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Tailoring single mesoporous carbon catalyst particles via pore-scale simulation for superior PEM fuel cell performance

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Mesoporous carbon
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Pore-scale model

ABSTRACT

Minimizing Pt loading while maintaining high performance is vital for commercializing proton exchange membrane fuel cells. Mesoporous carbon supports enable internal Pt placement, mitigating ionomer poisoning effect and mass transport limitations. However, this also increases proton transport resistance due to limited ionomer accessibility. This work presents a pore-scale model to simulate reactive transport in single catalyst particles. We evaluate the impacts of open pores, pore number, and Pt distribution on oxygen accessibility and performance. Results show that internal Pt outperforms ionomer-coated Pt when sufficient open pores promote mass transport, though performance drops if Pt is located too deeply. To address this issue, we propose a hollow-shell mesoporous carbon design that confines Pt near the outer surface. This approach enhances internal Pt utilization by up to 38% and enables a Pt loading reduction of as much as 50% at equivalent performance. These findings offer a practical strategy for ultra-low Pt catalysts.

1. Introduction

The shift toward sustainable energy systems has established proton exchange membrane (PEM) fuel cells as a promising technology, owing to their high efficiency, scalability, and zero emissions [1,2]. However, high costs and limited durability continue to hinder large-scale commercialization [3]. A major contributor to these challenges is the platinum (Pt) catalyst, which accounts for nearly half of the system cost and significantly influences performance and lifespan [4]. Enhancing the utilization efficiency of catalyst particles is therefore essential for achieving high fuel cell performance with reduced Pt loading [5]. In conventional catalyst layers (CLs), Pt nanoparticles are dispersed on carbon supports and partially coated with perfluorosulfonic acid (PFSA) ionomer to form the triple-phase boundary required for electrochemical reactions [6]. However, this configuration imposes inherent limitations, as schematically illustrated in Fig. 1. Extensive studies have shown that sulfonate groups in the ionomer adsorb strongly onto Pt surfaces, poisoning active sites and suppressing oxygen reduction reaction (ORR) activity by up to 80% [7–9]. Moreover, the low oxygen diffusivity and solubility within the ionomer film severely restrict oxygen transport to the Pt surface, especially at high current densities, leading to substantial mass transport losses and reduced the overall efficiency [10–12].

To address these limitations, mesoporous carbon has emerged as a promising alternative support material, enabling Pt particles to be hosted within internal pores and spatially separated from direct ionomer contact. This configuration is expected to mitigate sulfonate poisoning, enhance oxygen transport, and improve ORR activity, as illustrated in Fig. 1. Yarlagadda et al. [13] introduced the concept of "accessible pores", which allow proton transport without requiring direct ionomer contact. Mesoporous structures have demonstrated reduced local mass transport resistance and high catalytic activity, enabling up to 31% higher current density with 37% less Pt compared to conventional solid carbon supports. Subsequent studies reinforced these benefits. Lee et al. [14] showed that mesoporous carbon with interconnected ~63 nm channels exhibits superior mass transport. Yarlagadda et al. [15] further quantified local mass transport resistance for mesoporous carbon at only 3 s cm^{-1}, substantially lower than high-surface-area carbon (15.9 s cm^{-1}) and Vulcan carbon (8.3 s cm^{-1}). However, this benefit is accompanied by a notable trade-off: proton transport resistance in mesoporous carbon supports is substantially higher than Vulcan carbon at low relative humidity (RH < 50%), owing to the lack of direct ionomer pathways to internal Pt particles. Luo et al. [16] synthesized hierarchical interconnected pore networks for improved performance at low Pt loading, while Ortlieb et al. [17] developed a versatile synthesis platform for precise control over pore architecture and particle size. Leveraging such tools, Martin et al. [18] fabricated tailored mesoporous

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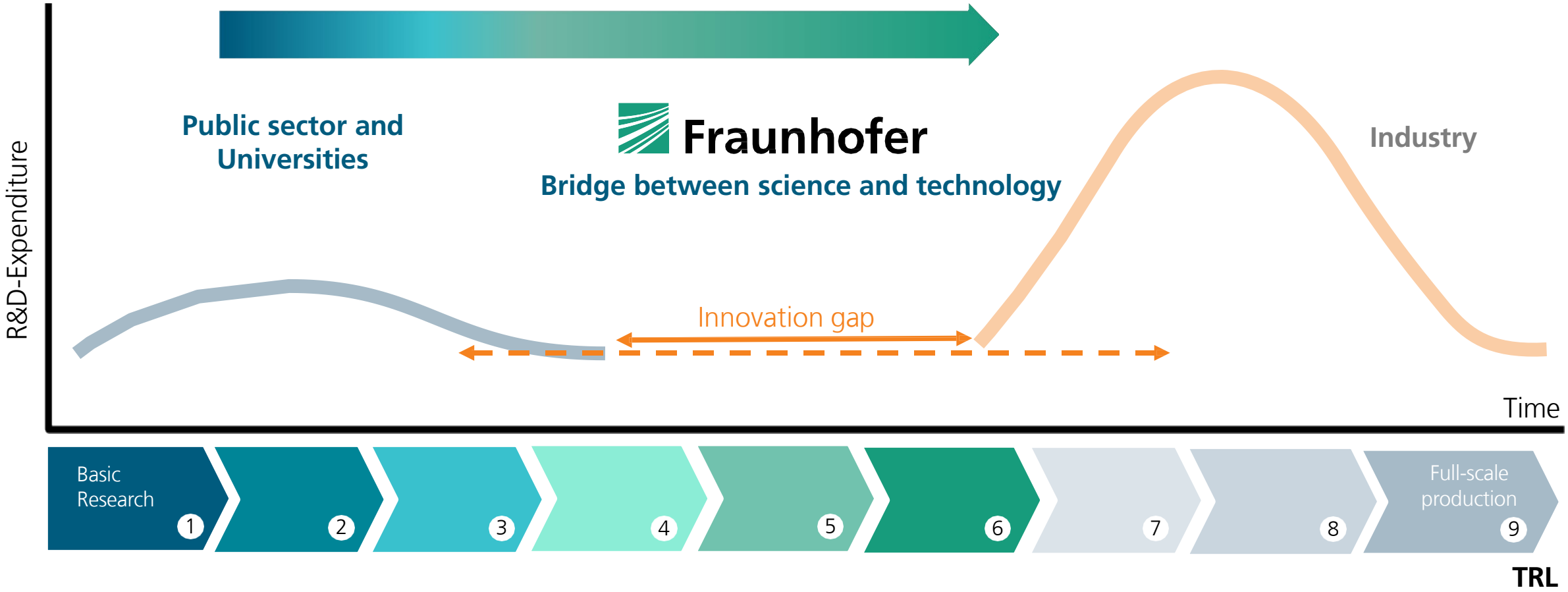
Tailoring Single Mesoporous Carbon Catalyst Particles via Pore-Scale Simulation

Speaker: Yuze Hou
Co-authors: Kläre Christmann, Nada Zamel
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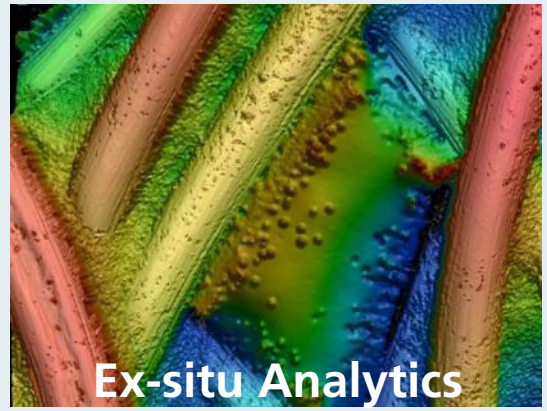
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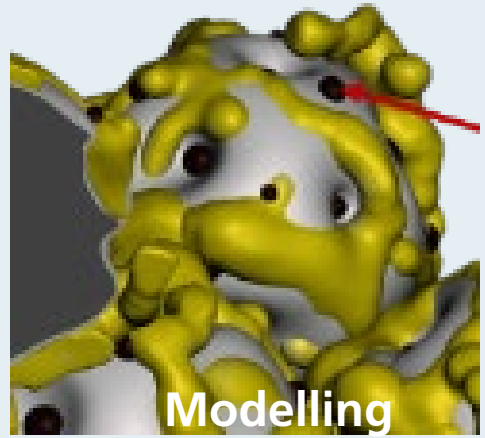
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- Focus on transport application

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Agenda

1. **Research Background**

2. **Pore-scale modeling platform**
   - Reconstruction model
   - Lattice Boltzmann model

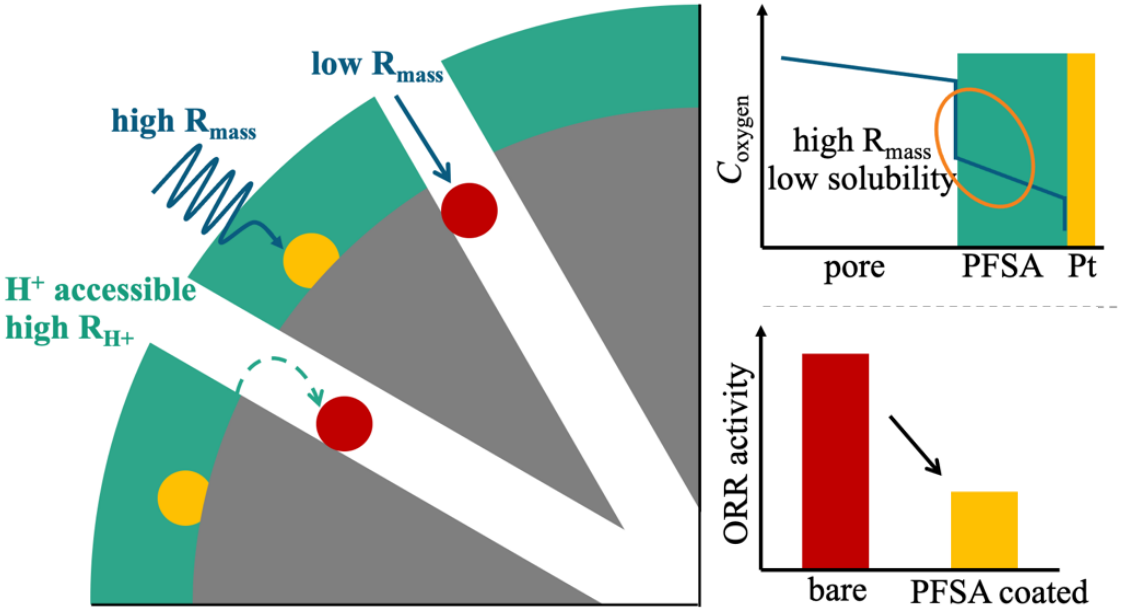
3. **Results & Discussion**

4. **Conclusions**

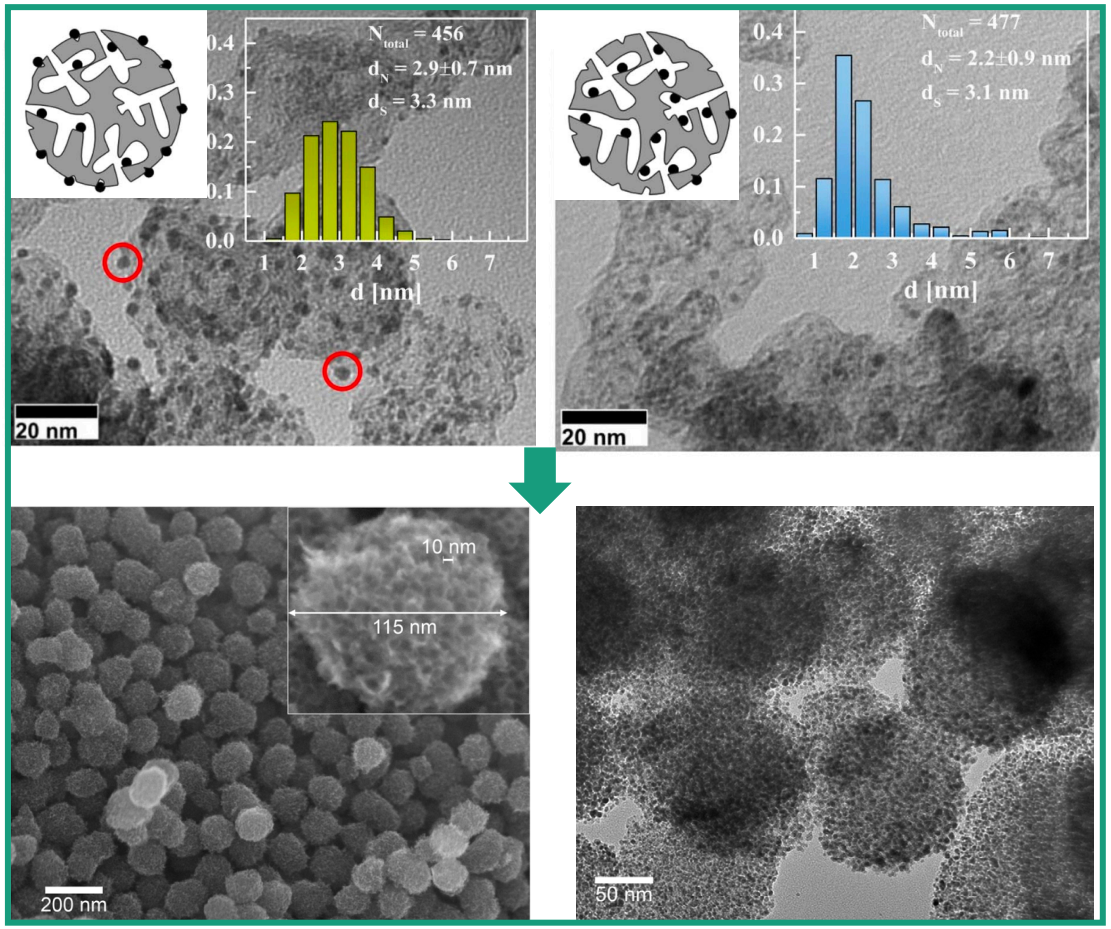
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Research background

Progress in carbon supported catalyst



- Ionomer coverage on Pt particles can significantly hinder mass transport and catalytic activity.
- Internal Pt is expected to deliver superior performance.



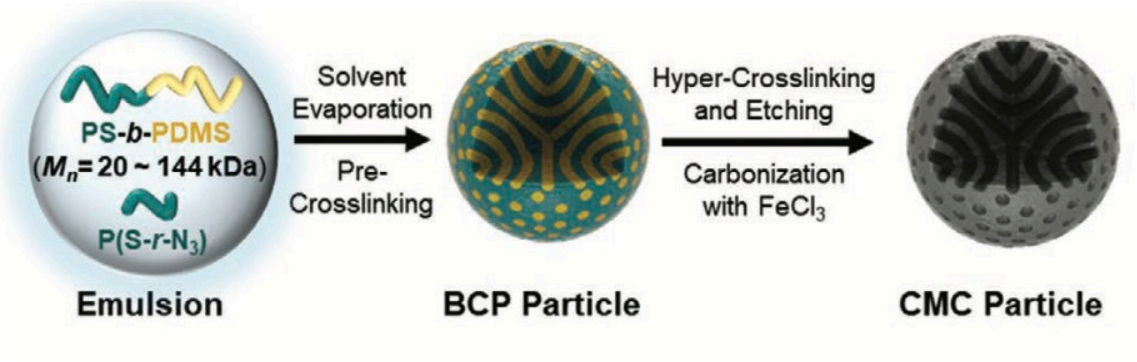
- Mesoporous carbon: promising catalyst support.

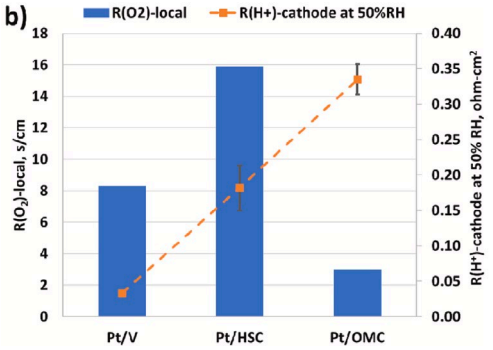
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Harzer, et al. J. Electrochem. Soc. 165.10 (2018): F770.
Martin, et al. Adv. Energy Mater. 15.36 (2025): 2500954.

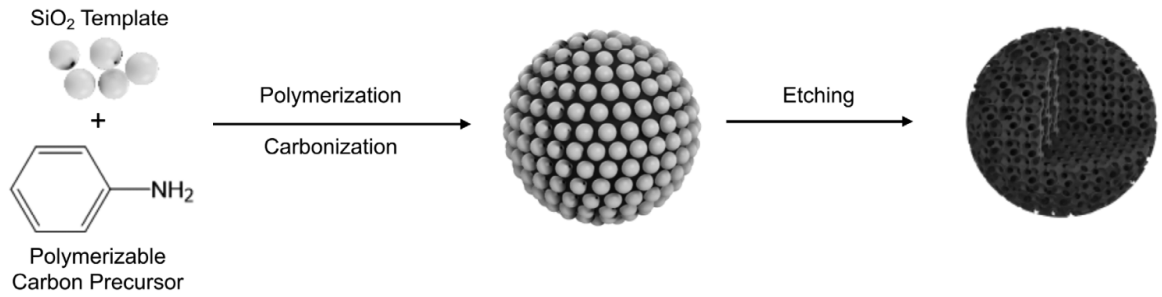
Research background

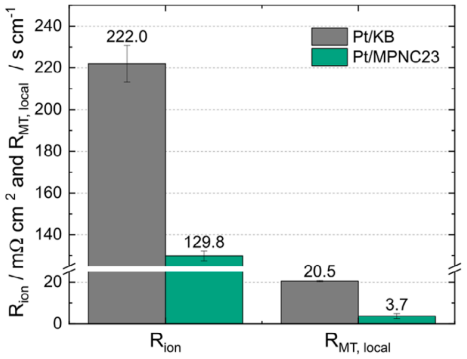
Mesoporous carbon support





Carbon ball with a network of straight cylindrical channels





N-doped carbon ball with interconnected spherical mesopores

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Lett, et al. Adv. Energy Mater. 11.48 (2021): 2102970. Yarlagadda, et al. J. of power sources 532 (2022): 231349. Ortlieb, et al. Small 21.2 (2025): 2407235.

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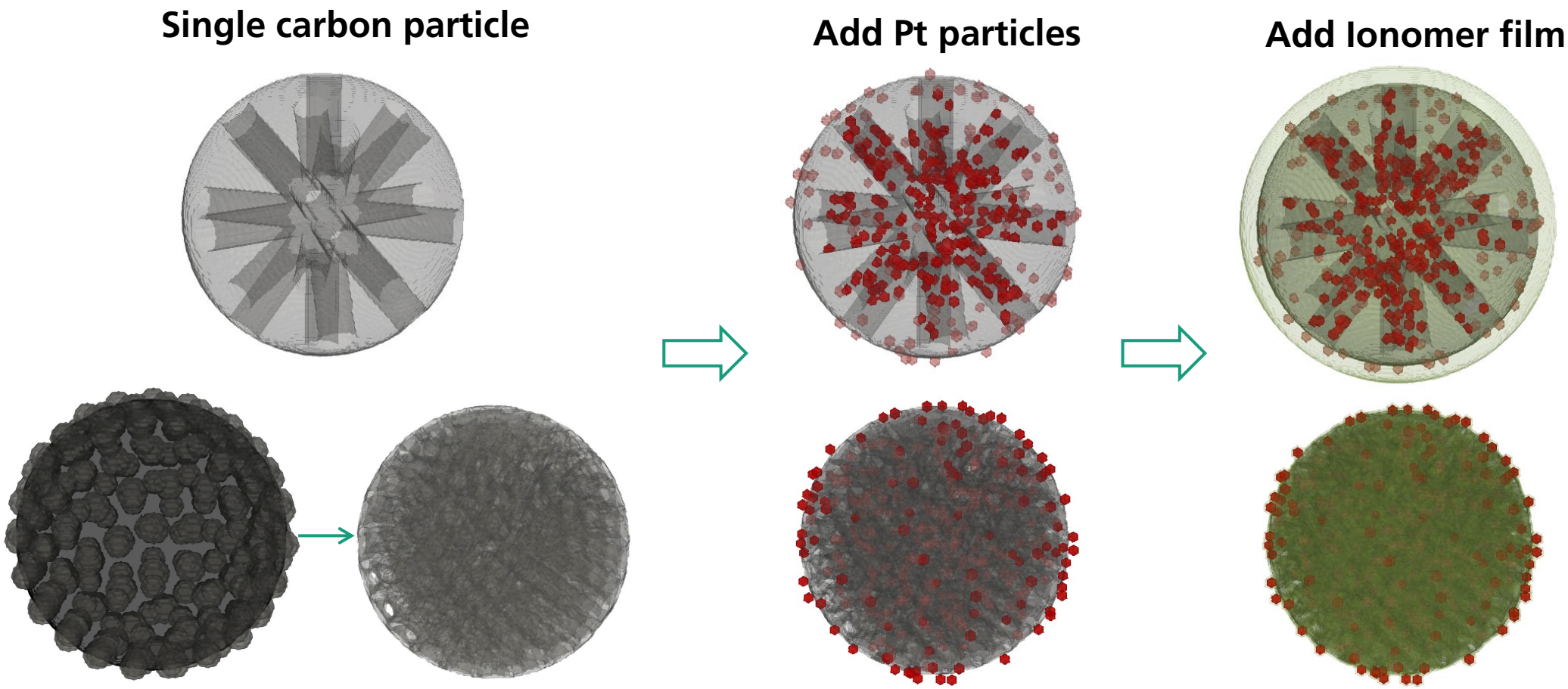
3. Results & Discussion

4. Conclusions

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Pore-scale modeling platform

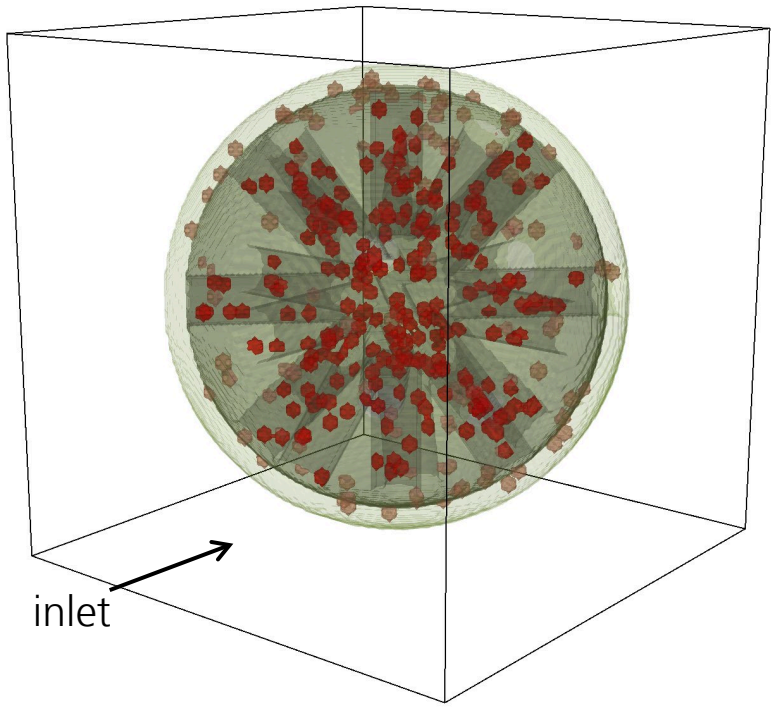
Reconstruction: Single mesoporous carbon particle



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Pore-scale modeling platform

Numerical model



R_{carbon} 50 nm; pore size 8 nm
I/C 0.6; Pt/C 0.6; Pt_{in}/Pt_{out} =1
Length of domain: 2.5 R_{carbon}
Resolution 1 nm, total ~1.9m grids

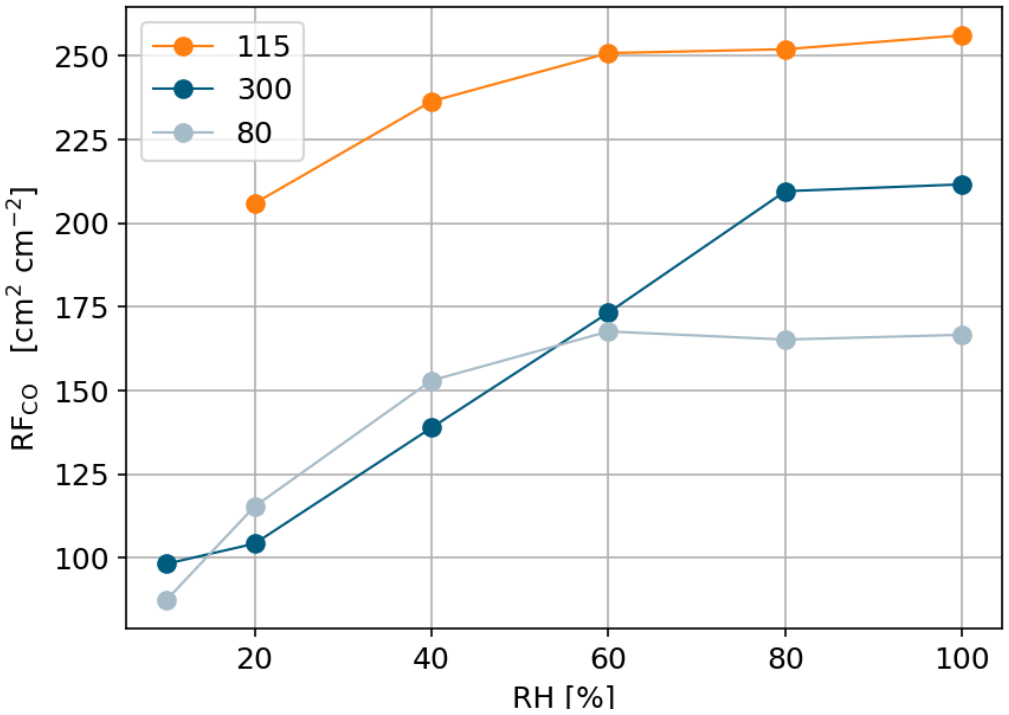
- Boundary condition:
  Inlet: C = 1 mol/m^3, outlet: no flux, rest: periodic

- Effect of ionomer poisoning: i_{ref} of ionomer-covered Pt is 1/2 of the ionomer-free Pt. (from literature: 1/4 ~ 1/2)

Shinozaki, K., Morimoto, Y., Pivovar, B. S., & Kocha, S. S. (2016). *Journal of Power Sources*, *325*, 745-751.
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Pore-scale modeling platform

Numerical model



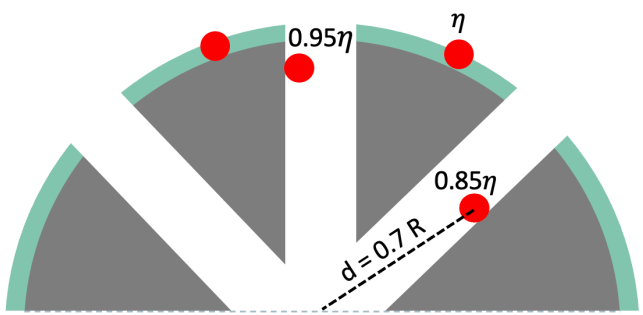
ECSA variation of catalyst with different particle size

- Boundary condition:
  Inlet: C = 1 mol/m^3, outlet: no flux, rest: periodic
- Effect of ionomer poisoning: i_{ref} of ionomer-covered Pt is 1/2 of the ionomer-free Pt. (from literature: 1/4 ~ 1/2)
- A 60% RH operating conditon (no flooding) is assumed, where inner Pt are activated.

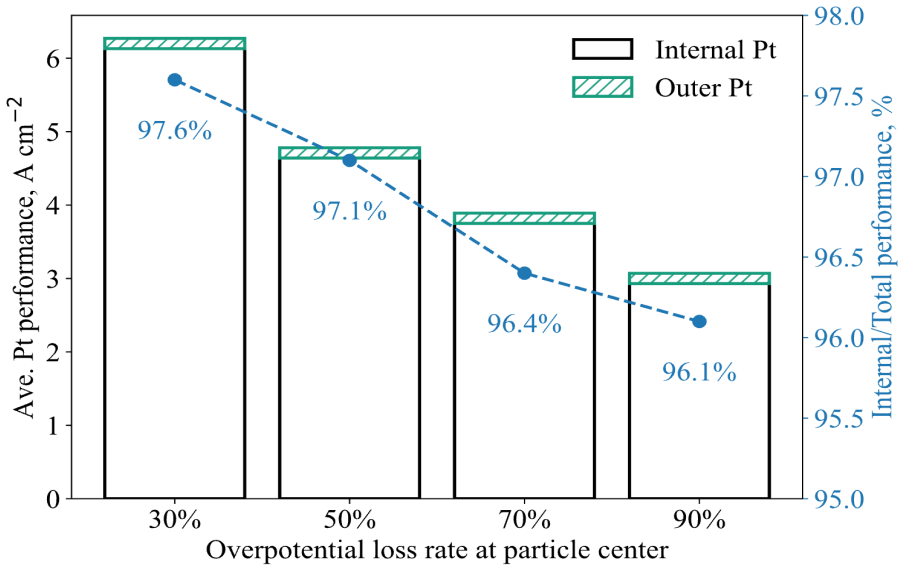
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Pore-scale modeling platform

Numerical model



$\eta_{local} = \eta - (R - d)/R * \eta * 50\%$

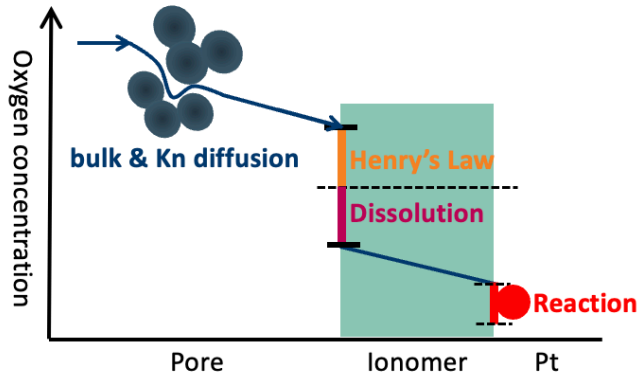


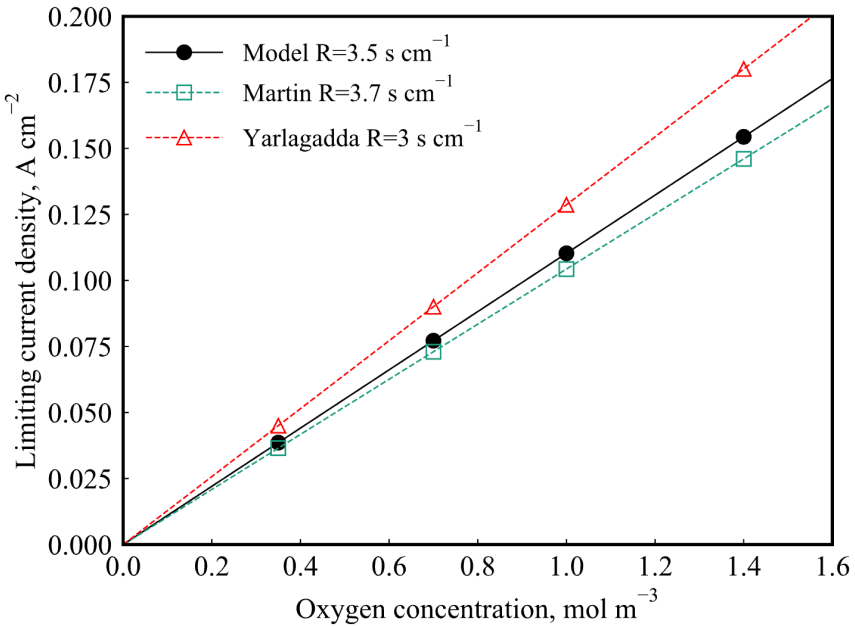
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- Uniform overpotential η is set for ionomer-covered Pt. η of internal Pt is lower due to R_{proton}, based on its specific location.

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Pore-scale modeling platform

Numerical model





- Boundary condition:
  Inlet: C = 1 mol/m^3, outlet: no flux, rest: periodic

- Effect of ionomer poisoning: i_{ref} of ionomer-covered Pt is 1/2 of the ionomer-free Pt. (from literature: 1/4 ~ 1/2)

- A 60% RH operating conditon (no flooding) is assumed, where inner Pt are activated.

- Uniform overpotential η is set for ionomer-covered Pt. η of internal Pt is lower due to R_{proton}, based on its specific location.
- A comprehensive LB model is utilized to simulate the reactive transport process. Distribution of C_{oxygen} and performance can be obtained to evaluate the mesoporous carbon design.

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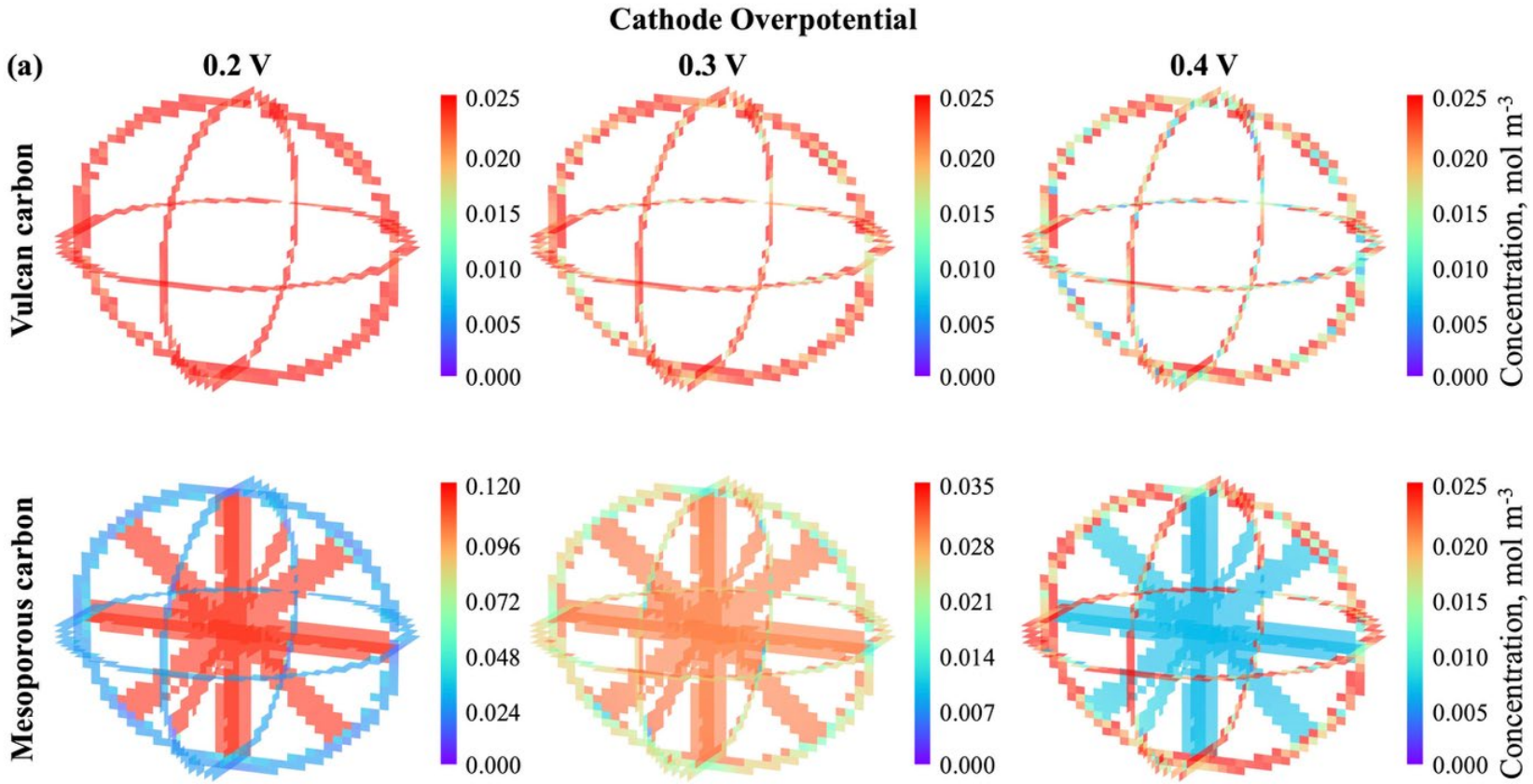
3. **Results & Discussion**

4. Conclusions

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Results & discussion

Vulcan carbon vs mesoporous carbon (pores blocked by ionomer)

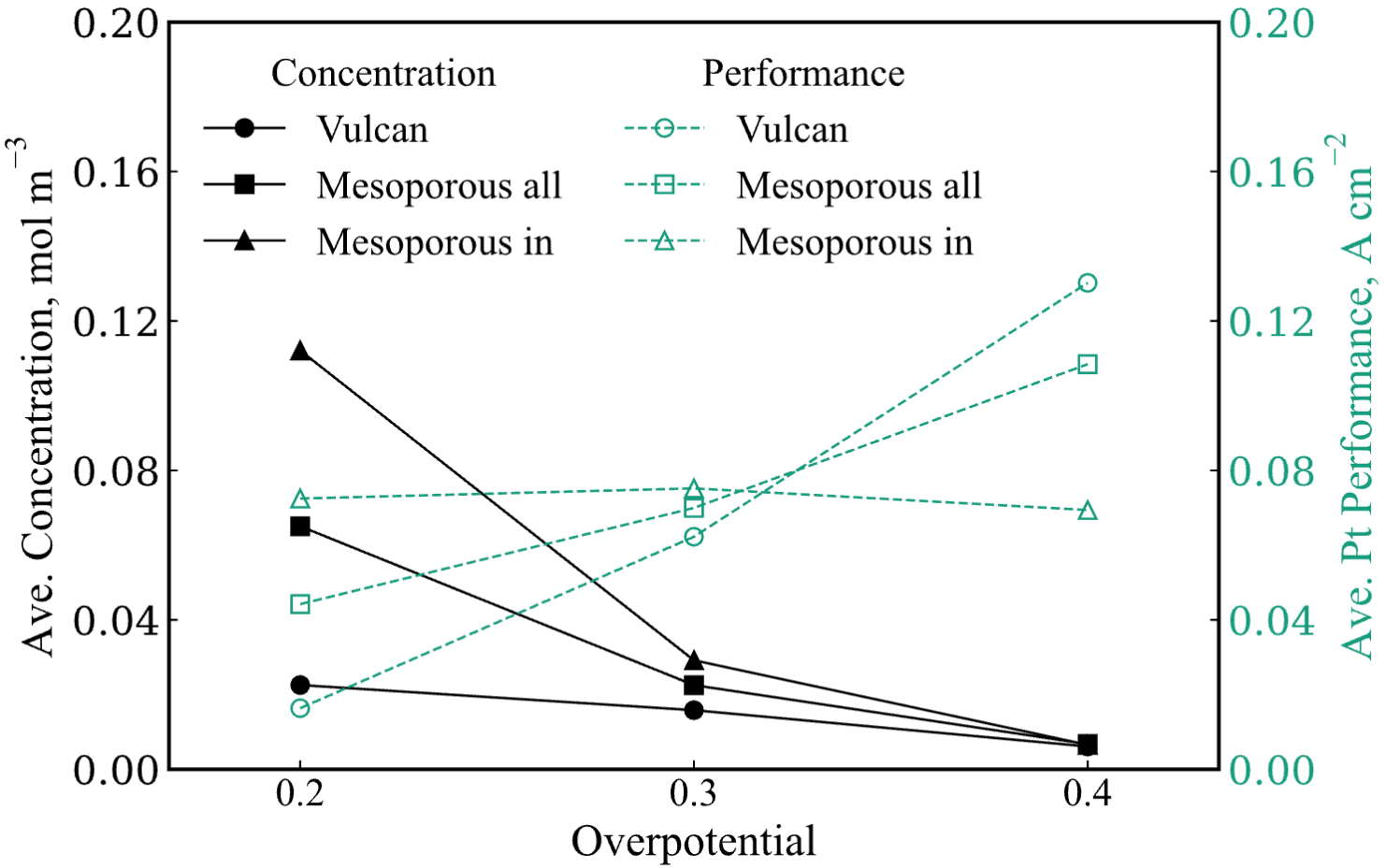


In high-performance mode, internal mesopores starve due to cross-ionomer resistance.
However, internal concentration can exceed the ionomer-limited value.

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Results & discussion

Vulcan carbon vs mesoporous carbon (pores blocked by ionomer)

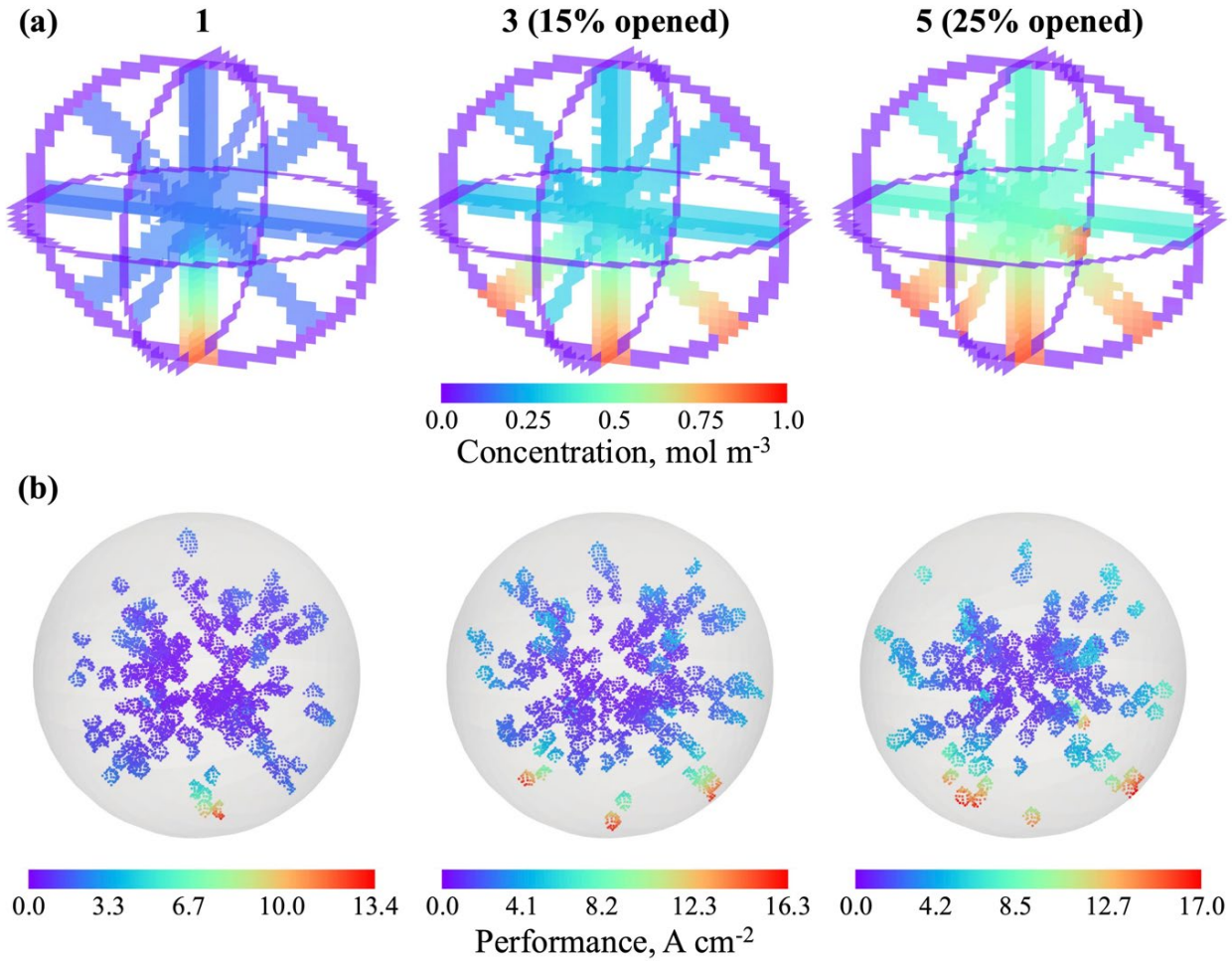


- At η 0.2 V, mesopore O_2 is not bound by Henry's law and exceeds ionomer levels, so internal Pt outperforms Vulcan.
- At η 0.4 V, O_2 must cross the ionomer into blocked pores; internal sites starve and the mesoporous particle falls behind Vulcan.
- Cross-ionomer resistance is the persistent bottleneck. Open pores are required to use internal Pt.

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Results & discussion

Effect of open pores

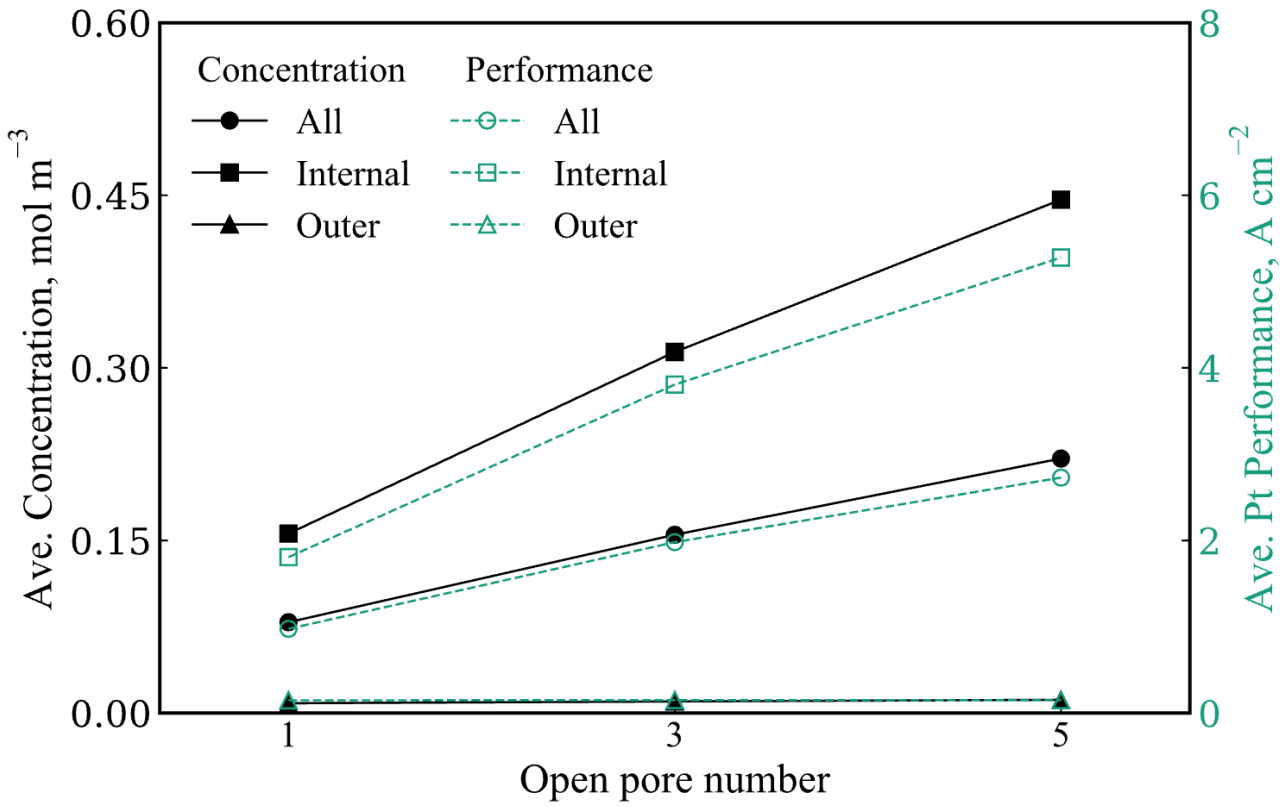


- Even one open pore substantially elevates the local C_{in}, which provides markedly superior local performance
- With increasing numbers of open pores, the C_{in} rises further, leading to a enhancement in internal performance

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Results & discussion

Effect of open pores

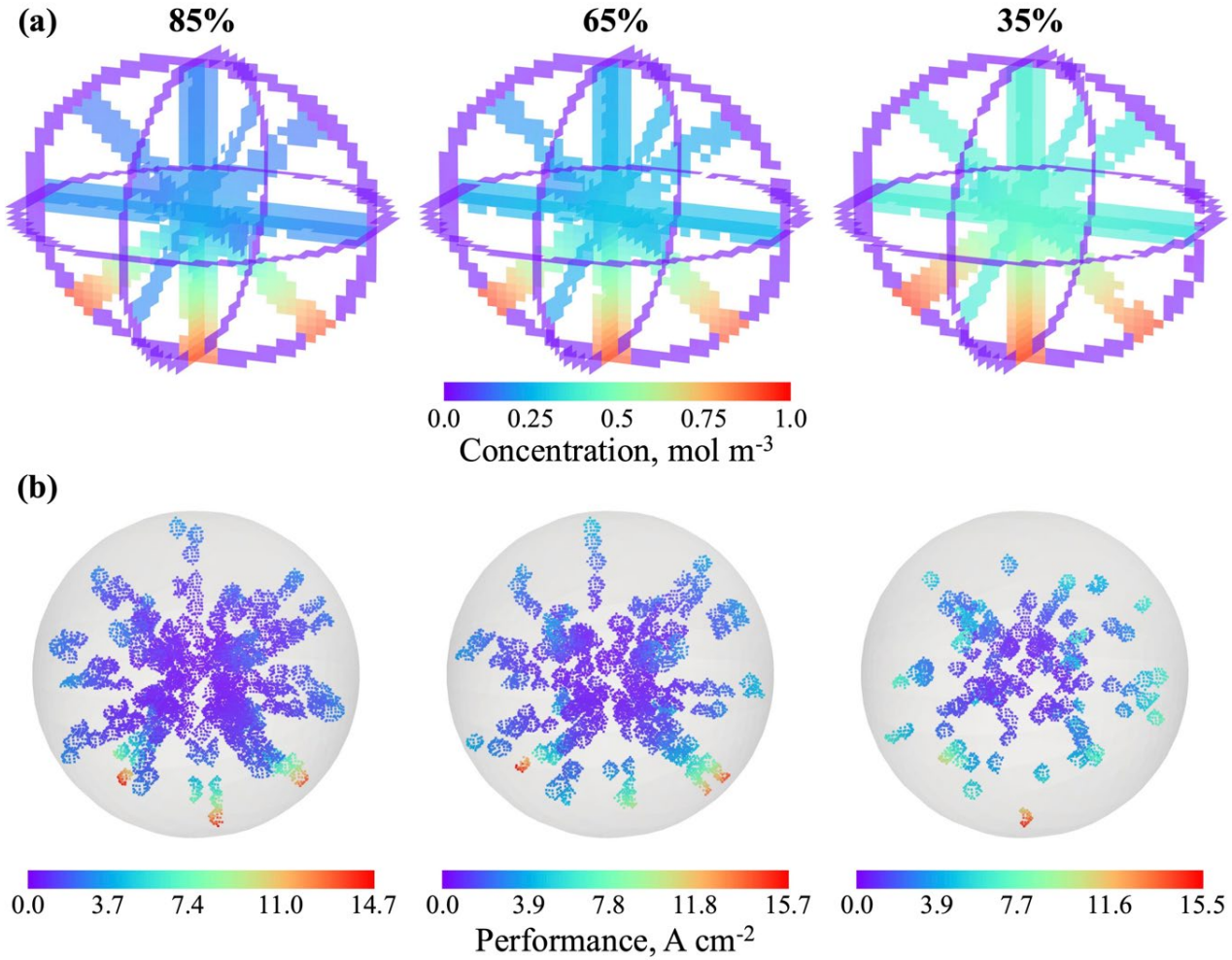


- Even one open pore substantially elevates the local C_{in}, which provides markedly superior local performance
- With increasing numbers of open pores, the C_{in} rises further, leading to a enhancement in internal performance
- Outer Pt particles coated by ionomer exhibit orders-of-magnitude lower performance and oxygen concentration compared to the internal Pt

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Results & discussion

Effect of internal Pt ratio

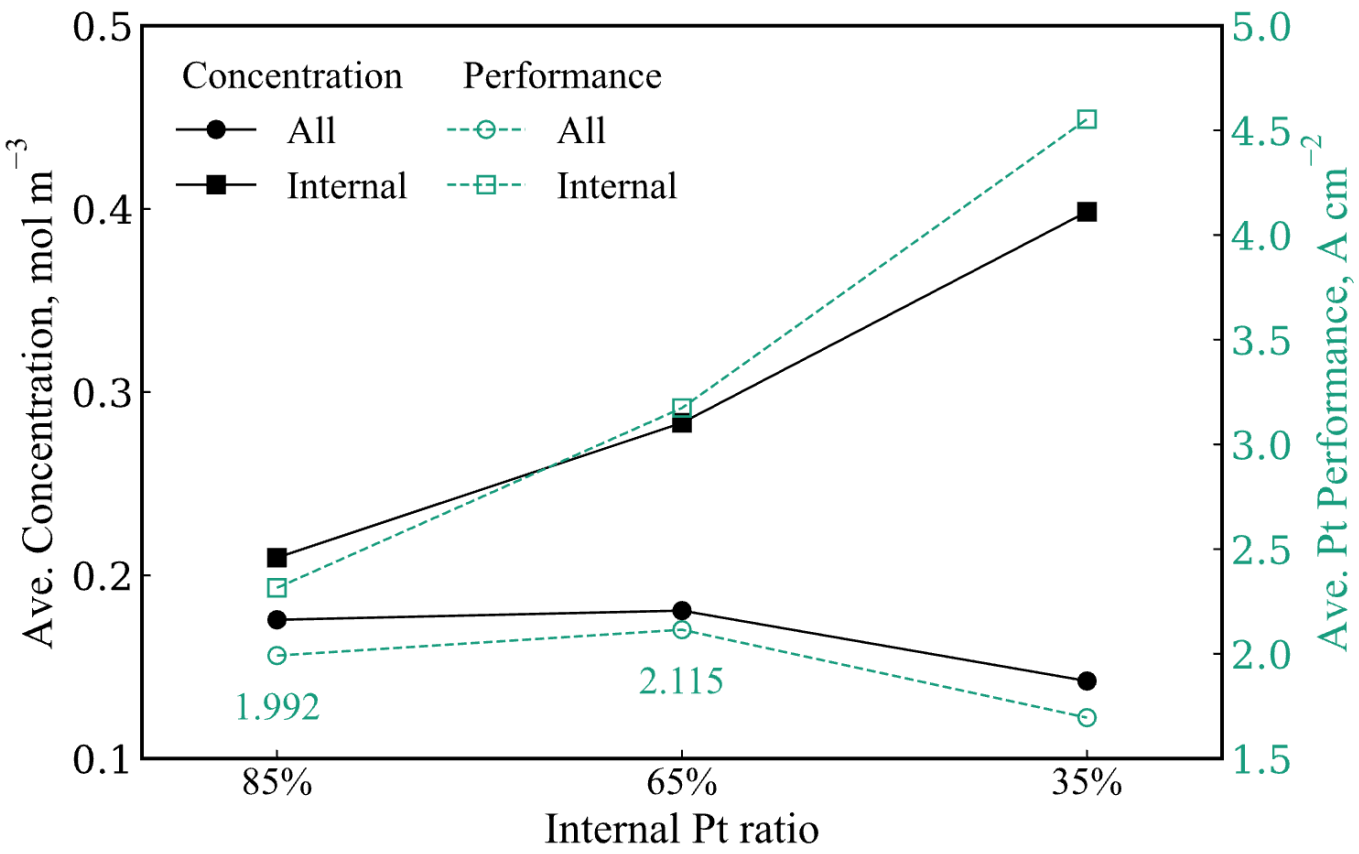


- A decrease in the internal Pt ratio from 85% to 35% reduces internal reactive sites, lowering oxygen consumption and increasing internal oxygen concentration.

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Results & discussion

Internal Pt ratio: overall vs internal performance

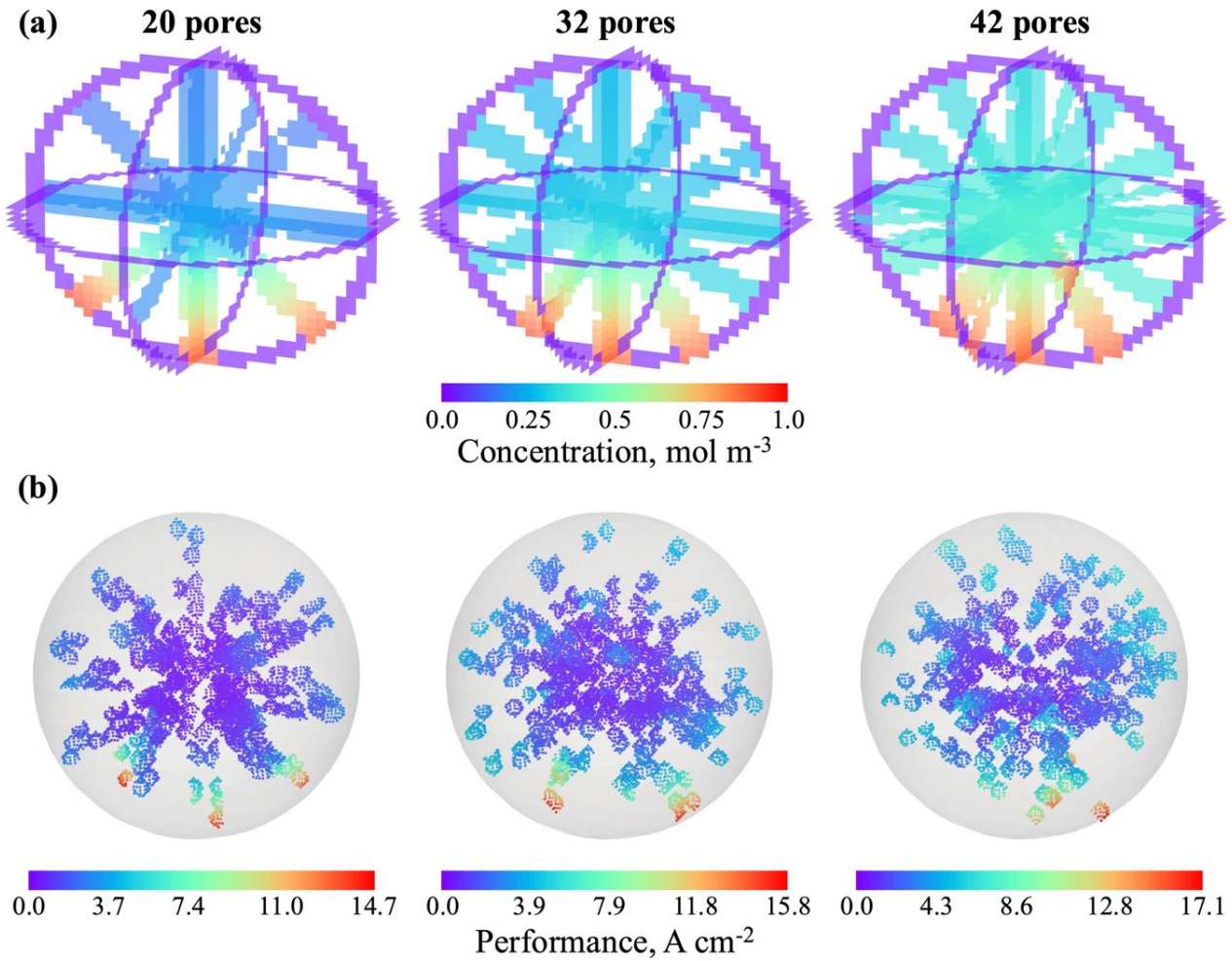


- A decrease in the internal Pt ratio from 85% to 35% reduces internal reactive sites, lowering oxygen consumption and increasing internal oxygen concentration.
- 85% internal Pt overcrowds blocked channels and lowers both internal and overall current.
- 35% internal Pt leaves most sites ionomer-coated and poisoned, so overall performance is the lowest.

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Results & discussion

Effect of internal pore number

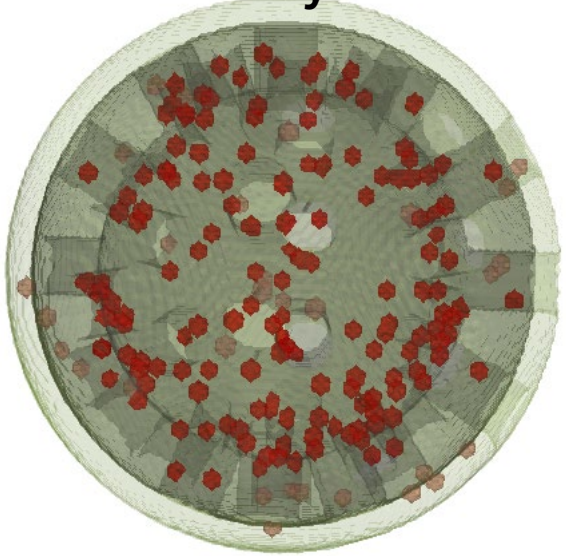


- As internal pores increase from 20 to 42, open pores rise, improving oxygen accessibility and elevating oxygen concentrations within the structure
- The internal Pt particles show a huge performance drop due to the proton transport resistance.

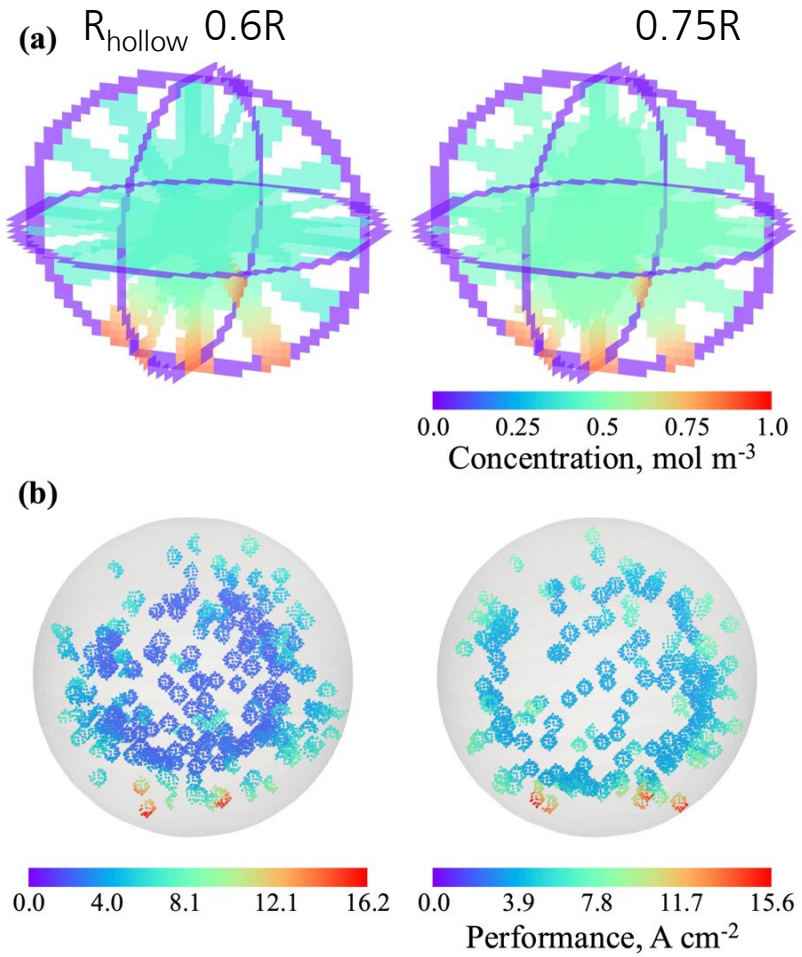
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Results & discussion
Hollow-shell carbon

Hollow-shell carbon catalyst



A hollow core keeps internal Pt near the outer ionomer.

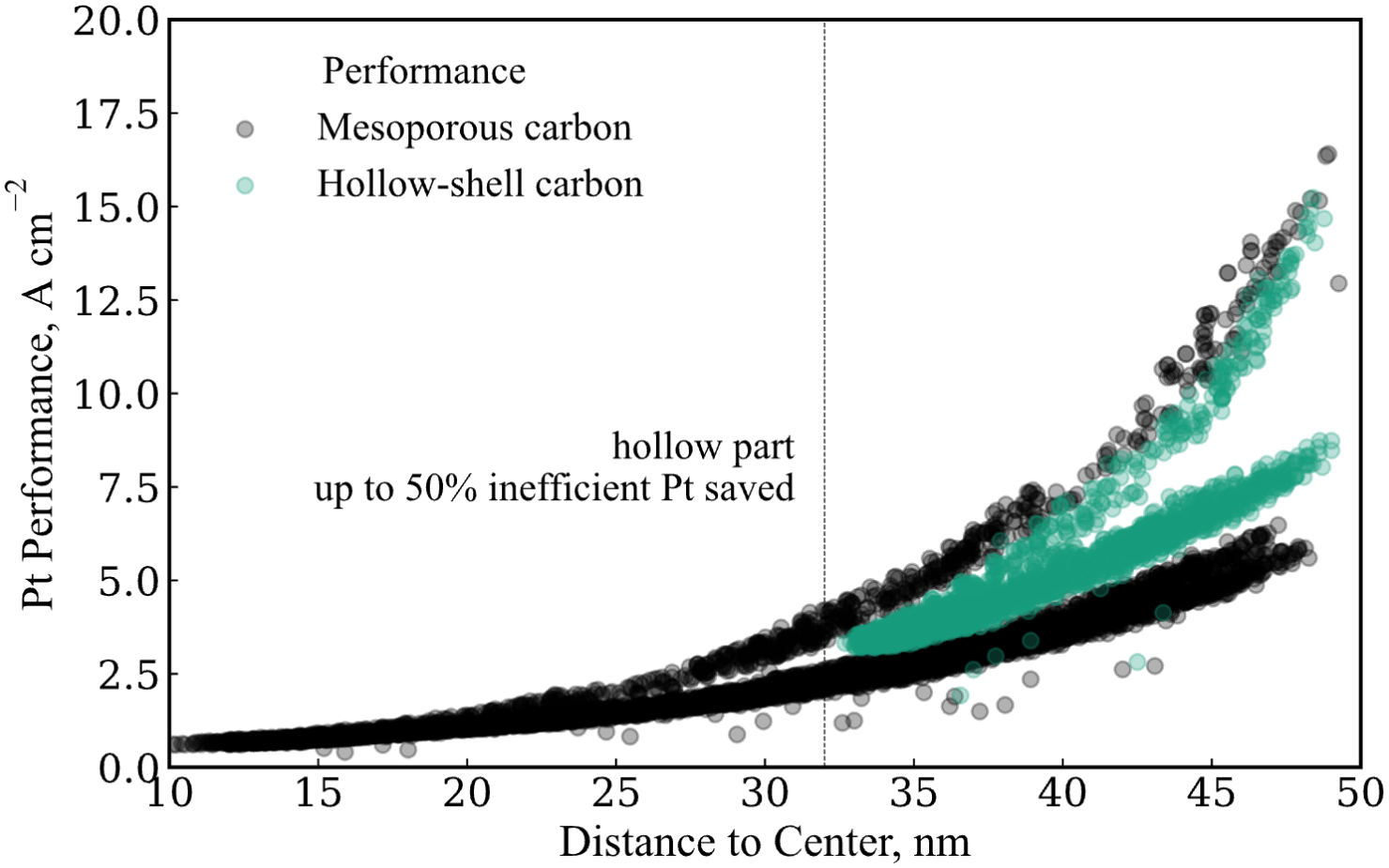


- The hollow-shell structure noticeably reduces the internal performance gap.
- A larger void space makes the internal performance both more uniform and higher.

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Results & discussion

Hollow-shell carbon vs mesoporous carbon



- Local performance rises toward the outer surface
- A high-performing cluster sits in open pores.
- Core-embedded sites stay low performance despite similar C_{O2} due to proton conduction.
- A hollow core removes that inefficient inner Pt (up to 50%) and parks remaining Pt in the proton sweet spot.

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Conclusion

- A pore-scale model is applied to optimize the microstrure of mesoporous carbon support.
- Internal Pt outperforms ionomer-coated Pt with adequate oxygen supply.
- Design guides: open pores provide efficient oxygen pathways; optimal internal Pt ratio depends on mass transport condition; proton resistance limits deeper internal Pt performance.
- Hollow-shell design can relocate the inefficient inner Pt to the high performance region, significantly reducing Pt loading.

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Thank You for Your Attention!

Dr. Yuze Hou
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