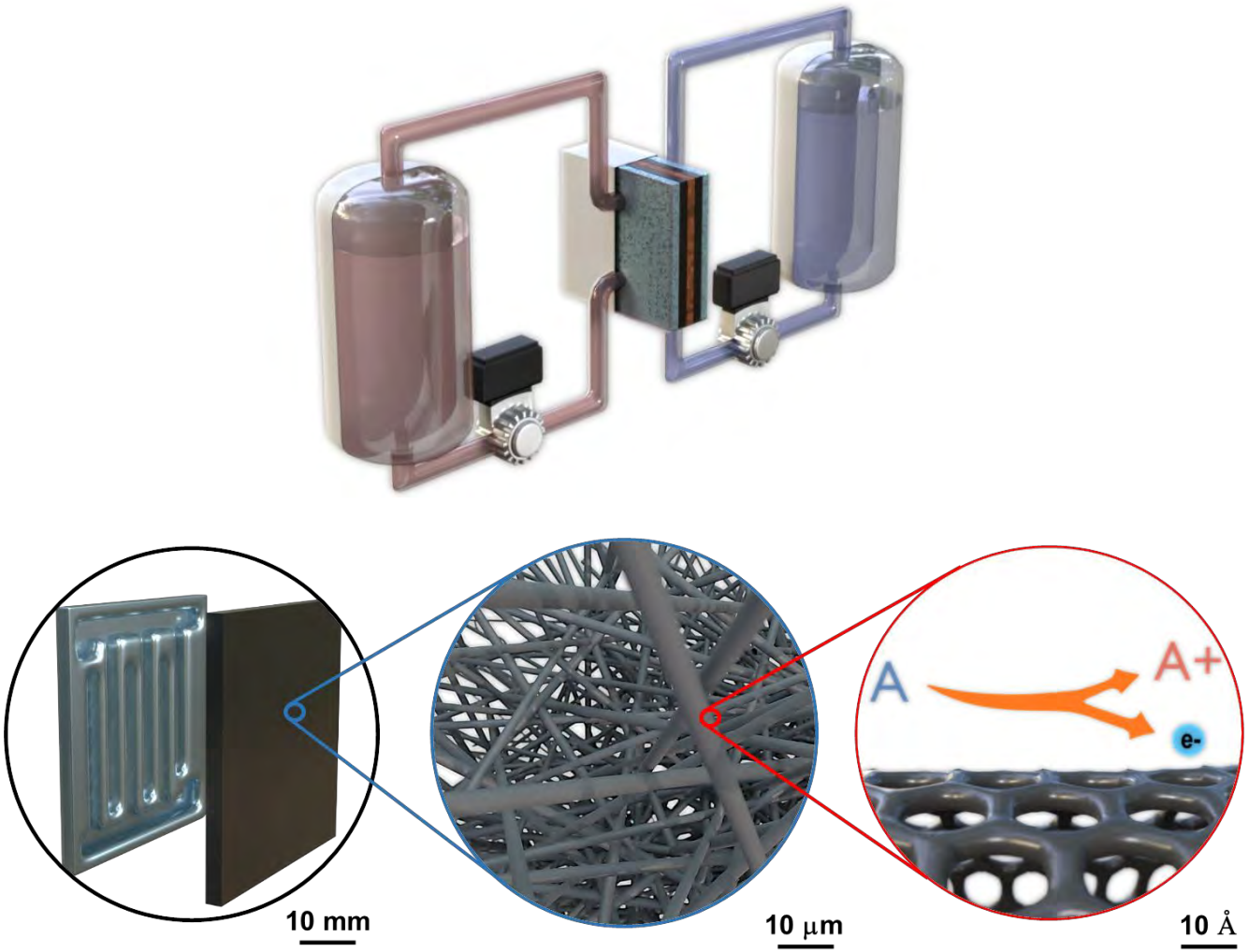




Minimizing area-specific resistance is a powerful strategy for reducing reactor cost contributions to the total system cost

References to TE analysis: Darling et al., *Energy Environ. Sci. 7, 3459 (2014), Noack et al., Energies 9(8) 627 (2016).*

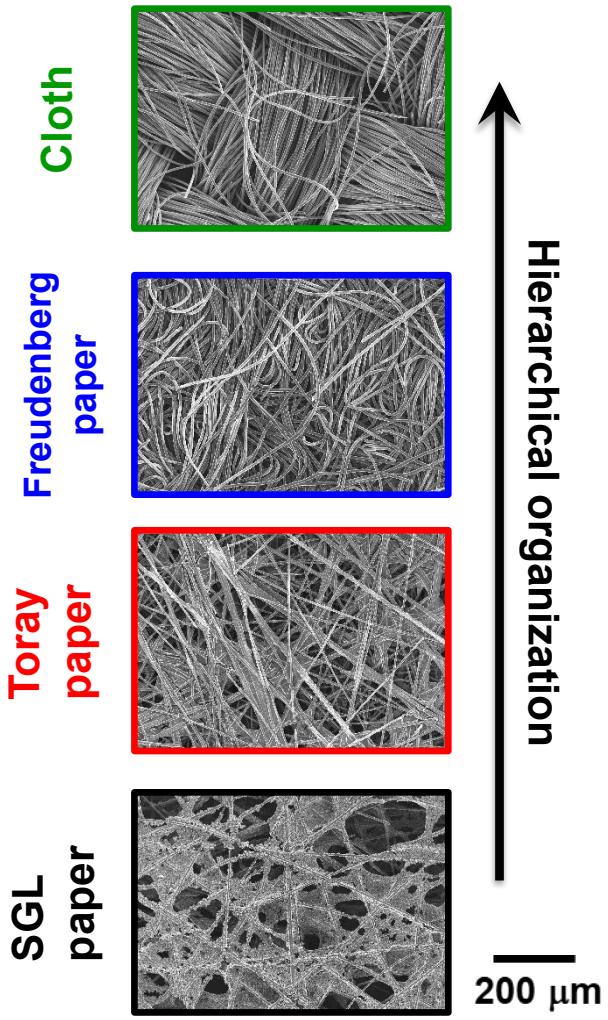
Understanding electrodes at multiple length scales

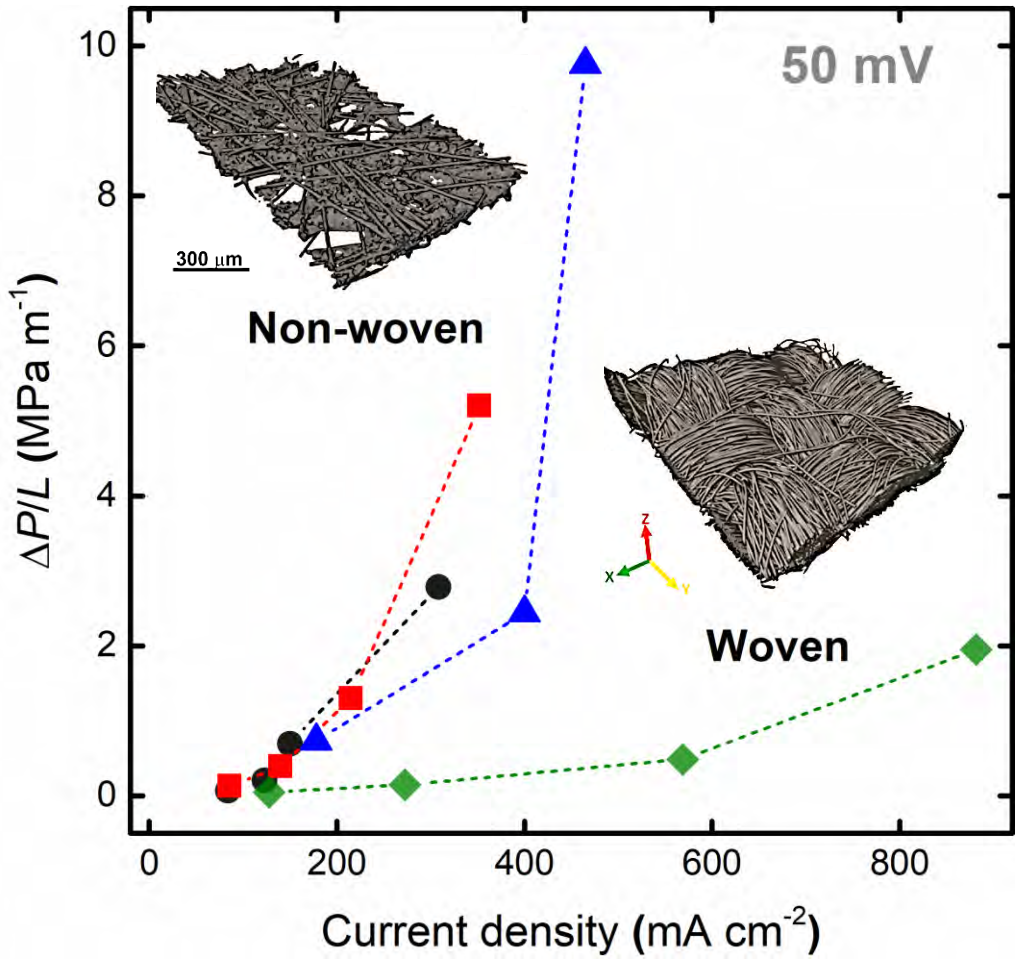


Minimizing area-specific resistance is a powerful strategy for reducing reactor cost contributions to the total system cost

Forner-Cuenca, *Current Opinion in Electrochemistry*, 18, 113 (2019)

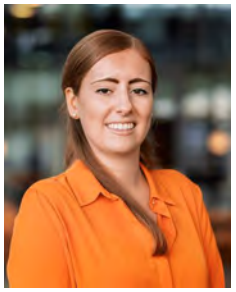
Electrode structuring improves mass transfer



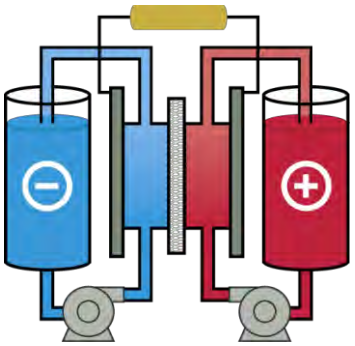


Forner-Cuenca et al., *Journal of The Electrochemical Society*, 166(10) A2230-A2241 (2019)

Towards predictive electrode design

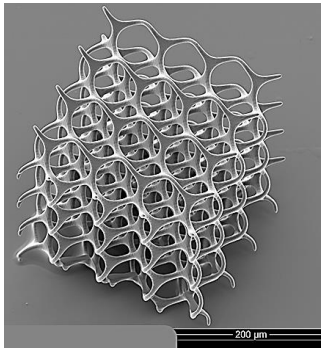


Redox flow battery



Modeling-assisted design

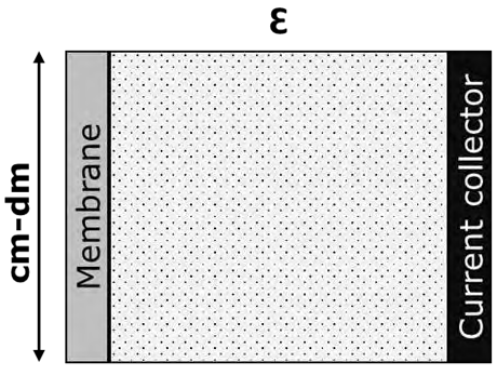
Advanced manufacturing



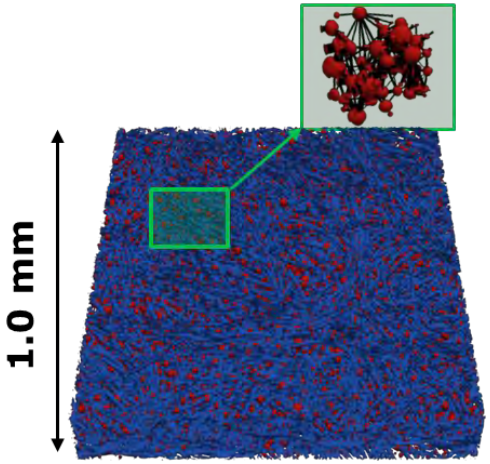
Chemistry-specific electrodes

Bottom-up design of electrode microstructures

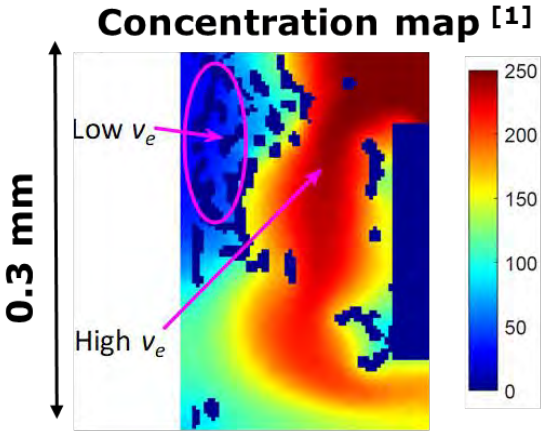
Level of complexity and detail



Macroscopic continuum model



Pore network model

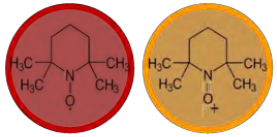


Lattice Boltzmann model
Finite Element model

Van der Heijden & van Gorp et al., *Journal of The Electrochemical Society* 169(4) 040505 (2022)

Model validation:
non-aqueous electrolyte

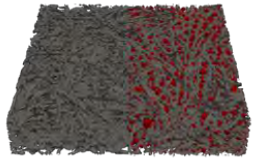
Active species: 0.1 M $TEMPO^{\cdot}$ / $TEMPO^{+}$



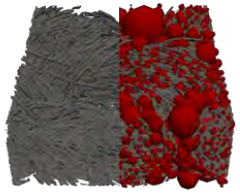
Salt: 1 M $TBAPF_6$

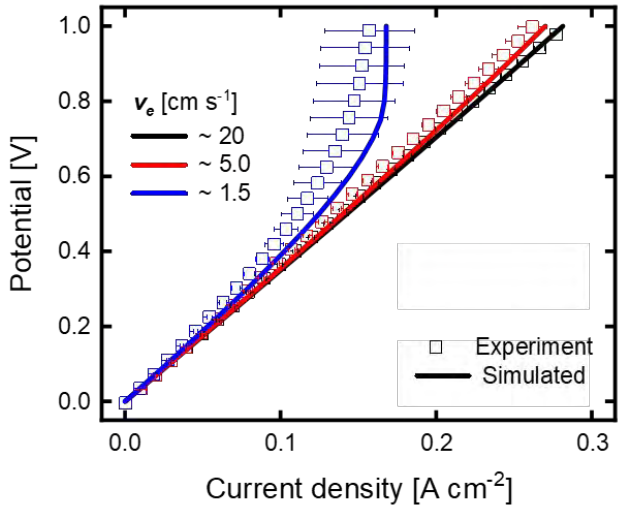
Solvent: Acetonitrile

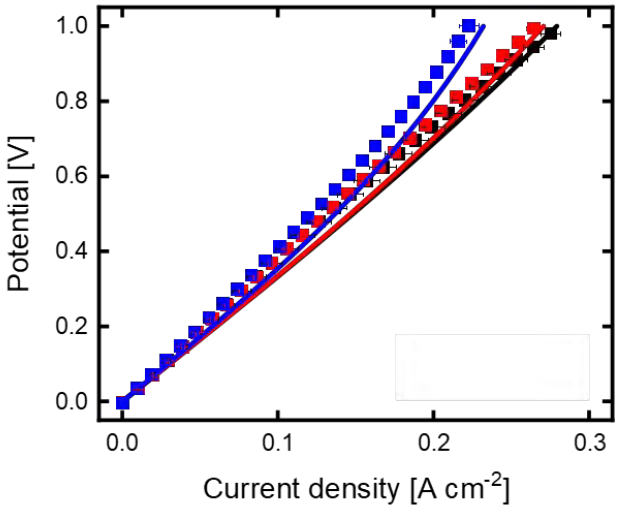
Electrode: Paper



Cloth



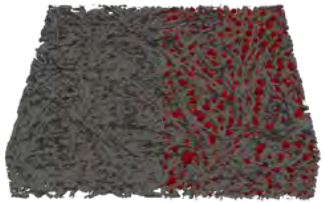


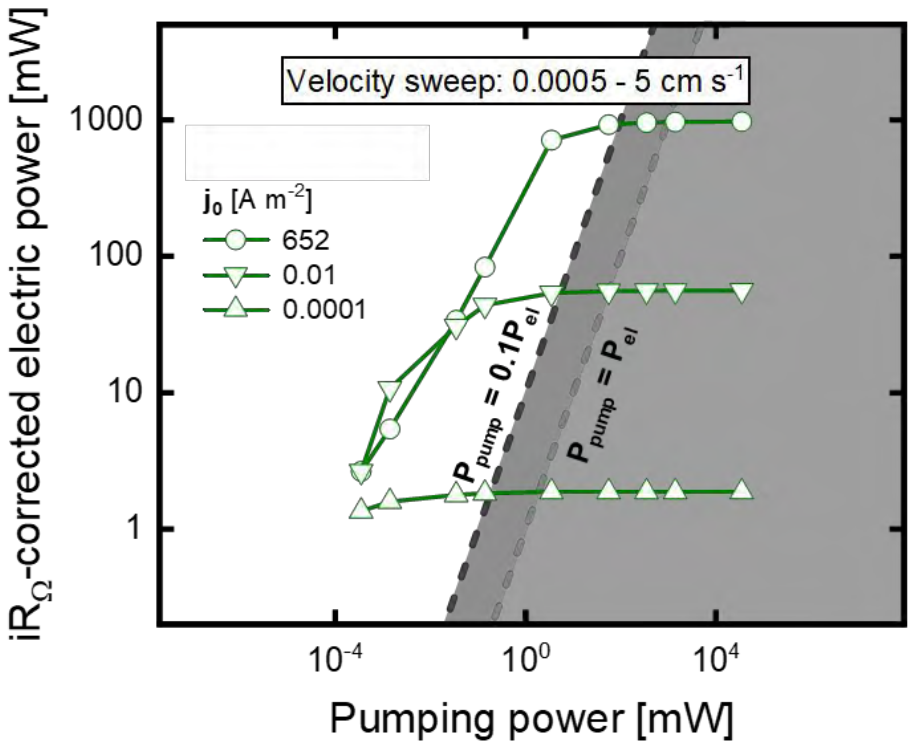


Van der Heijden & van Gorp et al., *Journal of The Electrochemical Society* 169(4) 040505 (2022)

Simulation can support engineers in selecting economical operating conditions

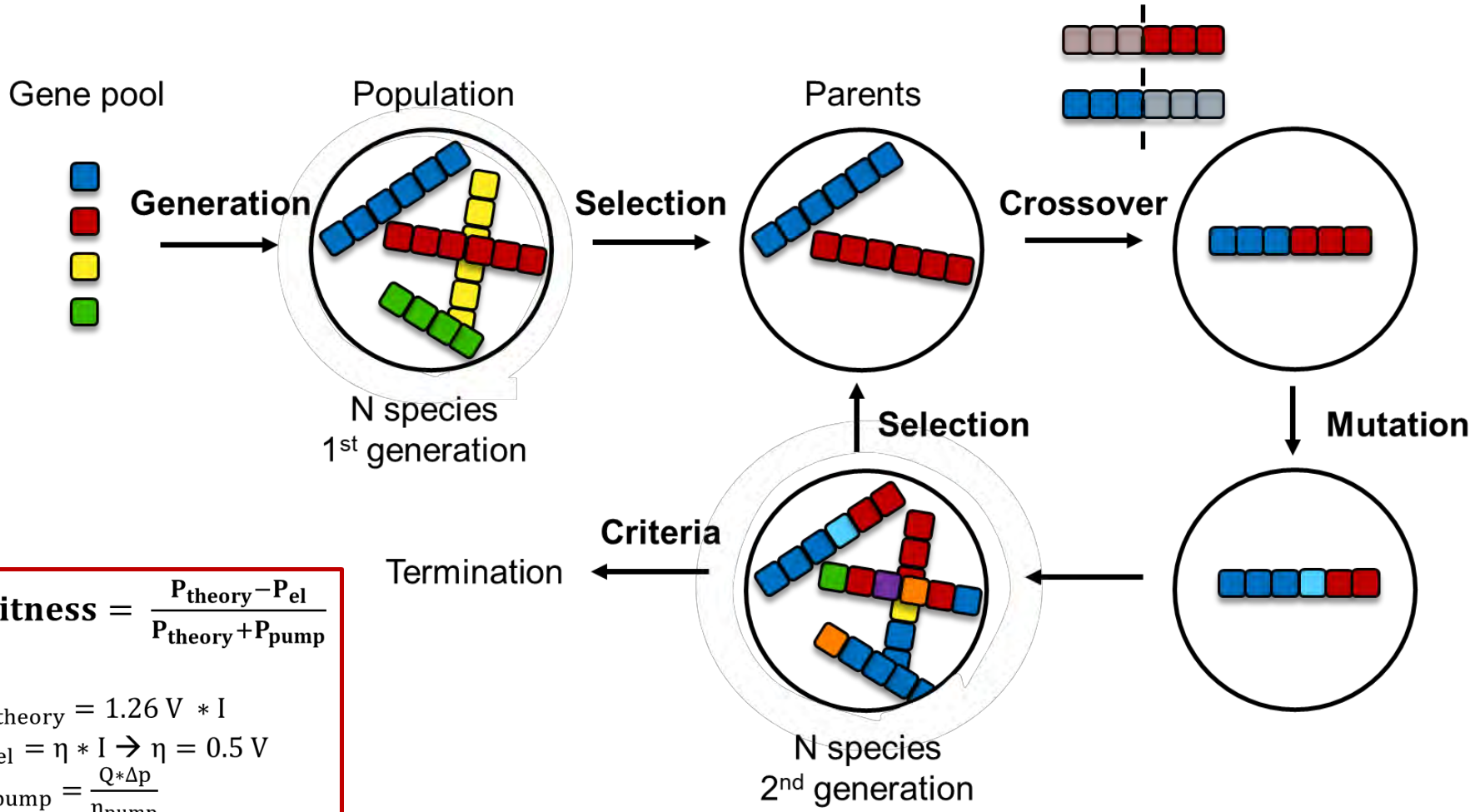
Paper electrode





Van der Heijden & van Gorp et al., *Journal of The Electrochemical Society* 169(4) 040505 (2022)

Coupling genetic algorithms with Multiphysics pore network modeling



$$\text{Fitness} = \frac{P_{theory} - P_{el}}{P_{theory} + P_{pump}}$$

$P_{theory} = 1.26\ V * I$

$P_{el} = \eta * I \rightarrow \eta = 0.5\ V$

$P_{pump} = \frac{Q * \Delta p}{\eta_{pump}}$

Van der Heijden & van Gorp et al., *in preparation*

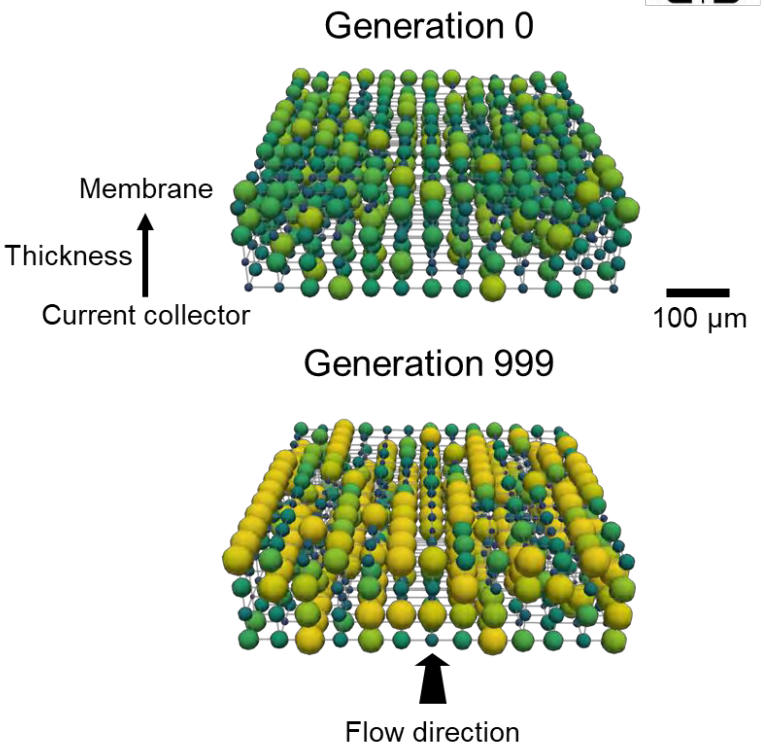
The microstructure evolves to generate longitudinal pathways of low tortuosity

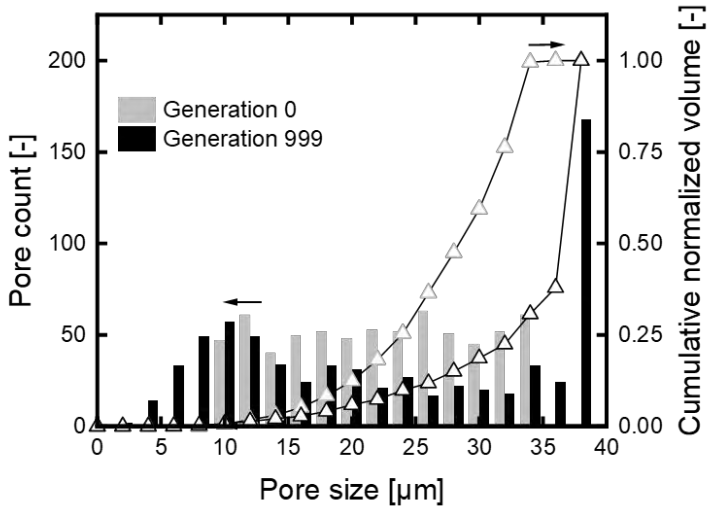
= 50

= 10

= 1000

= [13x13x4]

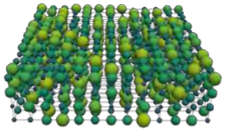
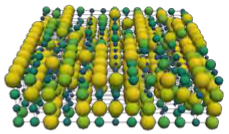




Tendency to form bimodal microstructures

Van Gorp, R. & Van der Heijden, M. et al., Chem. Eng. J., 455, 139947 (2022)

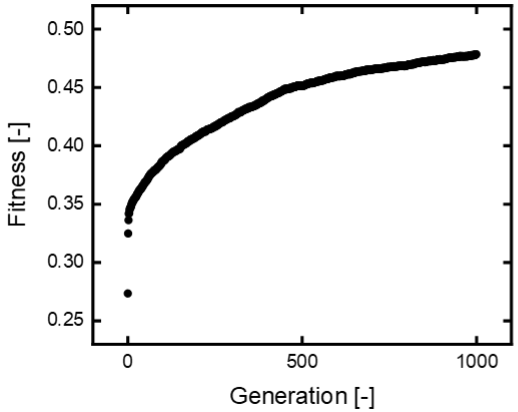
The microstructure evolves to generate longitudinal pathways of low tortuosity

 = 50  = 10  = 1000  = [13x13x4]  

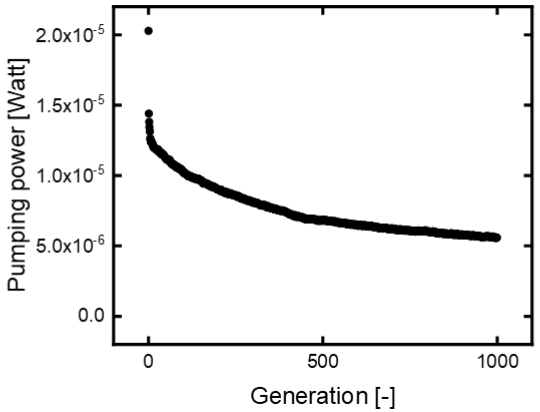
$$\text{Fitness} = \frac{P_{theory} - P_{el}}{P_{theory} + P_{pump}}$$

+ 75% Fitness
- 72% P_{pump}
+ 42% P_{el}

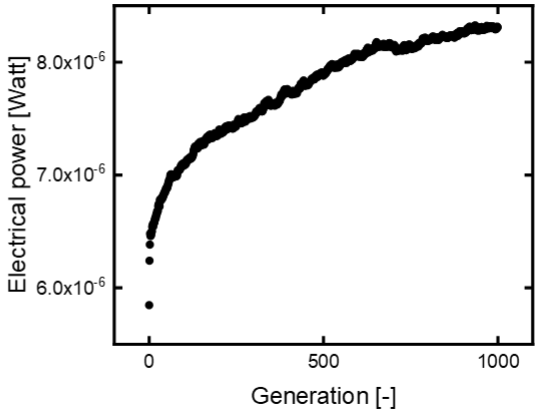
Fitness



Pumping power, P_{pump}



Electrical power, P_{el}

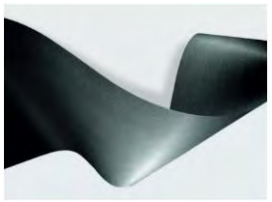


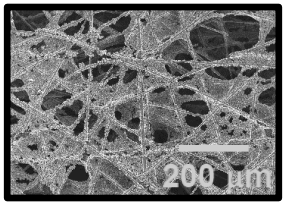
How do we predict electrode structures that can be manufactured with existing methods?

Van Gorp, R. & Van der Heijden, M. et al., Chem. Eng. J., 455, 139947 (2022)

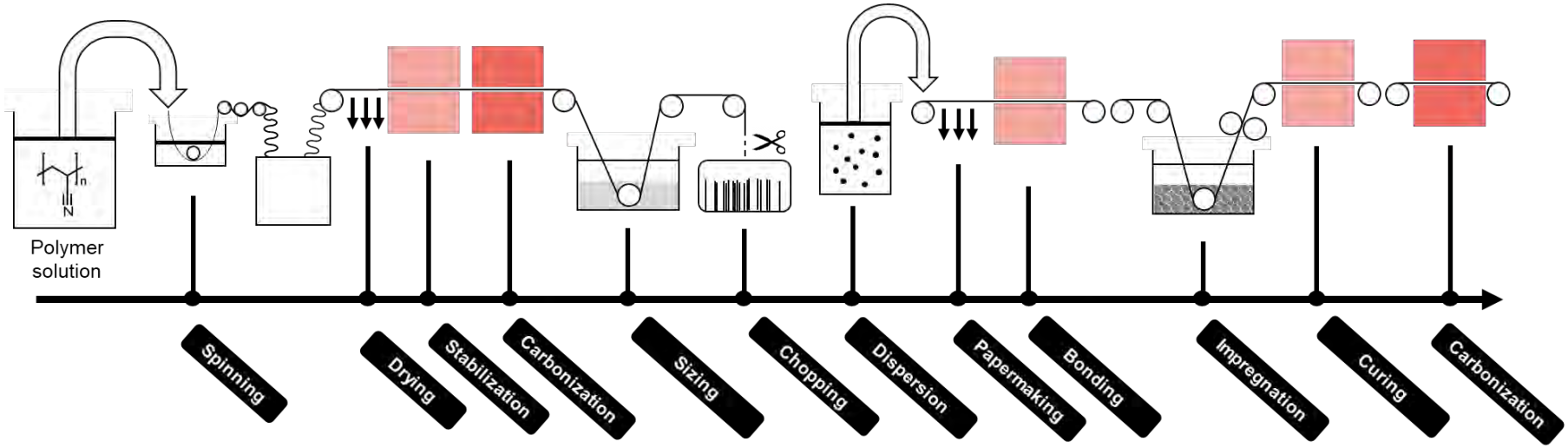
Carbon fiber electrode manufacturing

sgl carbon





Representative manufacturing route:

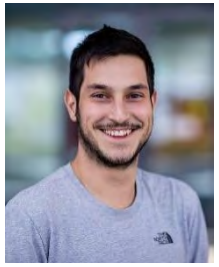


Estimated production costs: 20-80 € m^{-2}

Current state-of-the-art commercial manufacturing methods are complex and multi-step processes…can we consider alternative synthetic pathways?

From SGL white paper on gas diffusion layer manufacturing, C. Minke et al., *J. Power Sources* 324, 116, 2017

Bottom-up engineered microstructures with phase separation



Dissolve mixture → Cast → Phase Separate → Thermally Stabilize and Carbonize

PAN (Scaffold)

PVP (Pore-former)

DMF (Solvent)

Porous membrane

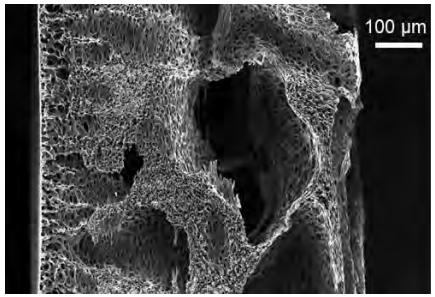
Air 270 °C

N_2 1050 °C

Conductive electrode

- ✓ Facile and practical synthesis procedure
- ✓ Versatile design space
- ✓ Multimodal interconnected microstructures

Macrovoids | Gradient | Isoporous



Tunable Microstructure

Estimated production costs: 5-12 € m^{-2}

Forner-Cuenca, Provisional Patent U.S. Serial No. 62/976,601; Wan & Jacquemond, Adv. Mater. 2021, 2006716