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Questions

Webinar staff to everyone

Welcome to "How Wildfire Smoke Impacts the Quality of Wine" with Associate Professor of Enology Elizabeth Tomasino of Oregon State University. This ACS Webinar is moderated by Gavin Sacks of Cornell University and co-produced with the ACS Division of Agricultural & Food Chemistry. Say "hello" to Elizabeth and Gavin in the questions window and tell us where you are joining us from today.

Webinar staff to everyone

Q: Hello! I'm from Oshkosh, Wisconsin

A: Glad you could join us!
1:54 PM

Webinar staff to everyone

Q: Good afternoon! I'm joining from Murfreesboro, TN.

A: Good to see you here.
1:54 PM

Webinar staff to everyone

Q: Hello! Doug here, Redding California.

A: Good to see you here Doug!
1:54 PM



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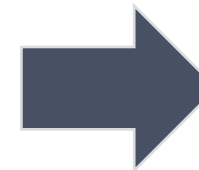
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hyperlinks from our team





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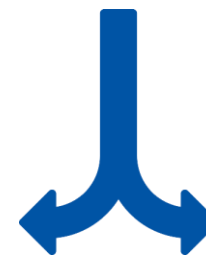


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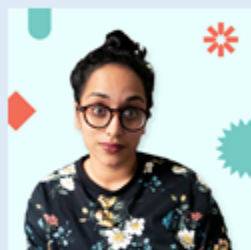
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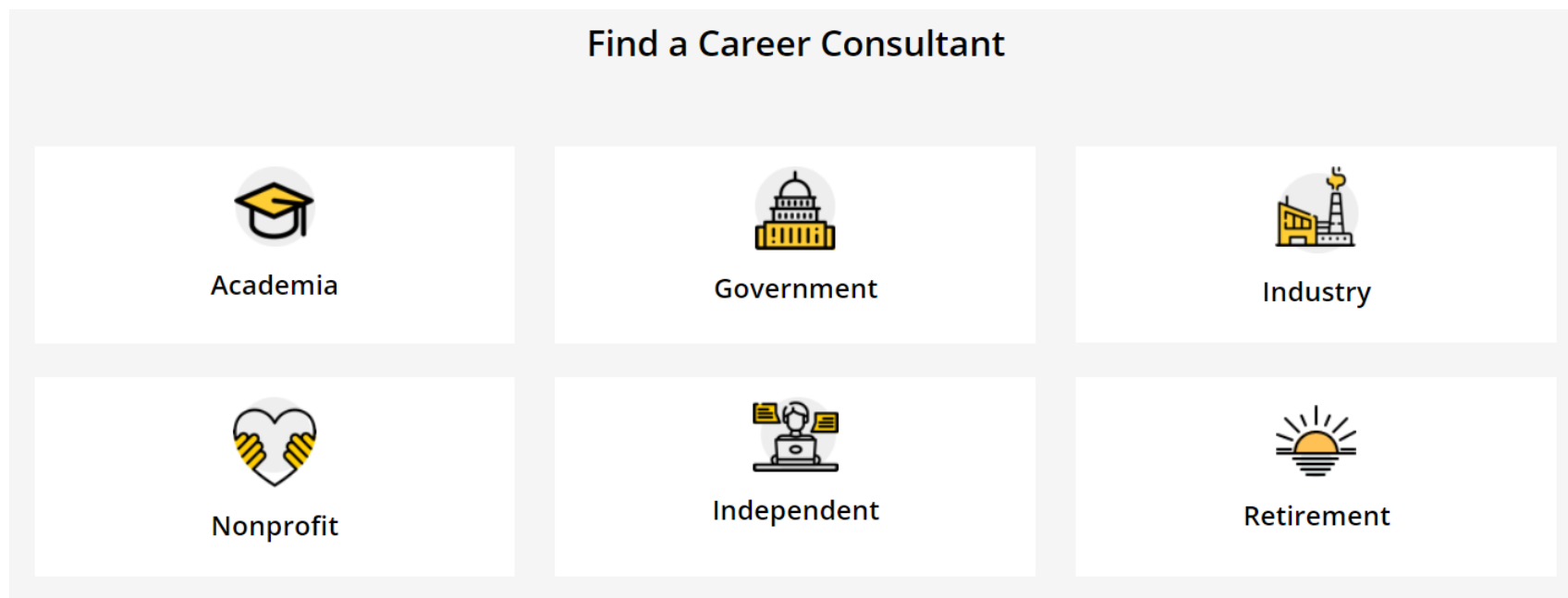
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BS, Massachusetts Institute of Technology, June 2021

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🕒 August 4, 2022

1
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NEXT WEEK!



Wed., May 11, 2022 | 2:00pm–3:00pm ET

Adapting to Climate Change: Insights from Indigenous Peoples

Co-produced with ACS Policy and the American Association
for the Advancement of Science

NEXT WEEK!



Thurs., May 12, 2022 | 2:00pm–3:00pm ET

Careers in Chemical Safety for Chemists

Co-produced with the ACS Division of Chemical Health and
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Tues., May 17, 2022 | 1:00pm–2:00pm ET

From There to Here: My Asian American Journey

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Role of Polymer Science in Water Purification Membranes



ABHISHEK ROY, Ph.D.

Senior Staff Scientist, National
Renewable Energy Laboratory



GEOFFREY GEISE, Ph.D. M.S.E.

Associate Professor of Chemical
Engineering and Materials Science and
Engineering (by courtesy), and ChE
Undergraduate Program Coordinator,
University of Virginia



SYED ISLAM, Ph.D.

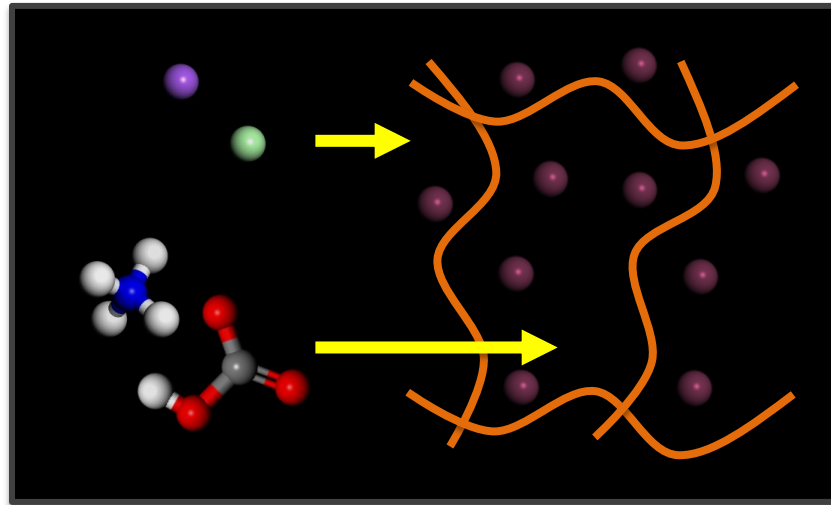
R&D Associate Staff, Chemical
Sciences Division, Oak Ridge
National Laboratory

This ACS Webinar[®] is co-produced with the ACS Division of Polymer Chemistry.

Controlling desalination via polymer membrane chemistry

Geoffrey M. Geise

The University of Virginia
Charlottesville, Virginia



Role of Polymer Science in Water Purification Membranes

May 5, 2022

Audience Survey Question

ANSWER THE QUESTION ON SCREEN IN ONE MOMENT



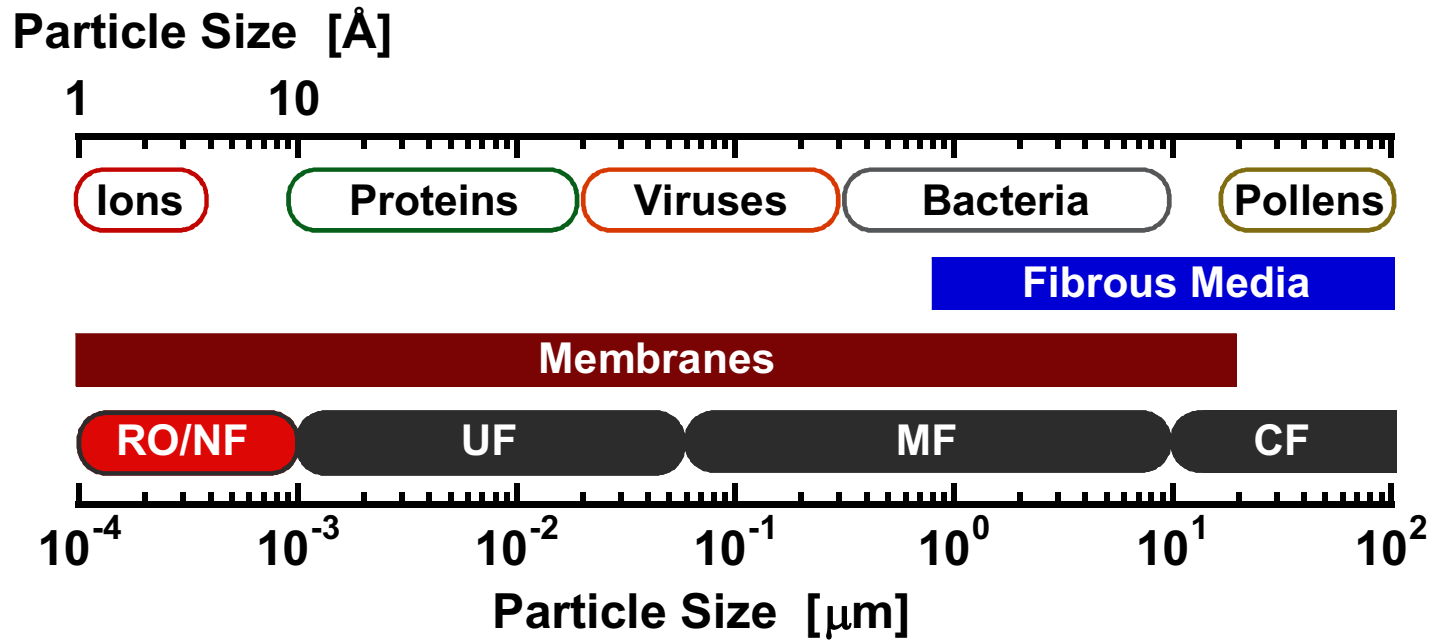
Which factors are most important for governing performance of polymeric desalination membranes (e.g., reverse osmosis membranes)?

- Thermodynamic factors
- Kinetic/diffusive factors
- Both
- None

** If your answer differs greatly from the choices above tell us in the chat!*

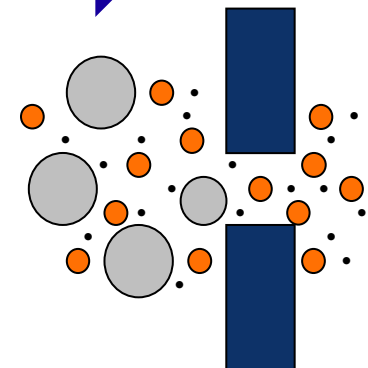
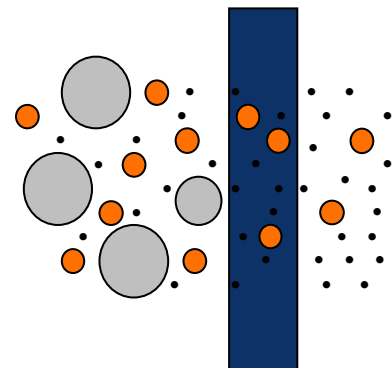
Generally, ion selective membranes are considered to be solution-diffusion materials

Geise, et al.,
J. Polym. Sci. Part B,
48 (2010)
1685-1718.



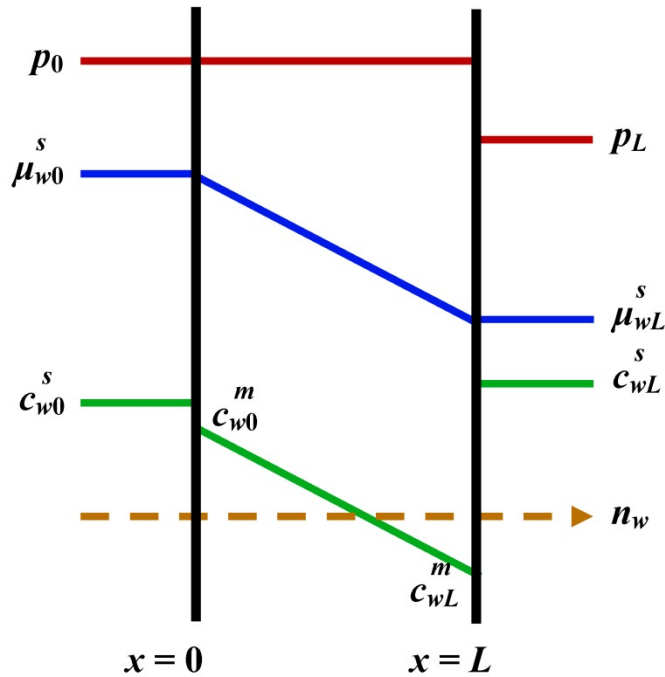
**Solution-Diffusion
(Non-Porous)
Membrane**

**Pore-Flow
Membrane**



Water and salt transport in non-porous polymers is described by a solution-diffusion mechanism

Water Transport

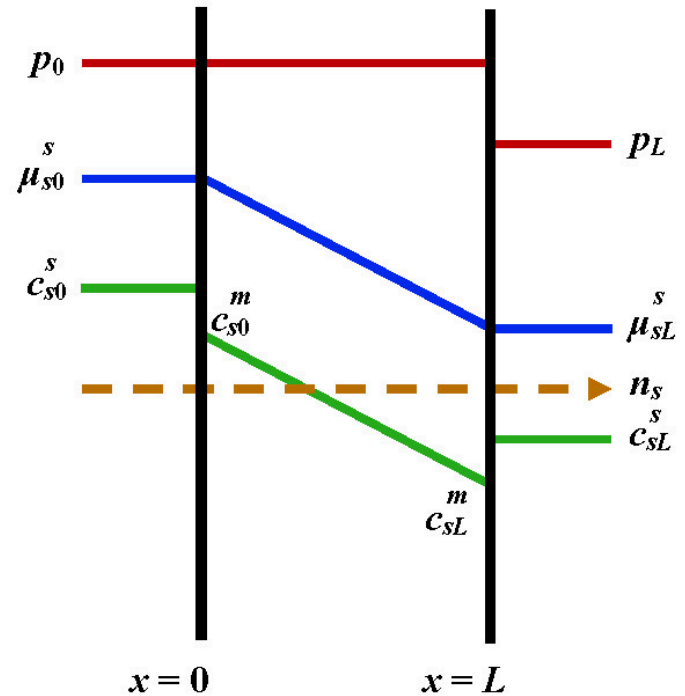


$$n_w = \frac{D_w}{L} \Delta c_w^m$$

$$P_i = K_i \times D_i$$

$$n_w = \frac{P_w}{L} \frac{\bar{V}_w}{RT} (\Delta p - \Delta \pi)$$

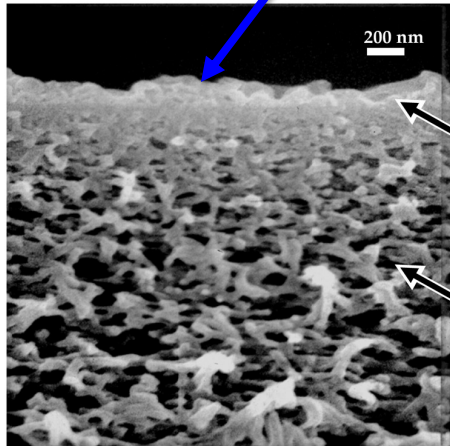
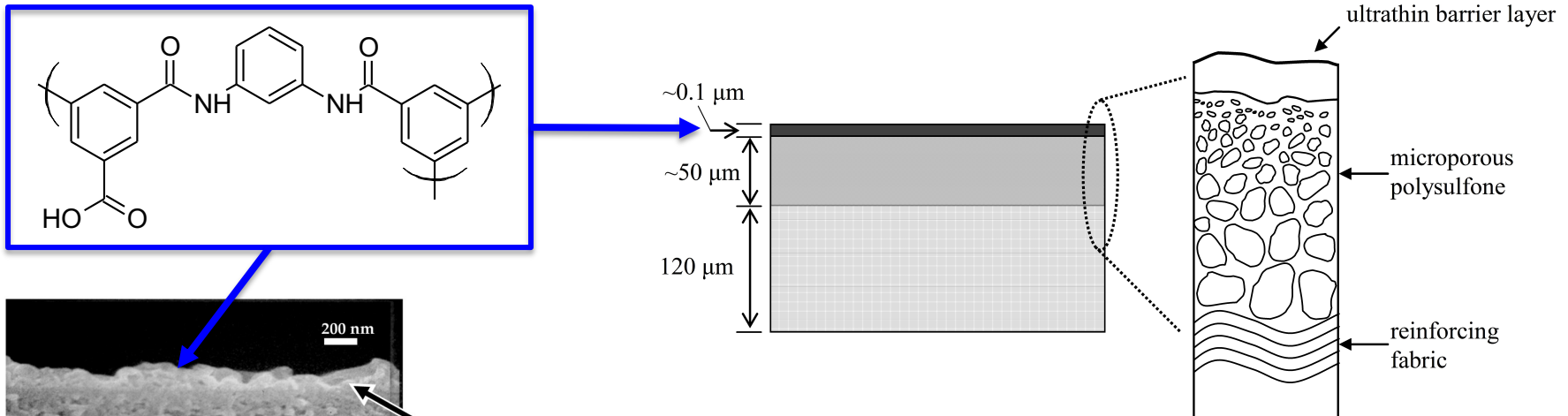
Salt Transport



$$n_s = \frac{D_s}{L} \Delta c_s^m$$

$$n_s = \frac{P_s}{L} \Delta c_s^s$$

Commercial RO membrane active layers sorb relatively little water



Ultrathin Polyamide Active Layer
Thickness: ~100 nm

Microporous Polysulfone
Thickness: ~50 μm

Geise, et al., *J. Polym. Sci. Part B: Polym. Phys.* **48** (2010) 1685.

Mass Fraction of Water in the PA Active Layer:

ESPA1 (low-energy RO): **0.02-0.08**

SWC1 (seawater RO): **0.04-0.06**

*Freger, *Environ. Sci. Technol.* **38** (2004) 3168.

DOW PA Active Layer Water Uptake ~5%

*A. Roy, Personal Communication, 2015.

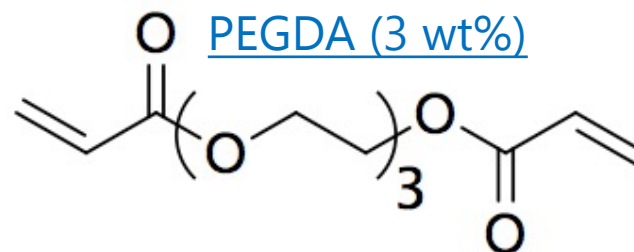
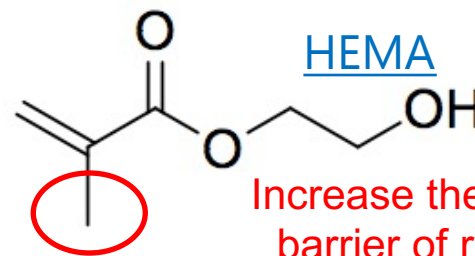
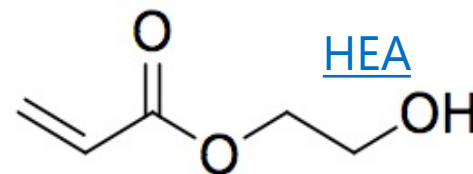
RO membrane polymer water content:

Different from ion exchange materials, such as Nafion (~30% water by volume)

*Paddison, Reagor, Zawodzinski, *Electroanal. Chem.* **459** (1998) 91.

We are interested in understanding the influence of polymer backbone rigidity on water/salt selectivity

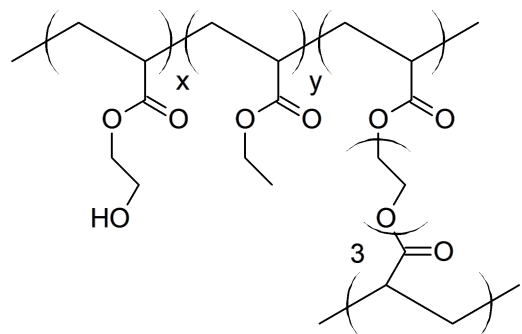
- **Choose materials with similar chemistry**
 - Ideally, only the backbone rigidities should be different
- **Prepare materials of comparable water content**
 - Transport properties are highly sensitive to water content
- **Consider ranges of water content that are relevant for desalination membranes**
 - 4-8% (by mass)
- **Study homogeneous polymers**
 - Avoid complications due to morphology



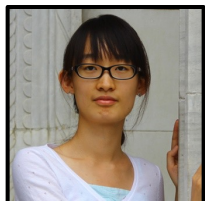
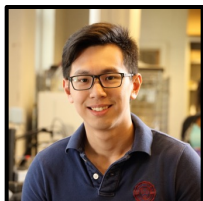
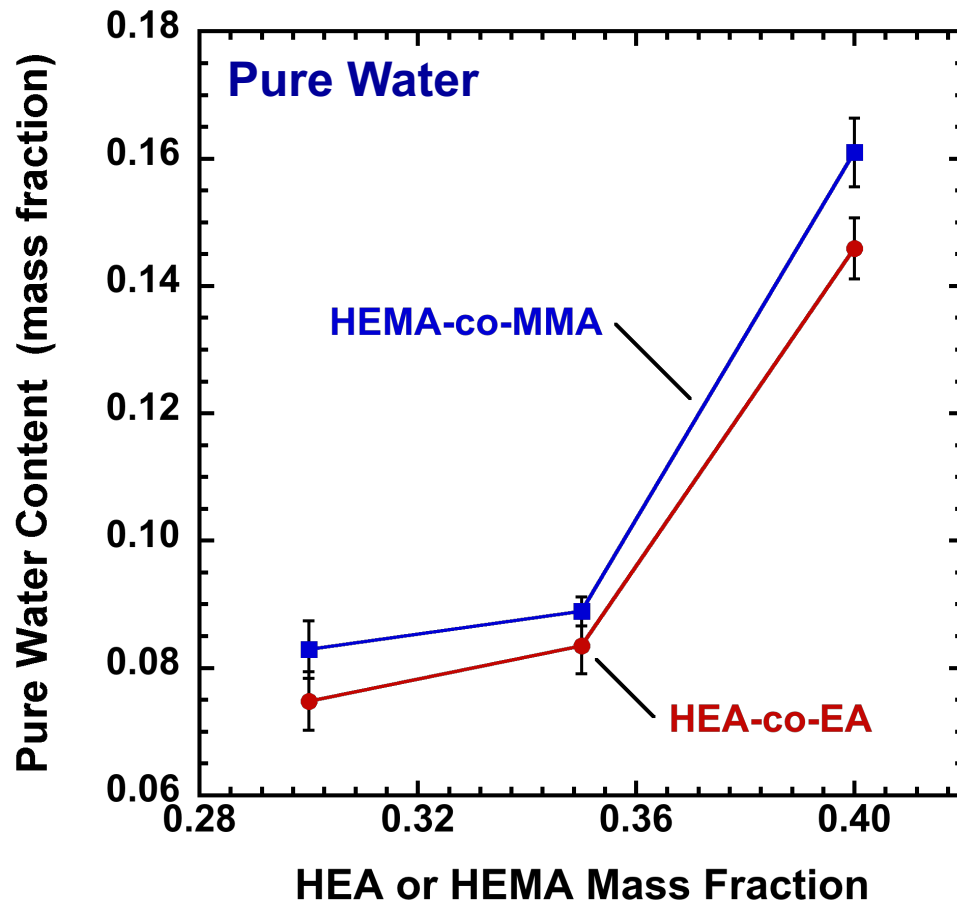
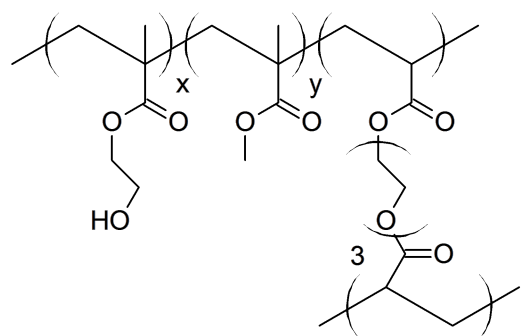
Crosslinked Polymer	Water Uptake [g(water)/g(dry polymer)]
XL-PHEA	1.6
XL-PHEMA	0.6

Copolymerizing HEA with EA and HEMA with MMA addressed the need to be able to prepare materials with comparable water content

Poly(HEA-co-EA)



Poly(HEMA-co-MMA)



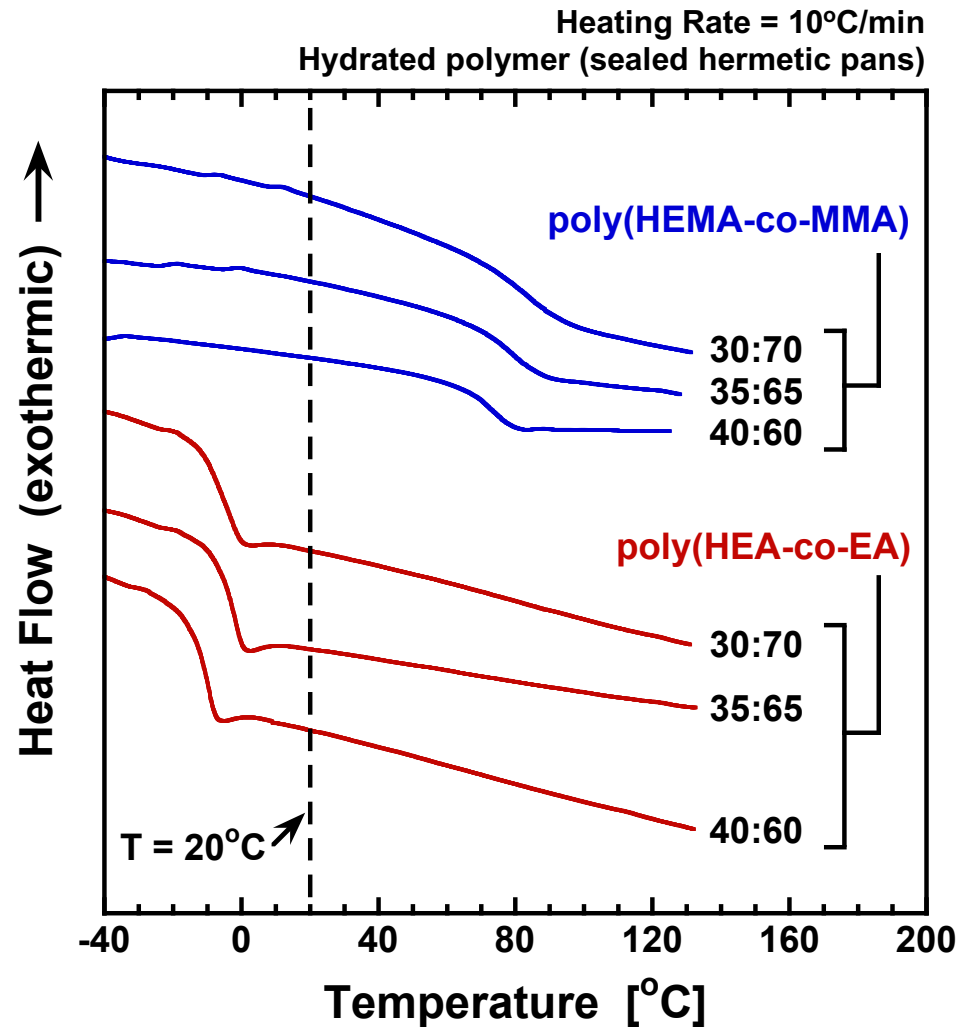
Kevin Chang Tianyi Xue (M.S. 2015)

Segmental dynamics and homogeneity were probed by making DSC measurements on hydrated films

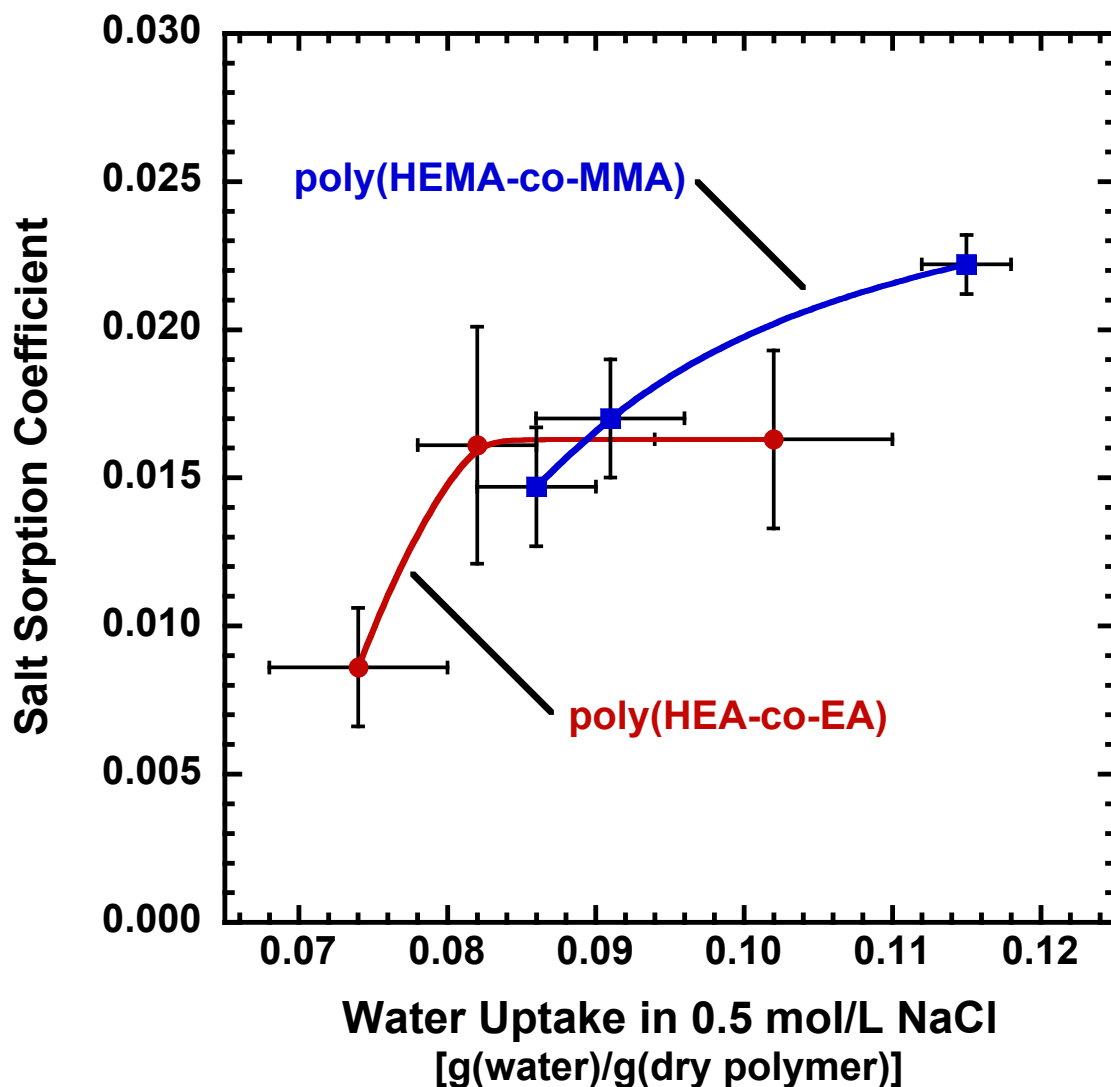
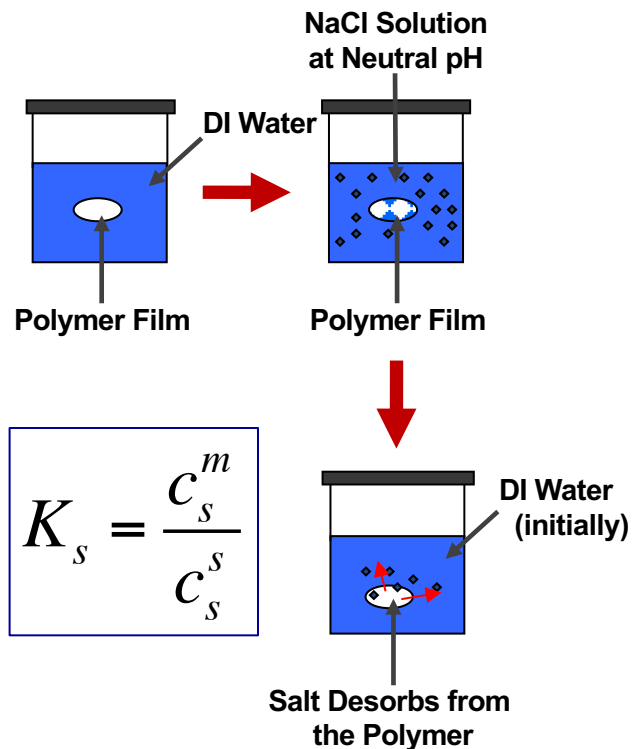
HEA-co-EA: Room temperature is above the glass transition meaning these films are in the *rubbery* state

HEMA-co-MMA: Room temperature is below the glass transition meaning that segmental dynamics are kinetically locked in a *glassy* state

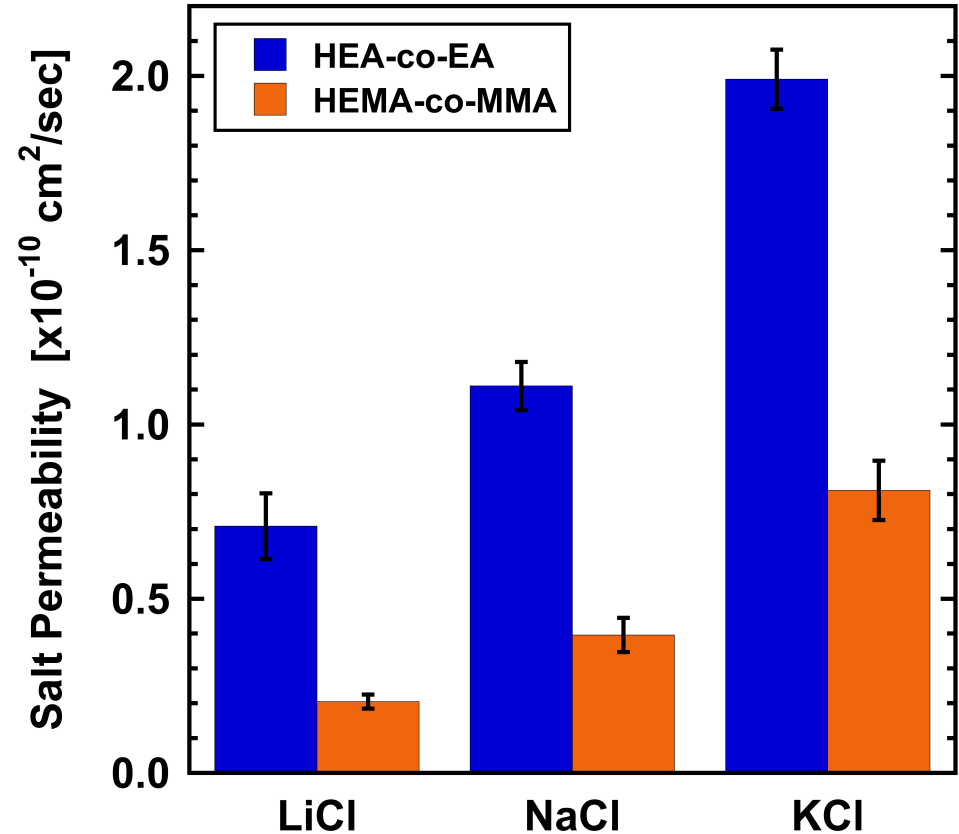
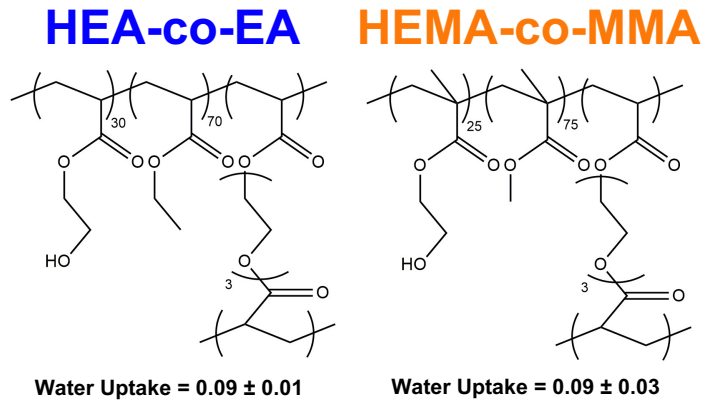
The observation of a single T_g in these copolymers suggests that they are relatively homogeneous



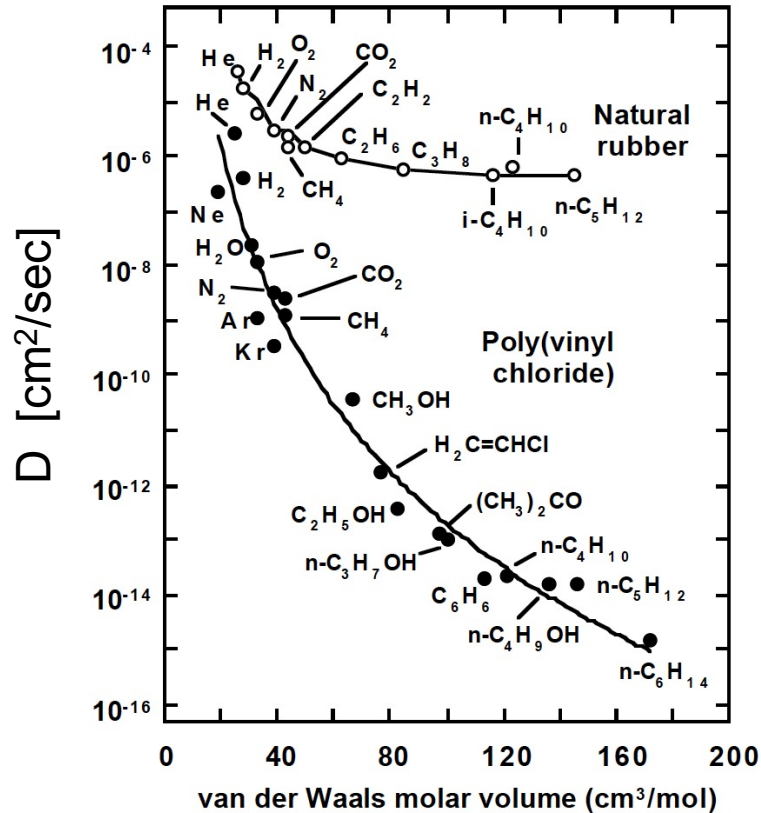
Salt sorption coefficient curves overlay suggesting that polymer chemistry (from a salt sorption perspective) is similar in our materials



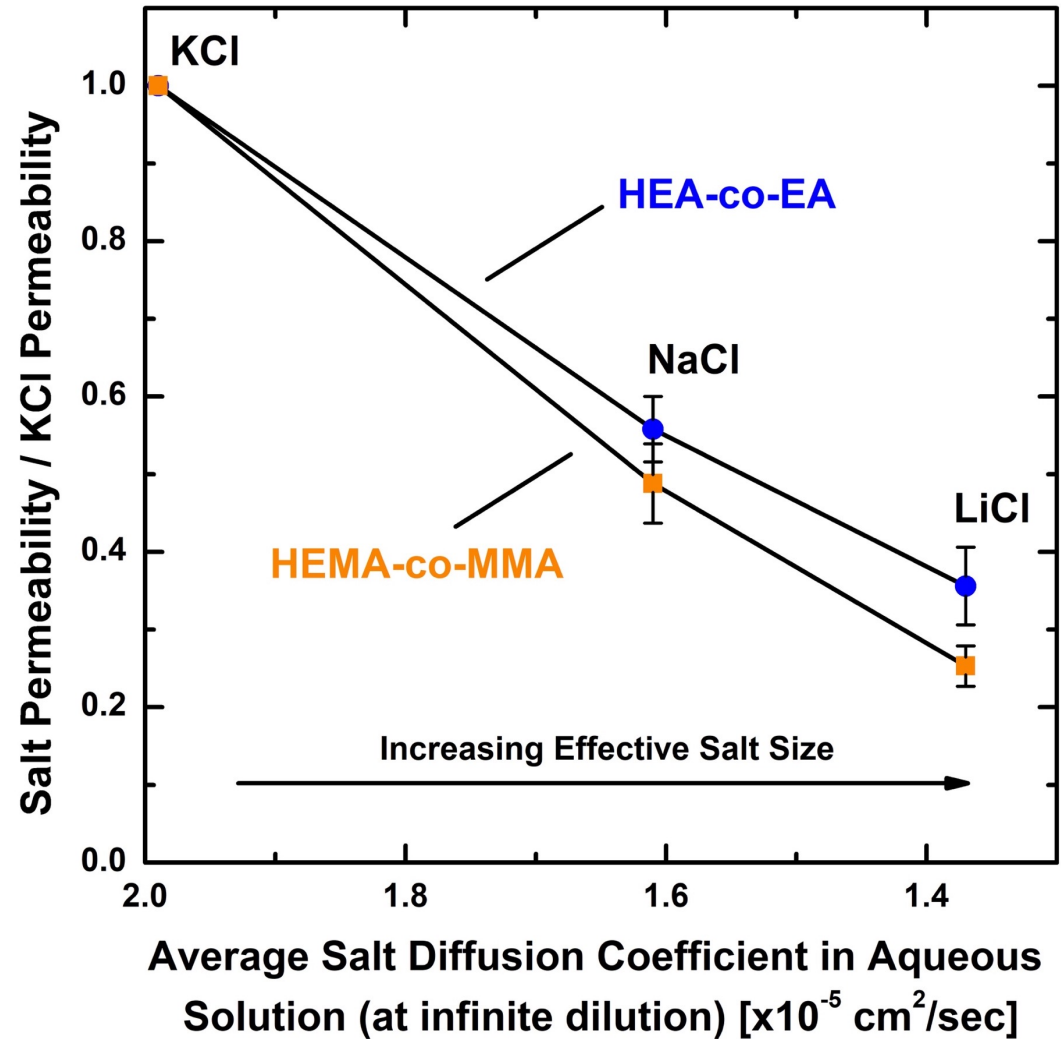
Salt permeation is faster in HEA-co-EA compared to HEMA-co-MMA



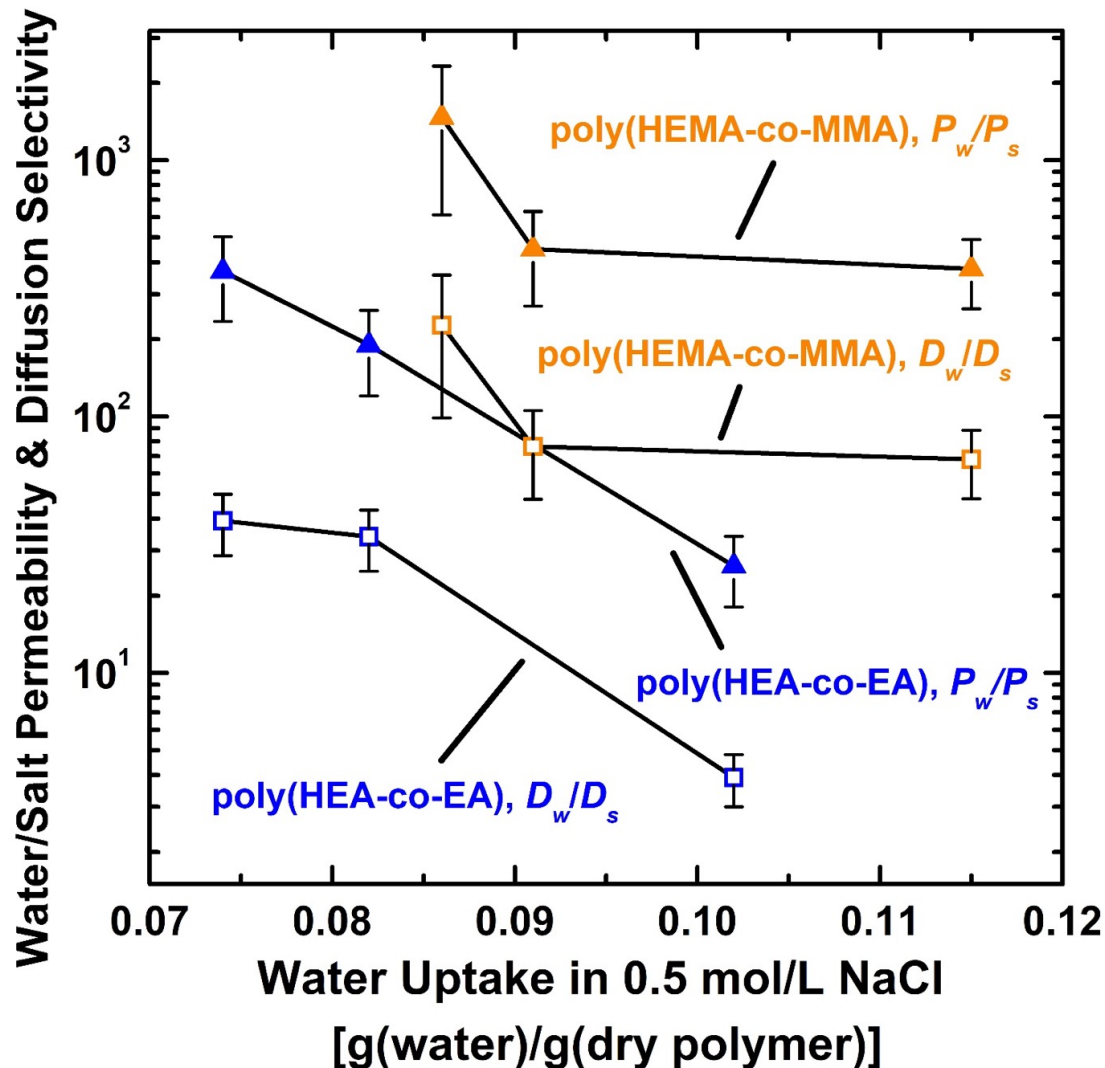
Polymer backbone rigidity also enhances size selectivity



Baker, R. W.; Wijmans, J. G., Membrane separation of organic vapors from gas streams. In *Polymeric gas separation membranes*, Paul, D. R.; Yampolskii, Y. P., Eds. CRC Press: Boca Raton, 1994; pp 353-397.

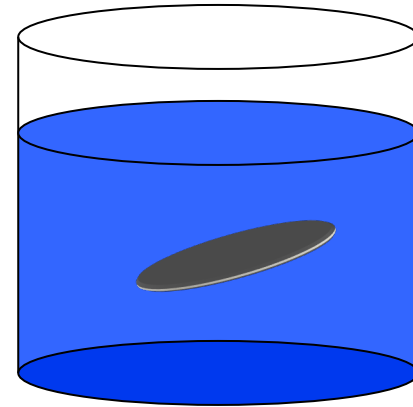


Water/salt permeability selectivity is higher in the more rigid copolymers compared to the more flexible copolymers



Structure-property relationship questions

Suppressing ion sorption is critical for preparing highly selective polymers for a wide range of membrane processes



Electrolyte Solution
(known composition)

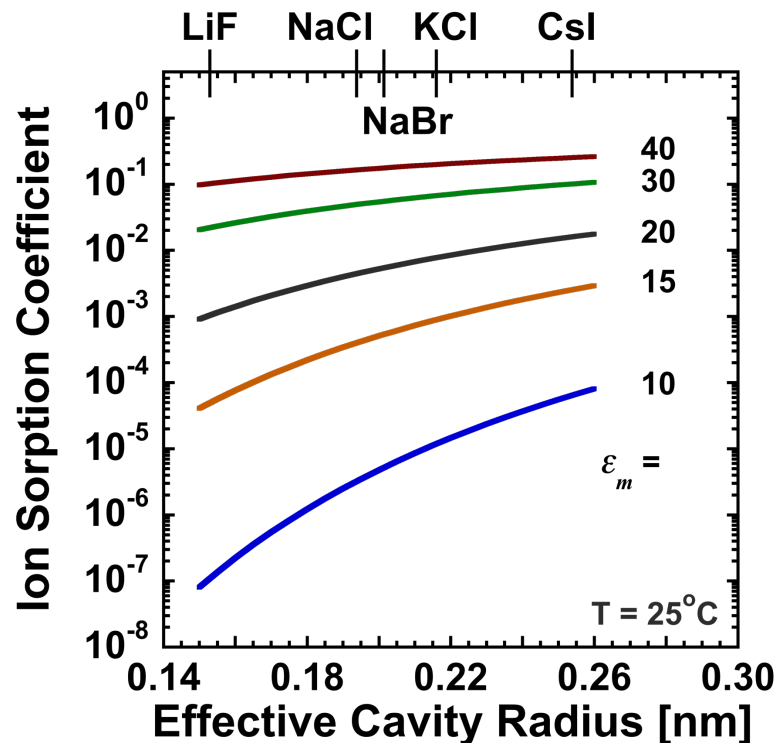
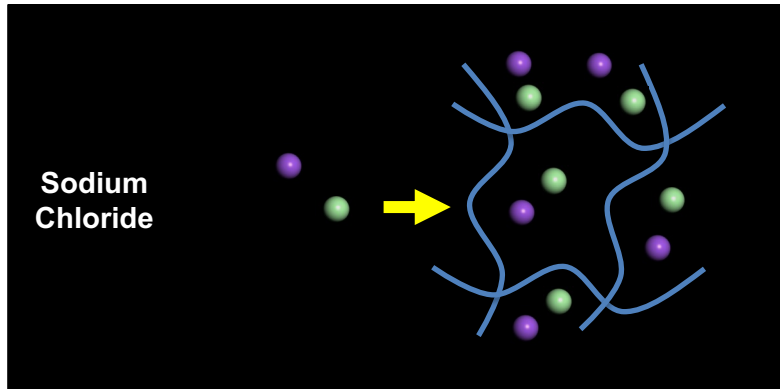
- **How do ions partition into the polymer?**
- **How do we control ion partitioning by controlling the molecular structure of the polymer?**

Thermodynamic view of ion sorption or partitioning

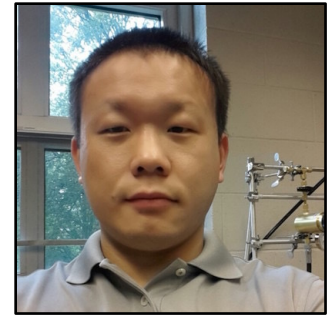
$$K_s \equiv \frac{c_X^m}{c_X^s} = \exp \left[-\frac{\Delta G_{X,sorption}}{RT} \right]$$

- **Electrostatics / charge density**
- **Dispersion forces**
- **Specific ion-polymer interactions**

Contribution of electrostatics to ion sorption



Huan Zhang
(M.E. 2015)



$$\Delta G_{Born} = \frac{z_i^2 e^2}{8\pi\epsilon_0 a_i} \left(\frac{1}{\epsilon_w} - \frac{1}{\epsilon_p} \right)$$

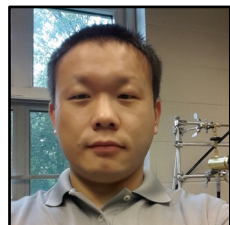
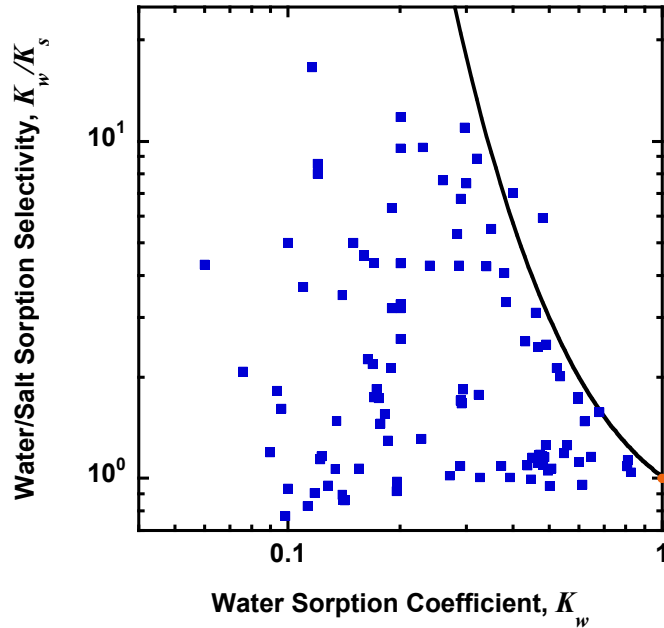
Charge density ↑

Hydrated Polymer Permittivity ↑

$$K_s = \exp \left[-\frac{z_i^2 e^2}{8\pi k T \epsilon_0 a_s} \left(\frac{1}{\epsilon_m} - \frac{1}{\epsilon_{sol}} \right) \right]$$

Need for relative permittivity information for hydrated polymers

$$\Delta G_{Born} = \frac{z_i^2 e^2}{8\pi\epsilon_0 a_i} \left(\frac{1}{\epsilon_m} - \frac{1}{\epsilon_w} \right)$$



Huan Zhang
(M.E. 2015)

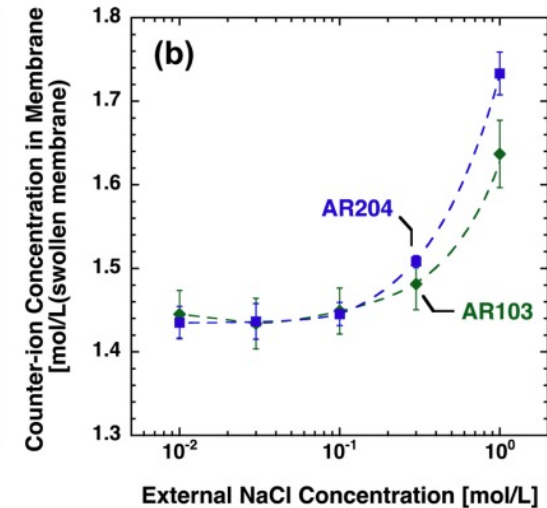
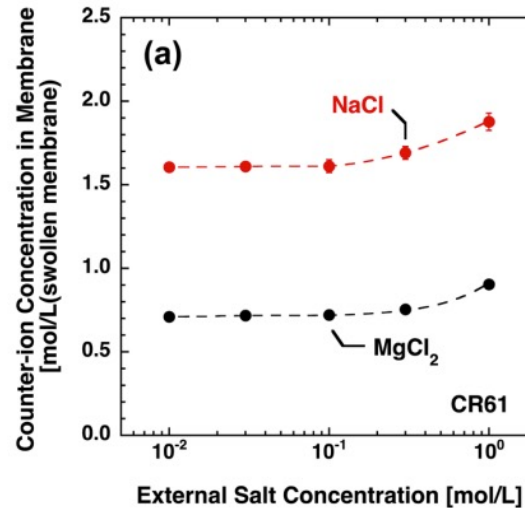
Zhang and Geise,
J. Membr. Sci.,
520 (2016) 790.

$$\gamma_+^m \gamma_-^m = \frac{\frac{C_A^m}{\xi C_-^m} + 1}{\frac{C_A^m}{C_-^m} + 1} \exp \left[\frac{-\frac{C_A^m}{\xi C_-^m}}{2 + \frac{C_A^m}{\xi C_-^m}} \right]$$

$$\xi = \frac{\lambda_B}{b} = \frac{e^2}{\epsilon k T b}$$

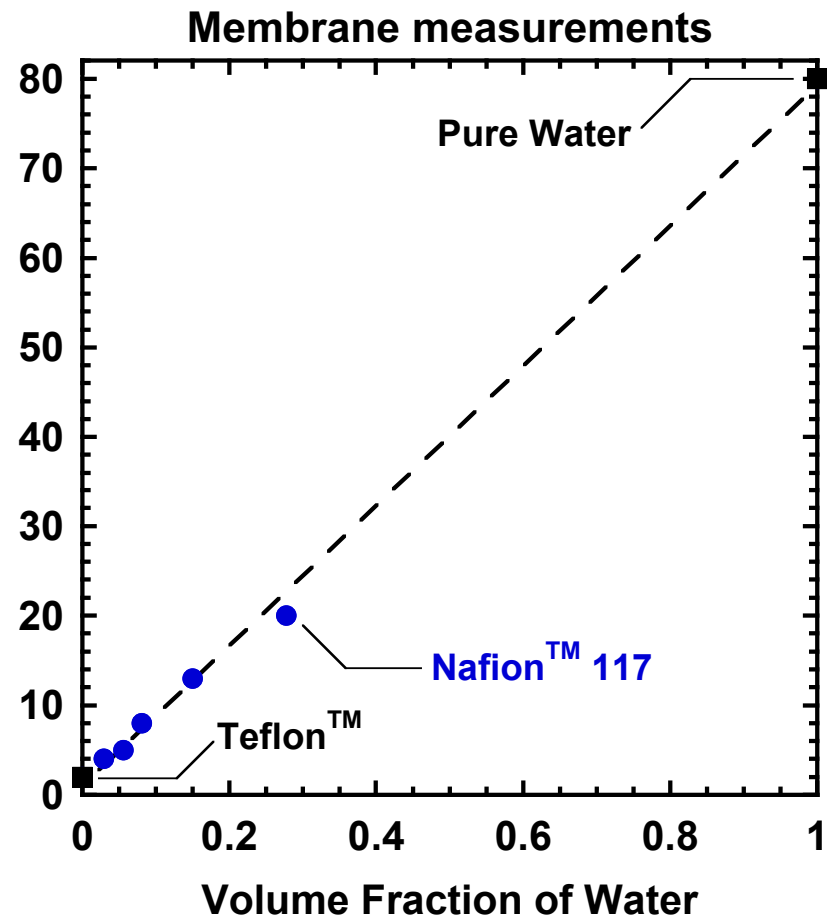
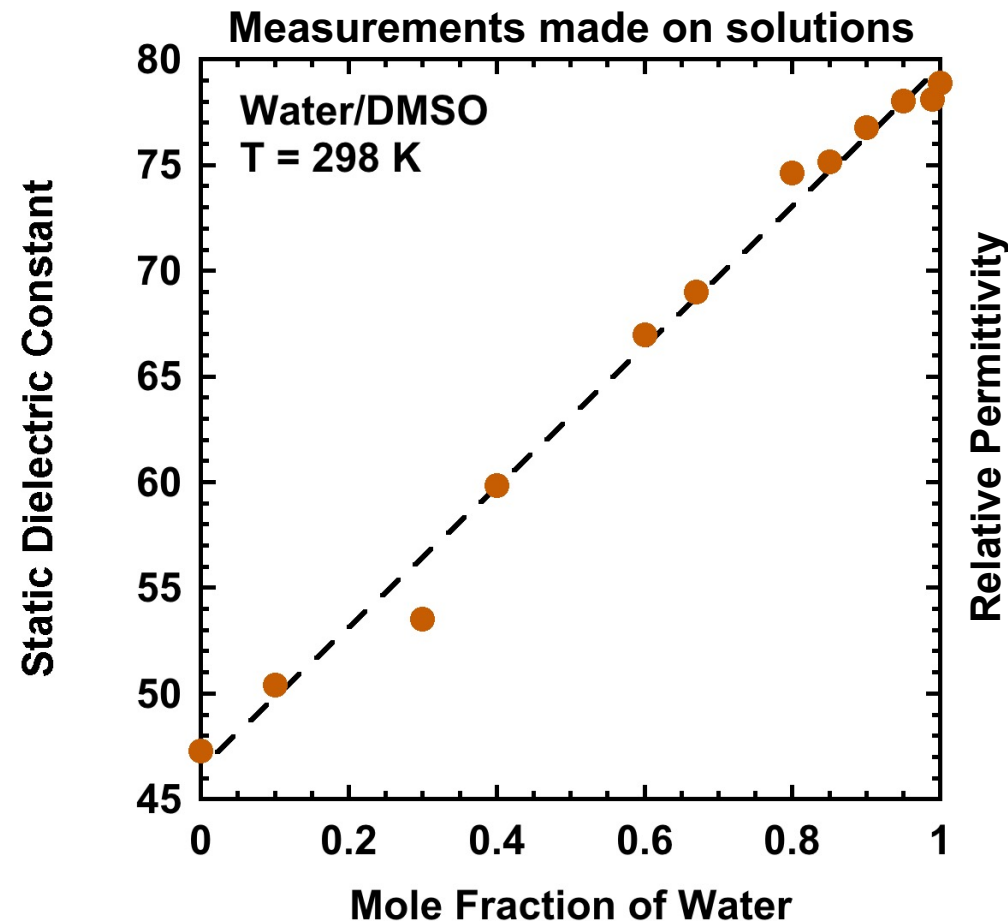
Bjerrum Length

Distance between fixed charges



Manning, *J. Chem. Phys.*, **51** (1969) 924.
Kamcev, et al., *ACS Appl. Mater. Interfaces*, **9** (2017) 4044.

Linear relationships between relative permittivity and water content are observed for some solvent and polymer systems

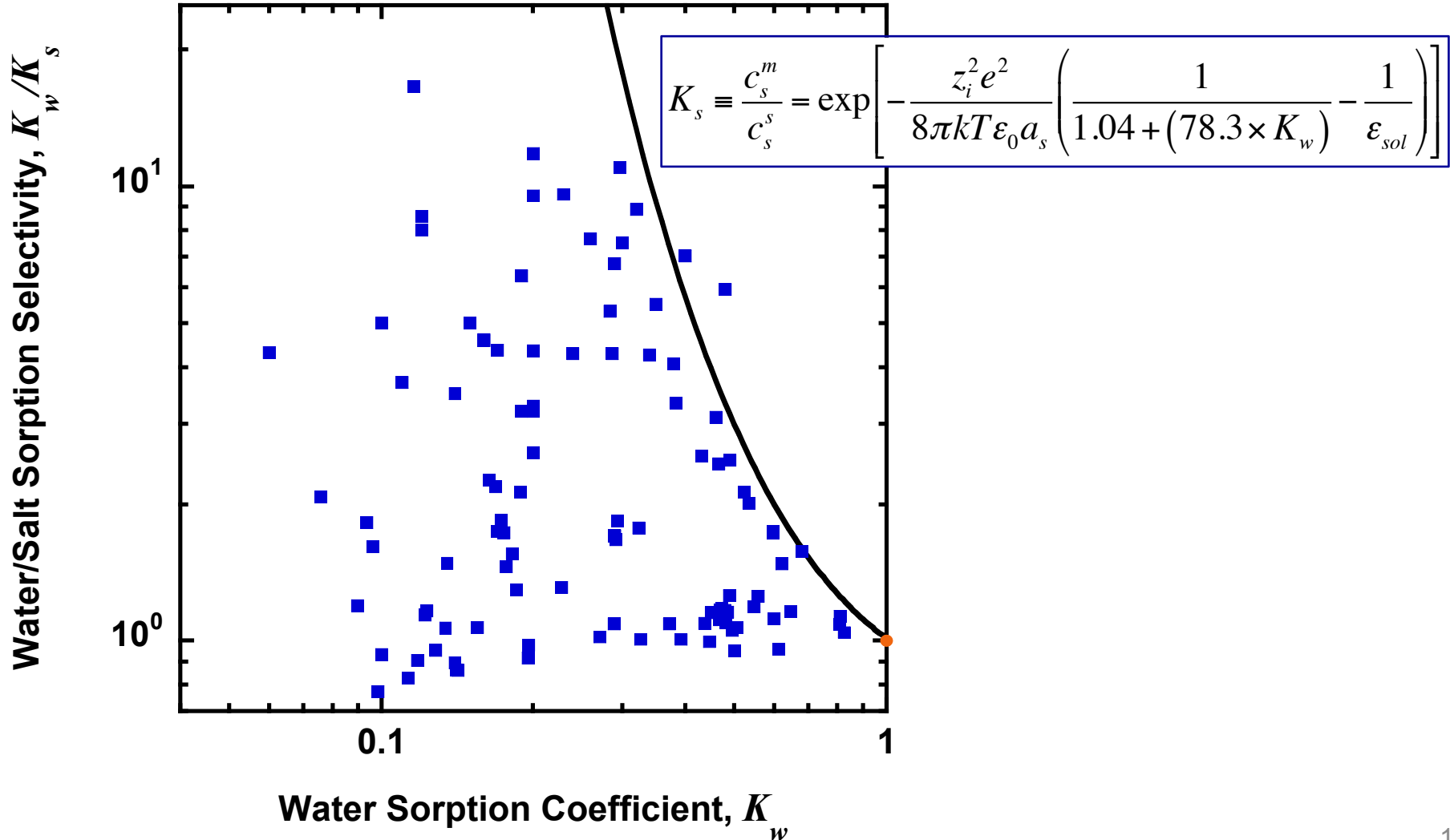


Zhang and Geise, *J. Membr. Sci.*, **520** (2016) 790.

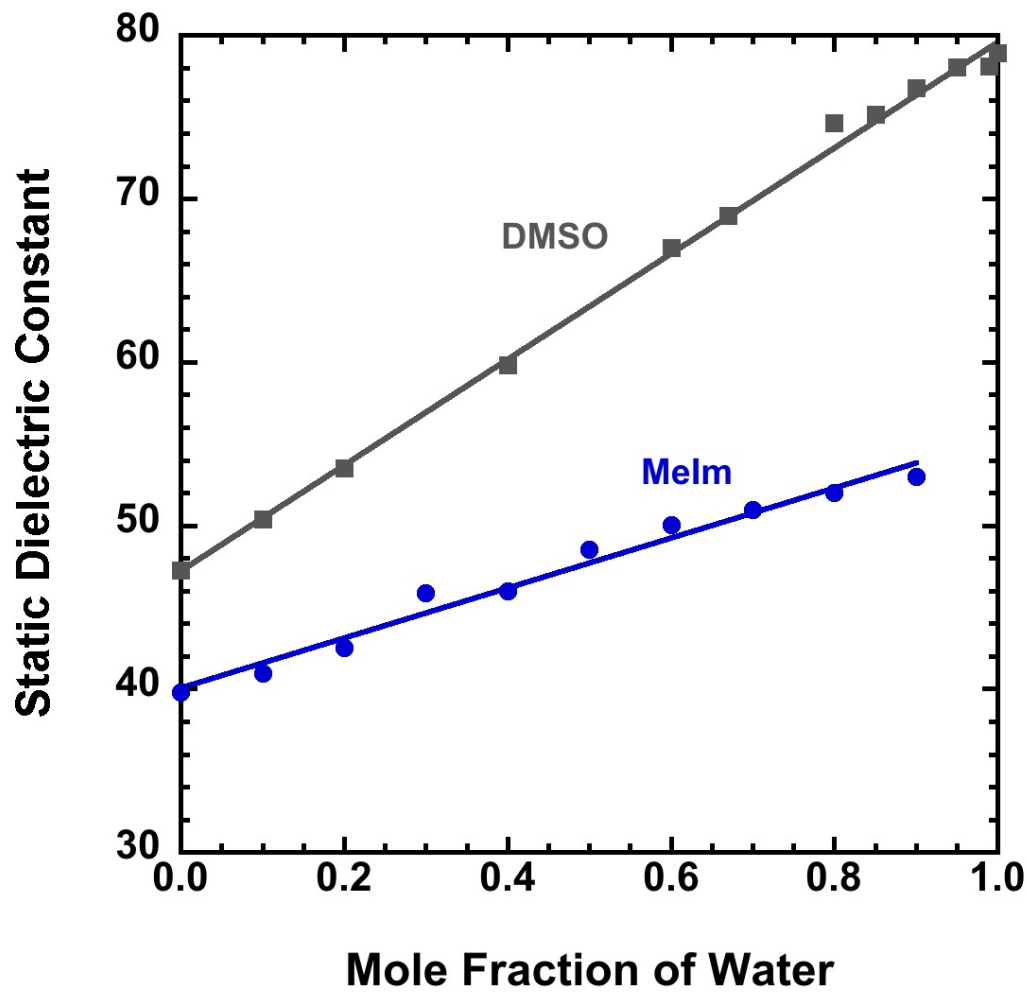
Paddison, Reagor, Zawodzinski, *J. Electroanal. Chem.*, **459** (1998) 91.

Lu, et al., *J. Phys. Chem. A*, **113** (2009) 12207.

Maximum co-ion sorption selectivity appears to be well described by the electrostatic model

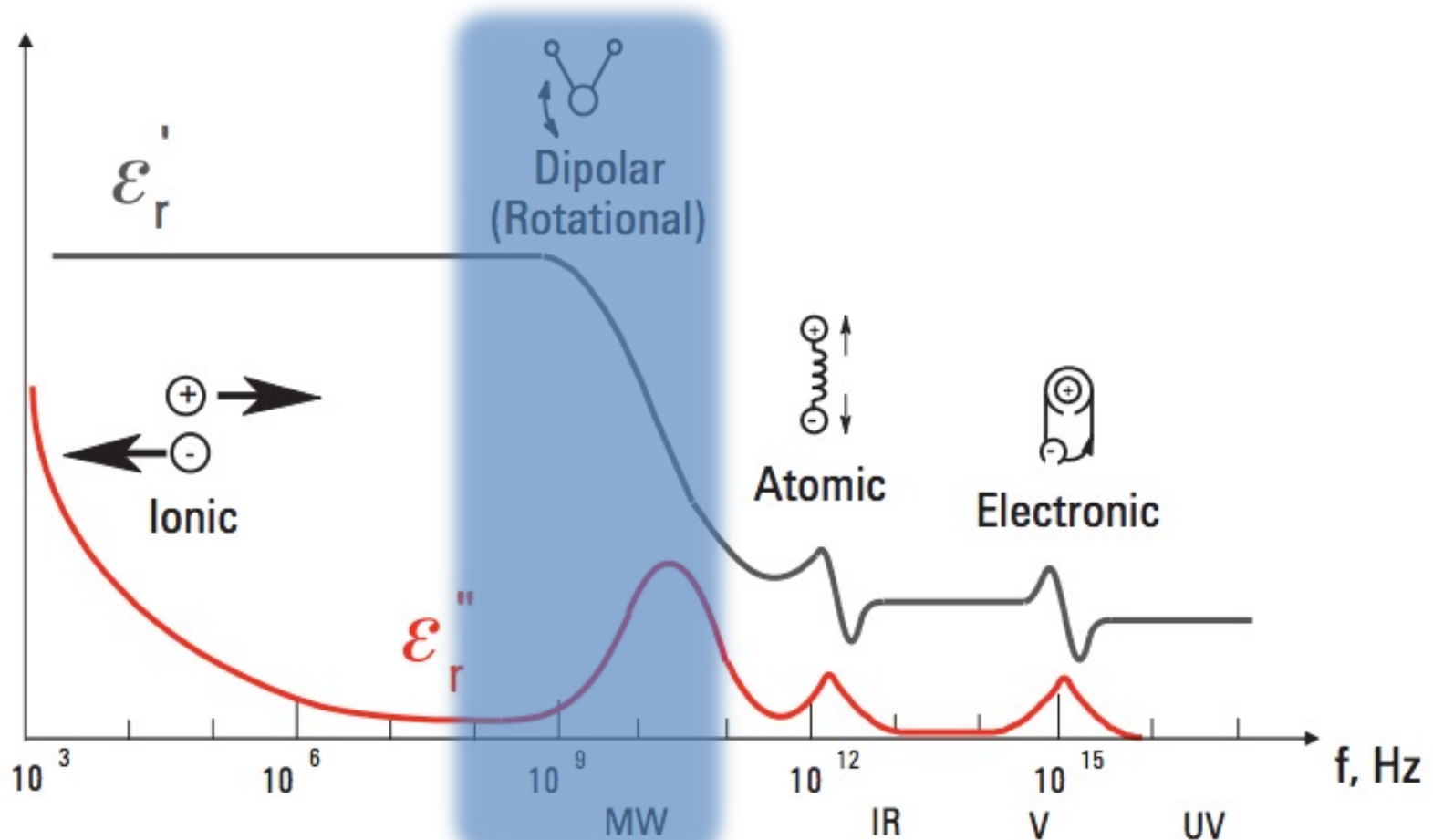


A linear variation in the relative permittivity from the dry polymer to the static dielectric constant of water may not always be realized



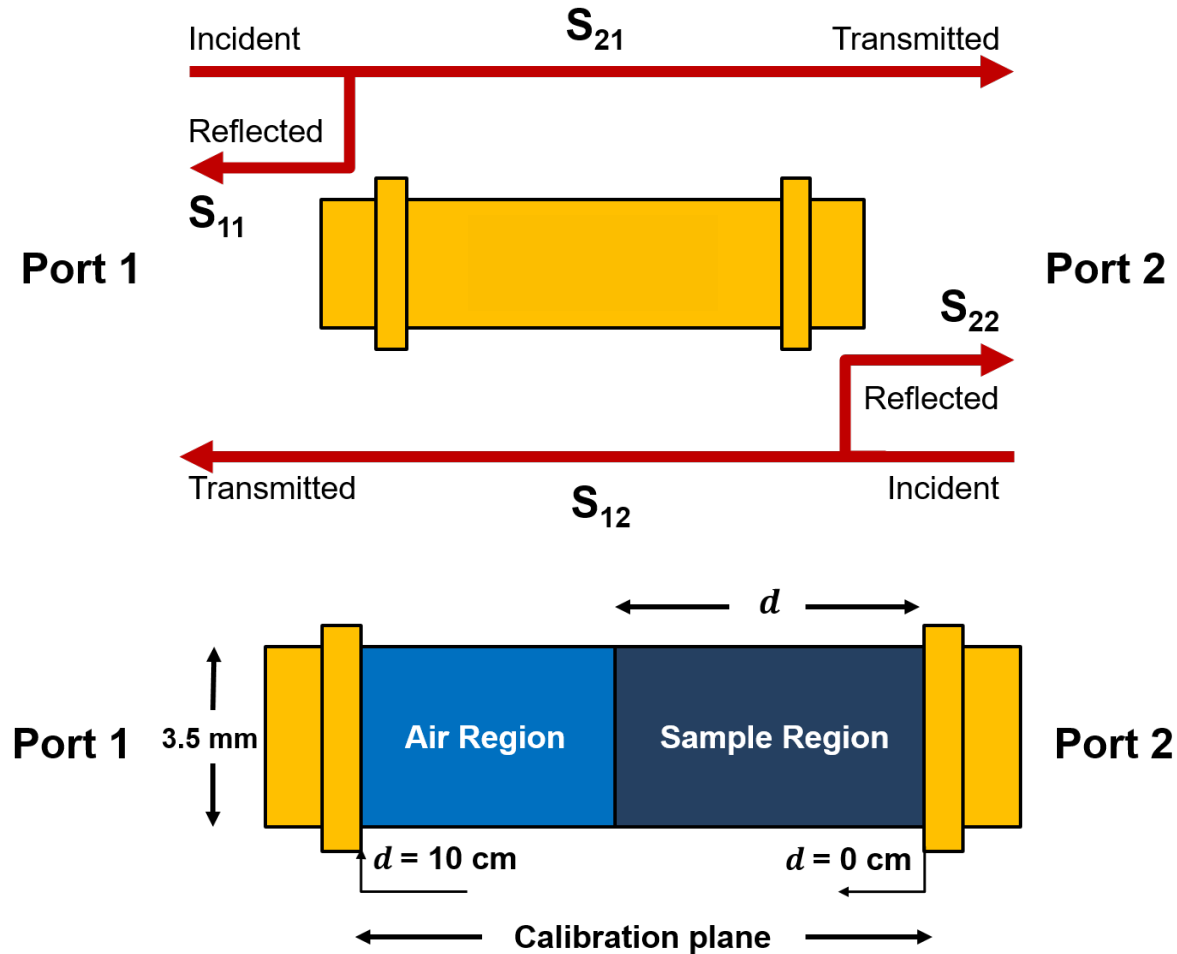
Zhang and Geise, *J. Membr. Sci.*, **520** (2016) 790.
Lu, et al., *J. Phys. Chem. A*, **113** (2009) 12207.
Liu, Jia, *Colloid. Polym. Sci.*, **293** (2015) 2053.

Molecular motions as a function of frequency

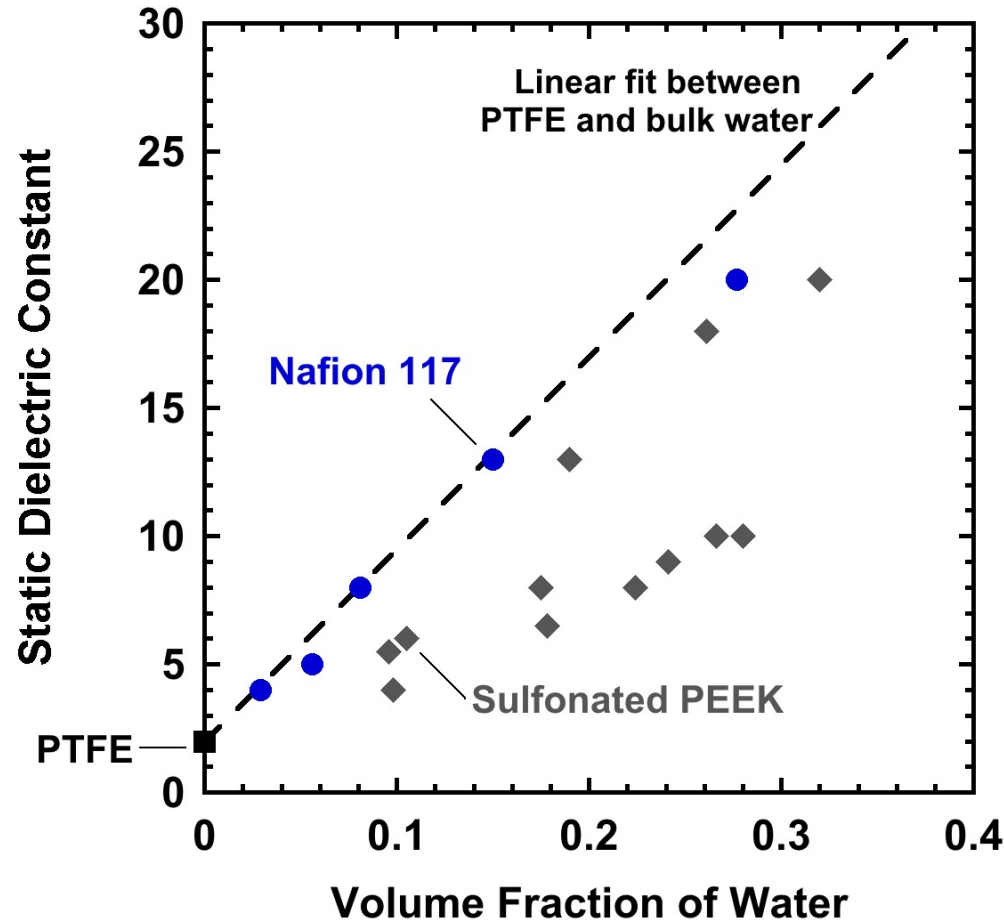


Keysight Technologies:
Basics of Measuring the Dielectric Properties
of Materials, April 27, 2015.

Measuring the dielectric properties of hydrated polymers in the microwave frequency region using a transmission line



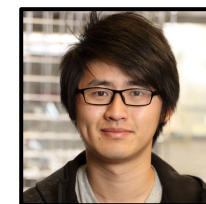
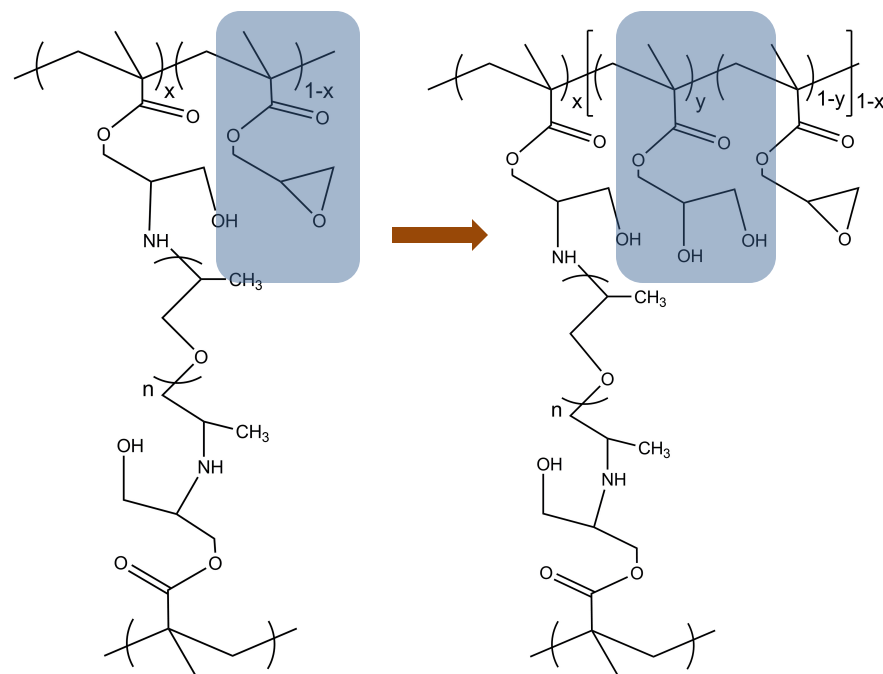
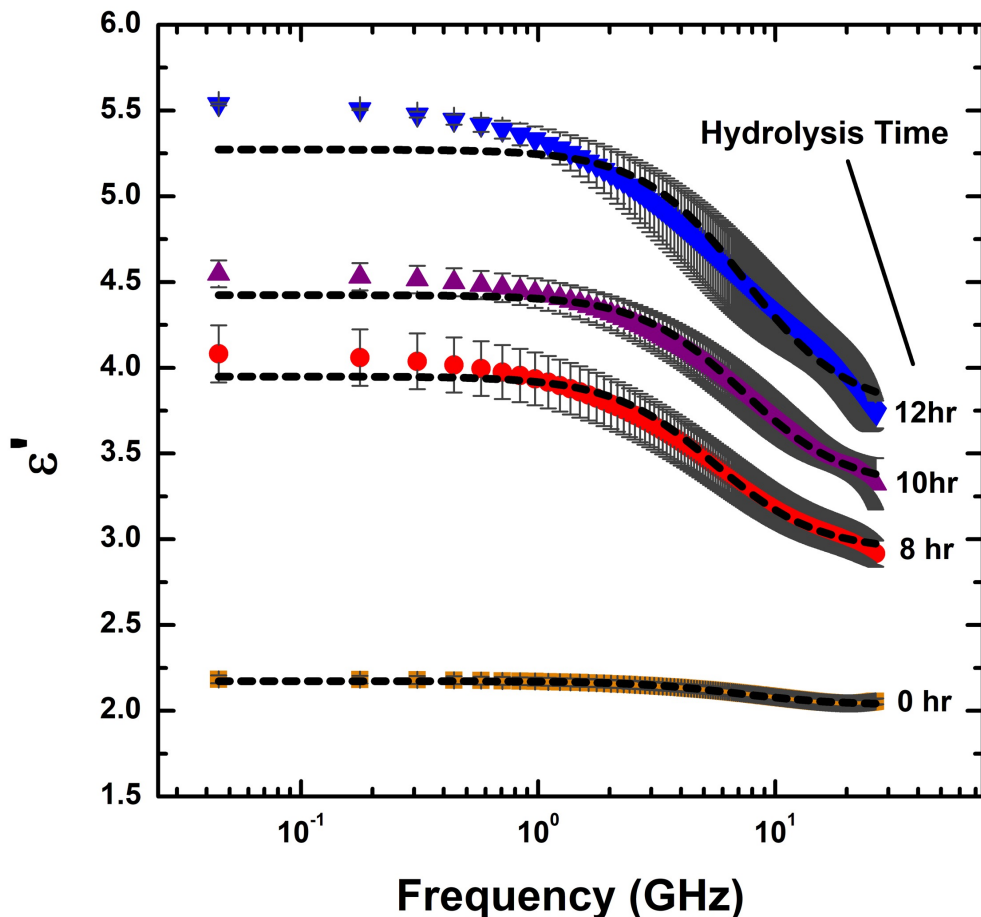
At a given water content, the static permittivity of hydrocarbon sulfonated polymers is often lower than that of Nafion



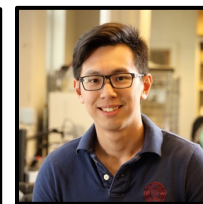
Paddison, Bender, Kreuer, Nicoloso, Zawodzinski, *J. New Mater. Electrochem. Syst.* **3** (2000) 293.

Paddison, Reagor, Zawodzinski, *J. Electroanal. Chem.*, **459** (1998) 91.

Hydrolysis increases both the water content and the relative permittivity of the polymer

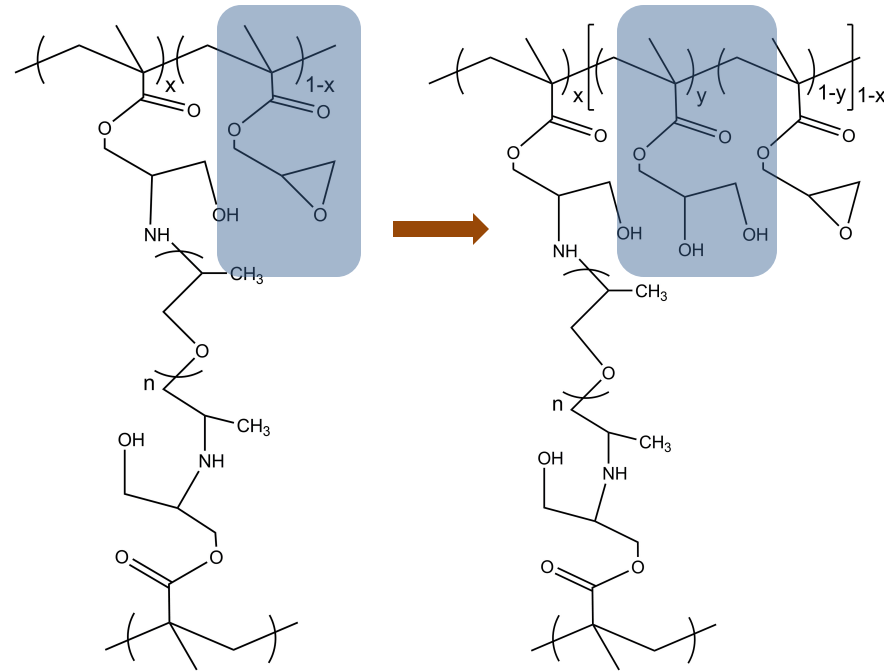
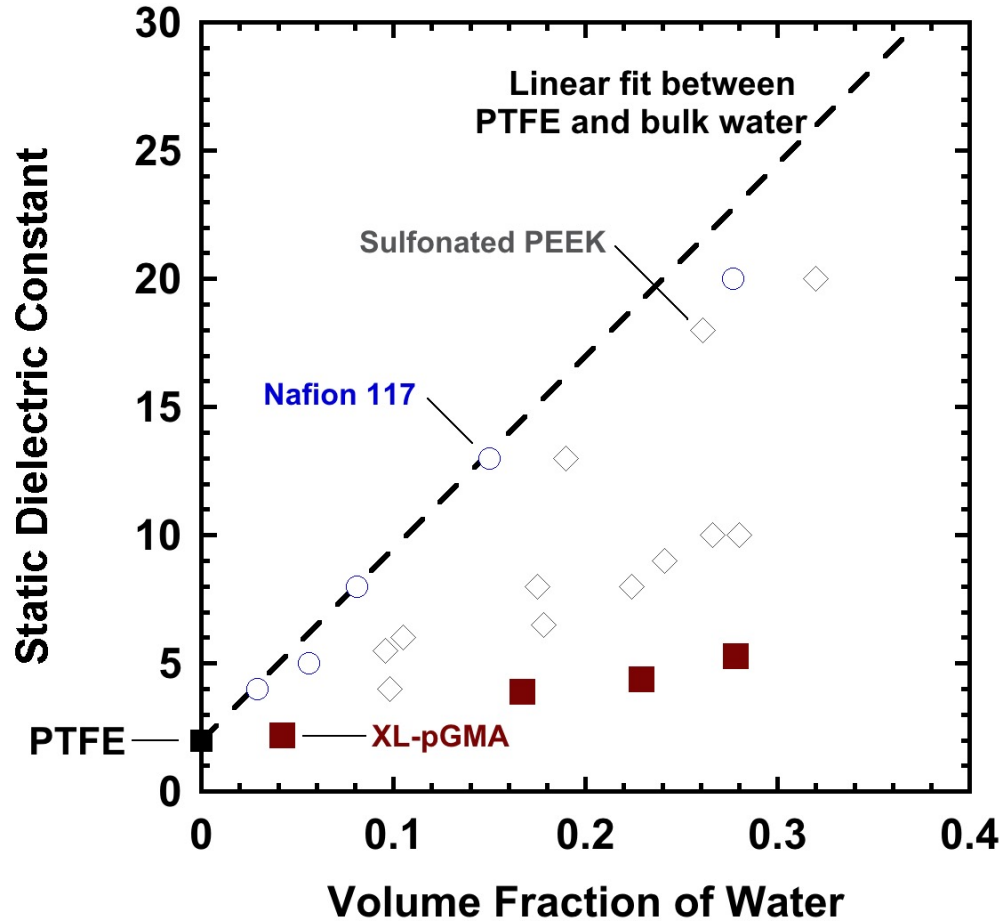


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Ring-opening hydrolysis of a crosslinked glycidyl methacrylate increases water content accompanied by a slow increase in permittivity

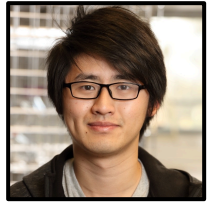


Paddison, Bender, Kreuer, Nicoloso, Zawodzinski, *J. New Mater. Electrochem. Syst.* **3** (2000) 293.

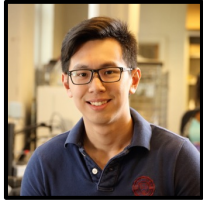
Paddison, Reagor, Zawodzinski, *J. Electroanal. Chem.*, **459** (1998) 91.

Chang, Luo, Geise, *J. Membr. Sci.*, **574** (2019) 24.

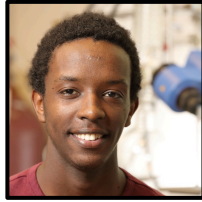
Can chemical functional group position be used to control desalination selectivity properties?



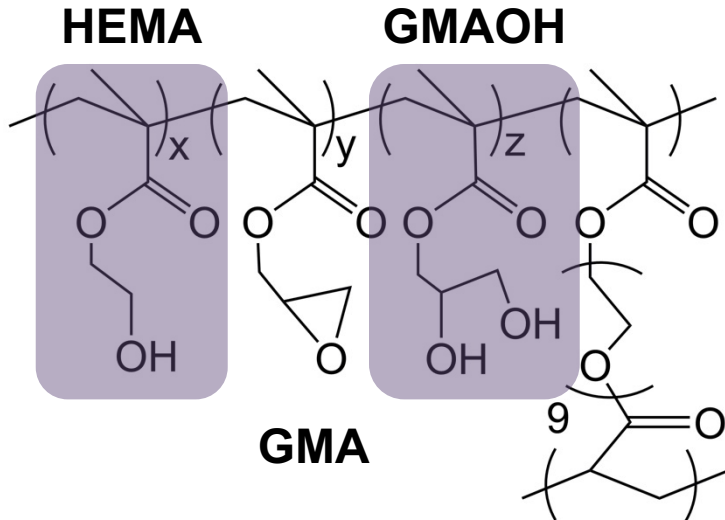
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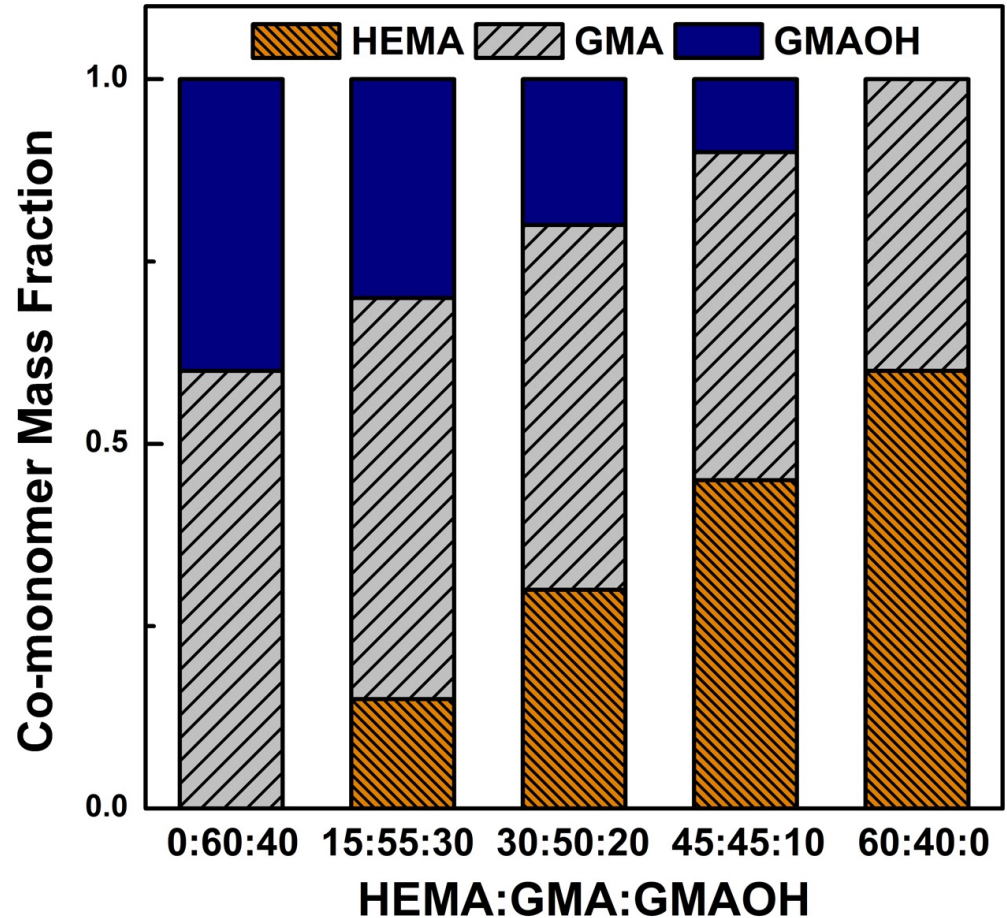
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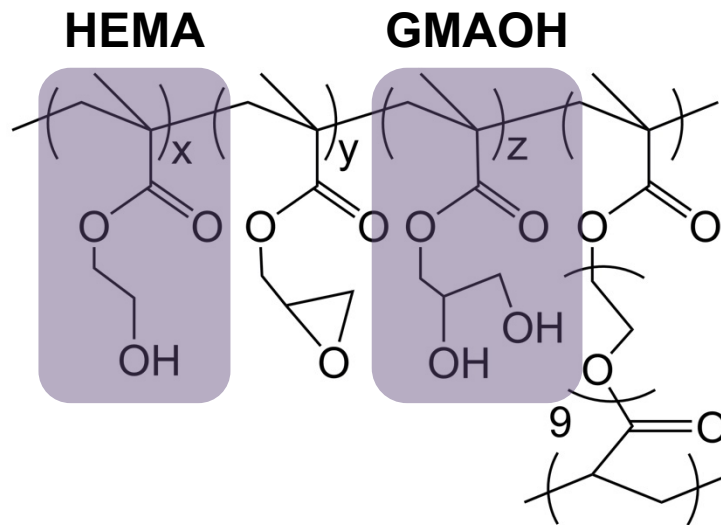
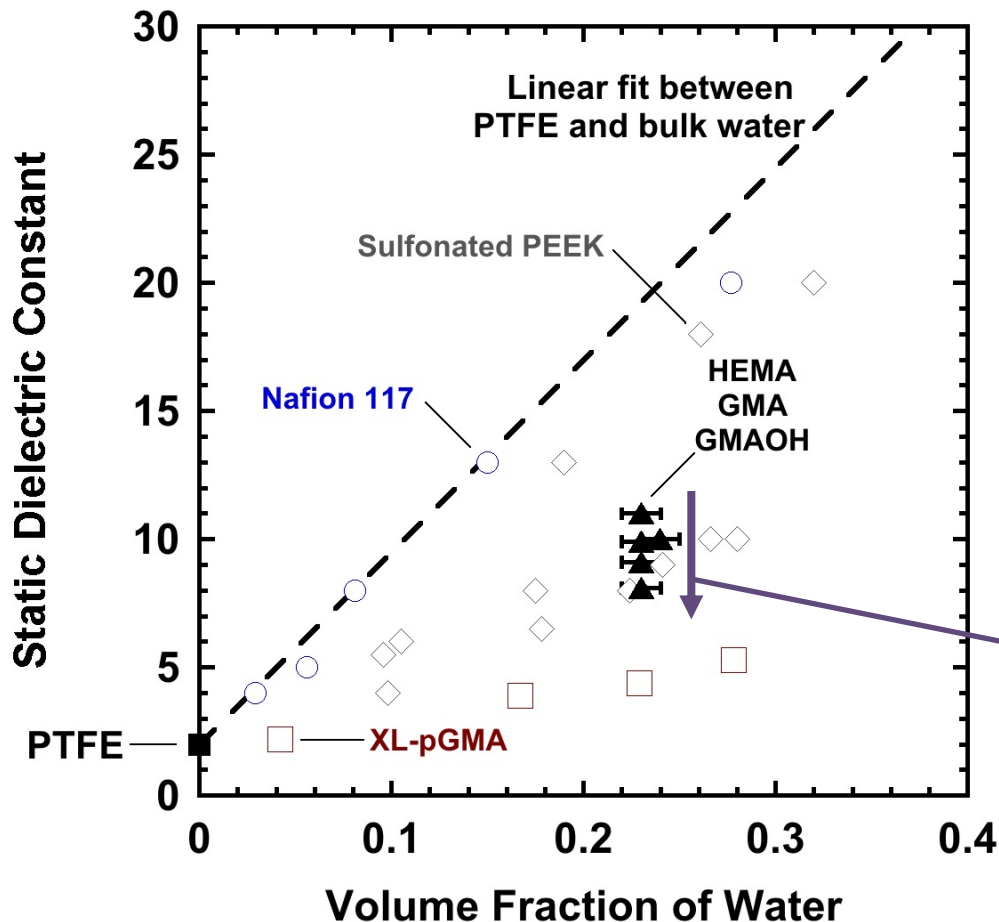
Kevin Bahati



All five materials contain equivalent amounts of water



Distributing –OH functionality throughout the polymer matrix drives a modest reduction in permittivity at equivalent water content



Increasing HEMA content

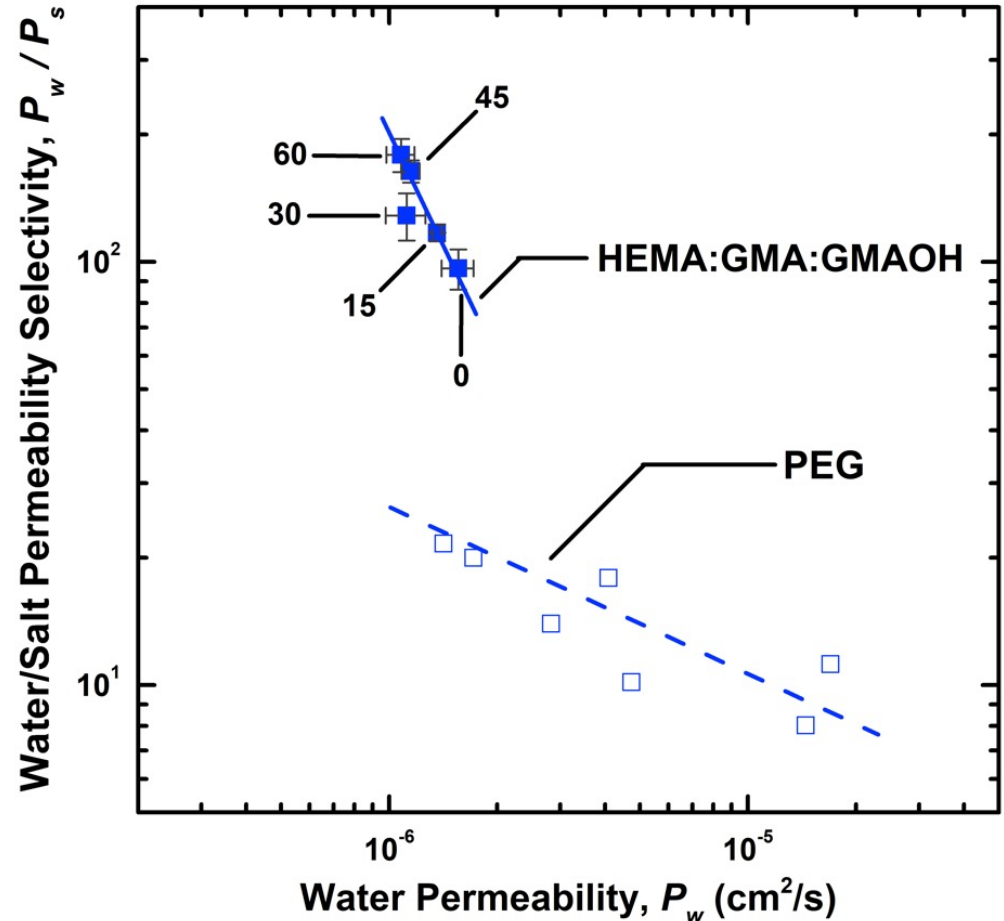
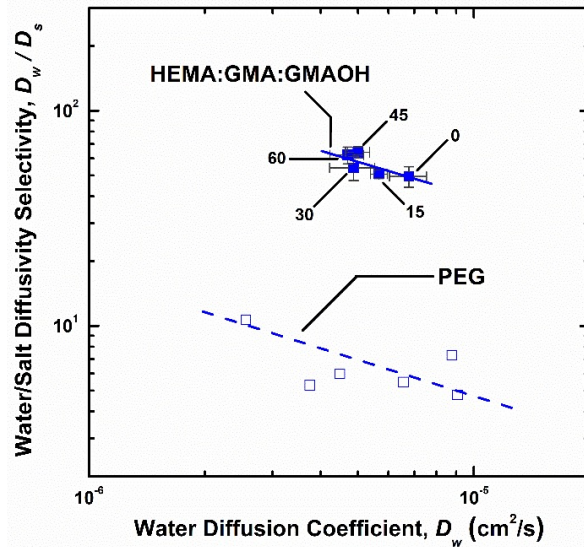
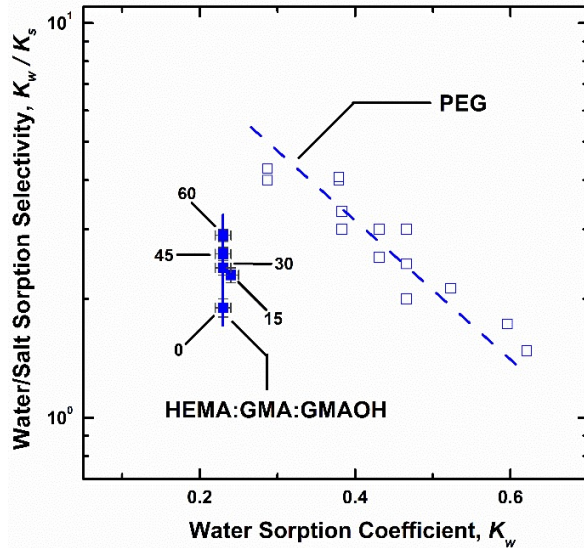
Paddison, Bender, Kreuer, Nicoloso, Zawodzinski, *J. New Mater. Electrochem. Syst.* **3** (2000) 293.

Paddison, Reagor, Zawodzinski, *J. Electroanal. Chem.*, **459** (1998) 91.

Chang, Luo, Geise, *J. Membr. Sci.*, **574** (2019) 24.

Luo, Chang, Bahati, Geise, *Environ. Sci. Technol.*, **6** (2019) 462.

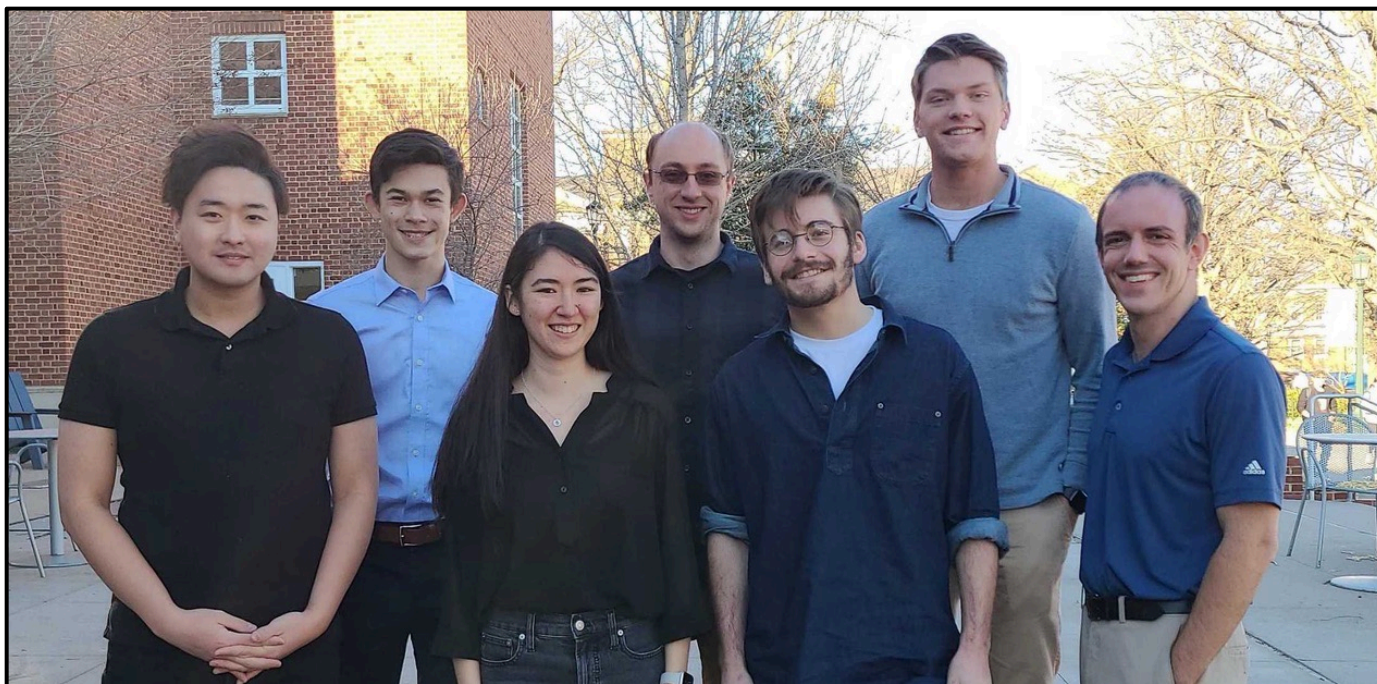
The increase in water/salt sorption selectivity coupled with an increase in diffusivity selectivity gives rise to favorable permeability selectivity properties



Summary

- **Polymer chemistry is important for desalination membrane applications**
 - Thermodynamics
 - Kinetics
- **Rigid polymer backbones are more desalination selective than flexible backbones**
- **Polymer chemistry and/or the position of functional groups can be used to manipulate thermodynamic factors that influence salt transport**

Polymer membrane research at UVA



Geise Research Group (L-R): *Top Row:* Ethan Kutner, Patrick McCormack, Charlie Leroux;
Bottom Row: Dr. Jung Min (Luca) Kim, Lena Keesecker, Sean Bannon, Prof. Geise



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UVA Sustainability Research Grant



American Chemical Society
Petroleum Research Fund
New Directions (ND) Award



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