



Membrane Databases – New Schema and Dissemination
(Supplement to: Development of Design Rules for High Hydroxide Transport in Polymer Architectures)

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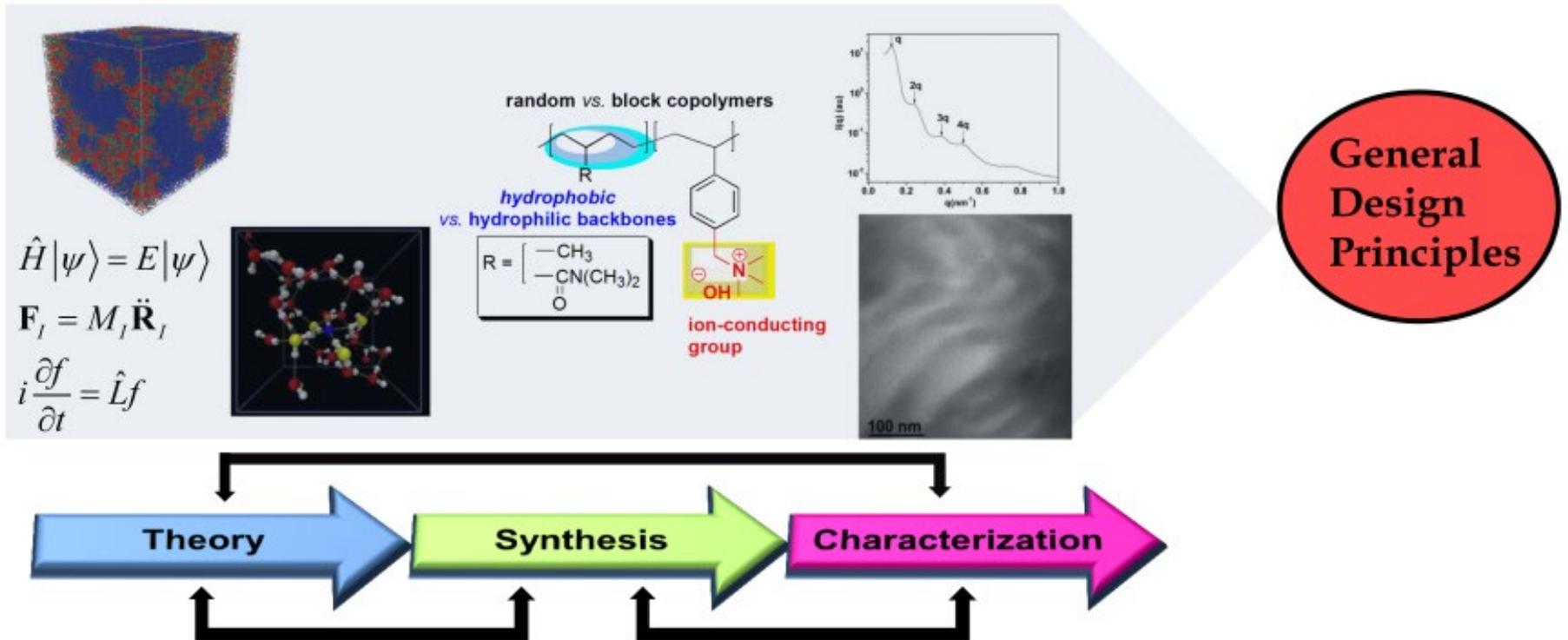
NSF – DMREF Program
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DOE Annual Merit Review
April 30th, 2019

Hydroxide Transport in Polymer Architectures

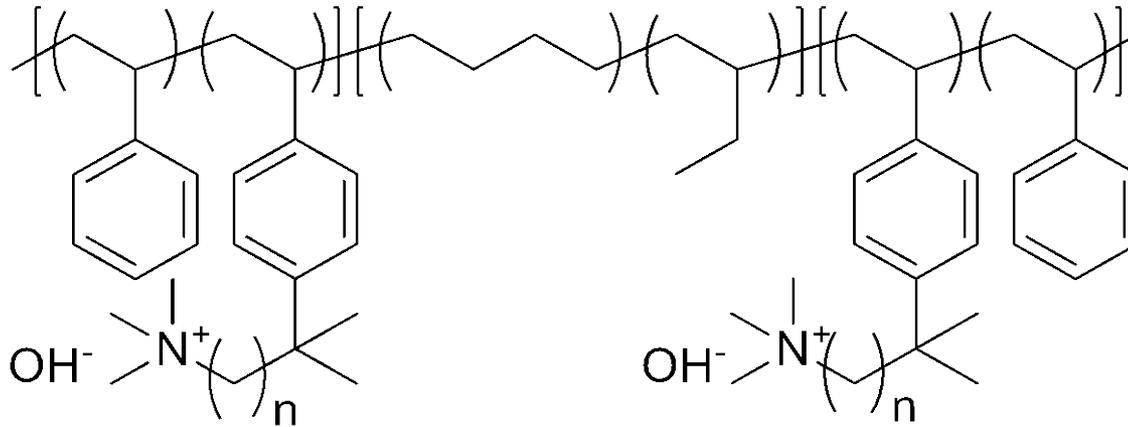
- How do we accelerate the design and development of new anion exchange membranes for electrochemical technology?
- How do we construct a thought paradigm, workflow, and set of analyses to attack the Materials Genome of membranes?
- How will large-scale simulation, data, and data analytics contribute to the rapid design and testing of new membranes?



AEM Synthesis & Characterization

Systematic variations in sidechain structures of AEMs

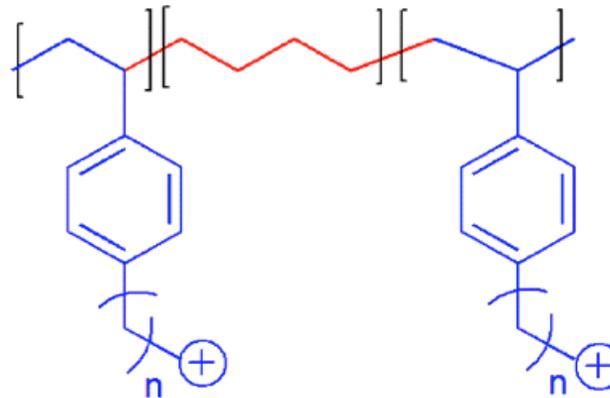
Investigate the effects of tether chain length and cation structure on hydroxide ion diffusion



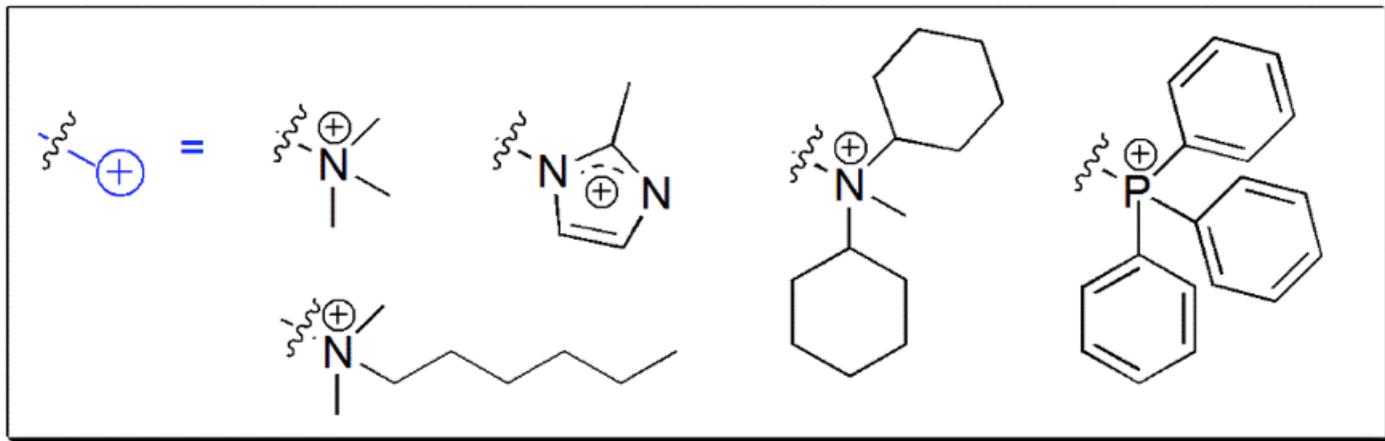
SEBS triblock copolymer
Styrene: 45 wt% (30 mol%)
 $M_w = 120$ kg/mol, $M_w/M_n = 1.1$

(n = 1, 3, 5)

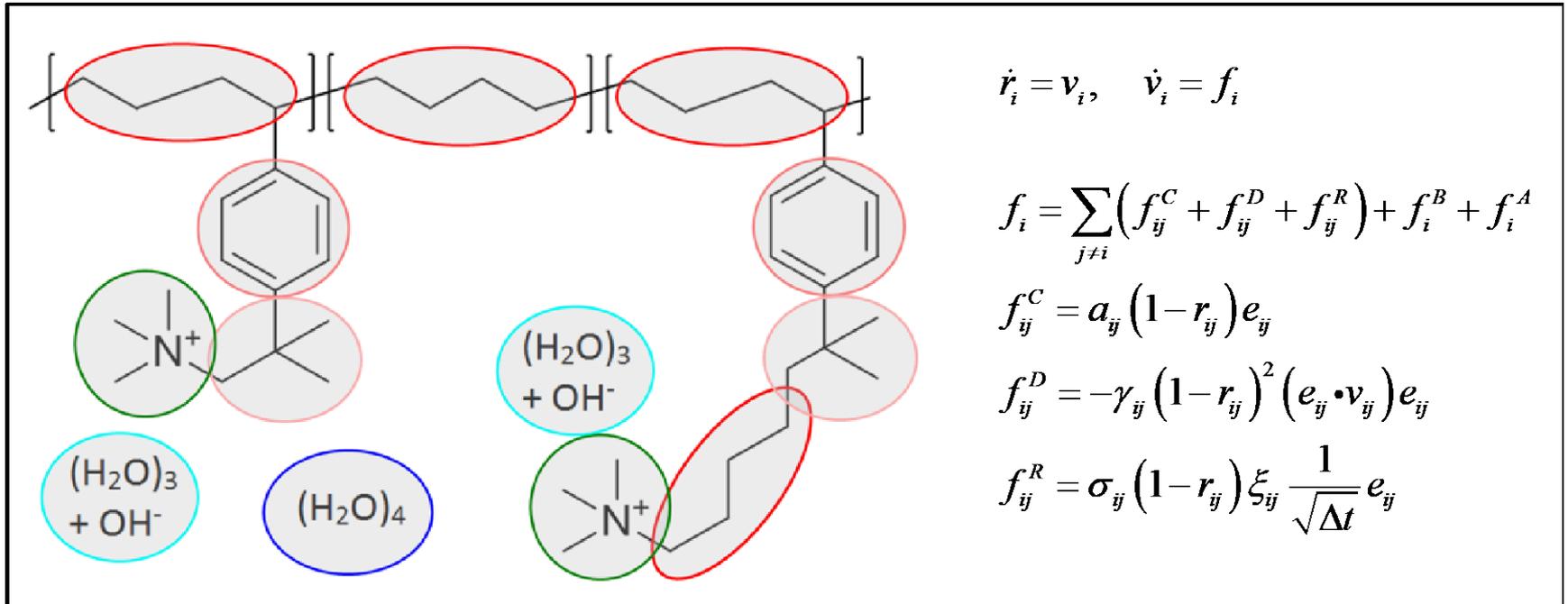
How Does Tether and Cation Influence Morphology and Properties?



SEBS AEMs
(n = 1, 3, 5)

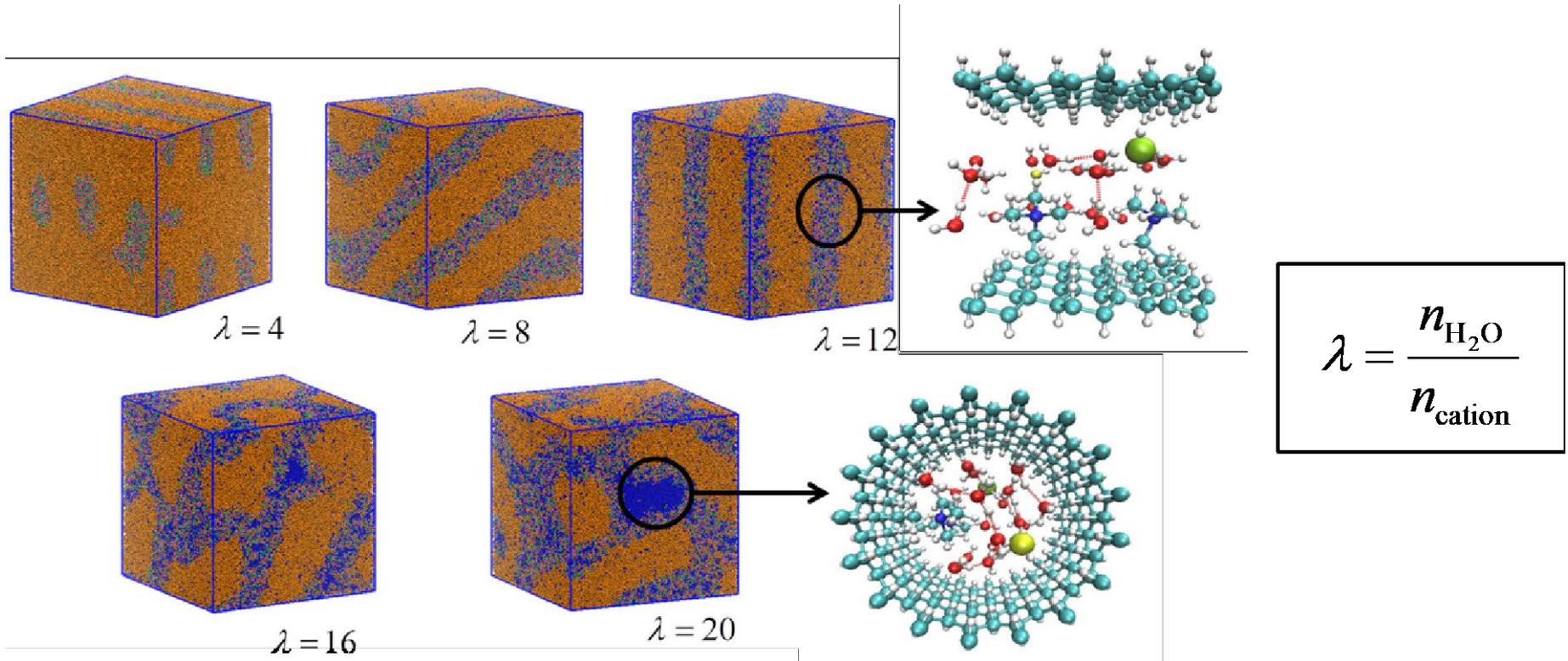


Mesososcopic Modeling of Anion Exchange Membranes



Sepehr, F., H. Liu, X. Luo, C. Bae, M. E. Tuckerman, M. A. Hickner, S. J. Paddison, "Mesoscale Simulations of Anion Exchange Membranes Based on Quaternary Ammonium Tethered Triblock Copolymers," *Macromolecules* **2017**, 50(11), 4397-4405.

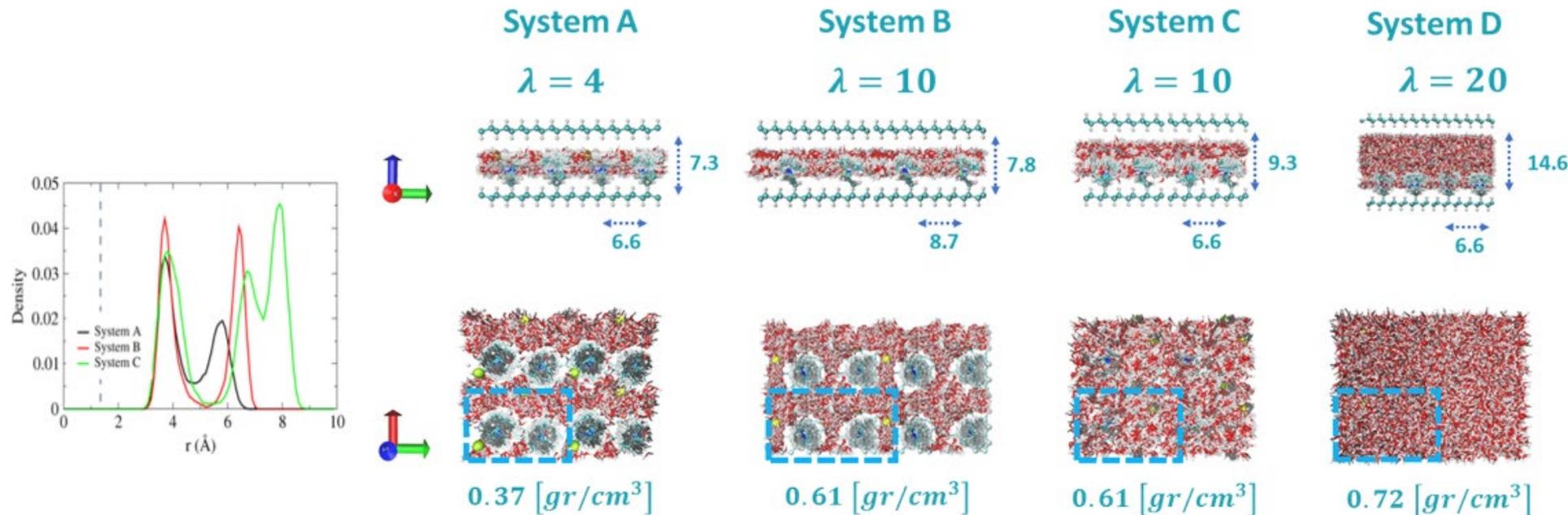
DPD Simulations of Morphology Provide Characteristic “Pores” for Detailed AIMD Models



T Zelovich, Z Long, MA Hickner, SJ Paddison, C Bae, ME Tuckerman
“Ab initio Molecular Dynamics Study of Hydroxide Diffusion Mechanisms in Nano-Confined Structural mimics of Anion Exchange Membranes”
The Journal of Physical Chemistry C **2019**.

DPD Simulations of Morphology Provide Characteristic “Pores” for Detailed AIMD Models

Connecting hydroxide diffusion to cation and tethering group chemistries from first principles



- Aqueous hydroxide transport is governed by both vehicular and structural diffusion (see figure below) mechanisms.^{4,5}
- *Ab initio* molecular dynamics simulations used to study effect of cation spacing, water content, size of pore, and temperature on hydroxide diffusion.
- Results of local-scale interactions guide further synthesis.

Membrane Databases

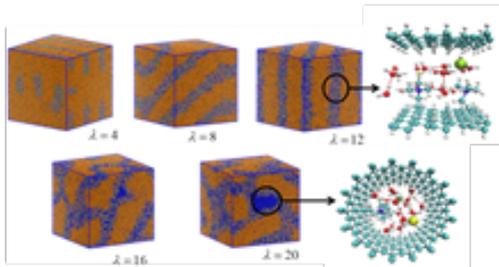
New Schema and Dissemination

- Take DMREF knowledge and literature observations and construct new membrane database.
- Make large database available to HydroGEN and EMN users for device work.

NSF DMREF Team



Anion Exchange Membrane Database



Data and fundamental materials characterization



HydroGEN Data Hub

Testing of DMREF materials for low temperature water splitting performance



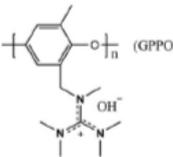
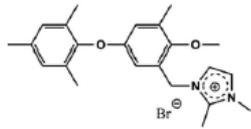
Polymer nomenclature and schema

NIST National Institute of Standards and Technology
U.S. Department of Commerce



Analysis and Feedback Across All Partners

Membrane Database

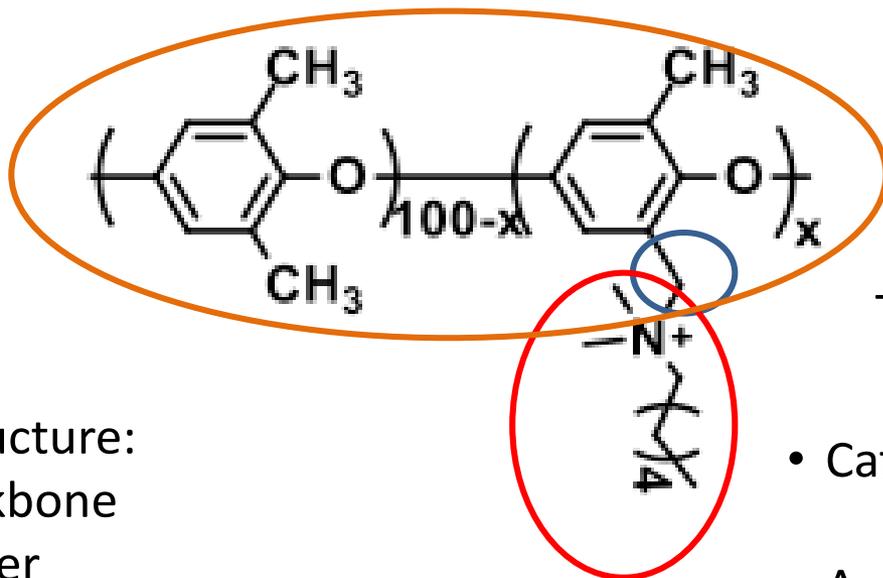
	Cation Structure	Backbone Structure	IEC (mmol/g)	Anion conductivity (mS/cm)	Swelling ratio (%)	Water uptake (%)	Alkaline stability	Ref
1.	 (GPPO)	PPO	2.69	71 (25°C)	12.5 (25°C) 18.9 (80°C)	49.9 (25°C) 72.9 (80°C)		1
2.			2.23	64 (25°C)	25.0 (25°C) 45.0 (80°C)	77.1 (25°C) 98.7 (80°C)	1M KOH @ 25°C, 8 days, no degradation	
3.	BTMA		2.65	44 (25°C)	37.5 (25°C) 75.6 (80°C)	100.6 (25°C) 430.1 (80°C)	20-40% loss of QA (come from other refs)	
4.	 (DMI)		2.8	40 (25°C) 75 (60°C)	37.5 (20°C)	136.7 (20°C)		2
5.			2.5	35 (25°C) 65 (60°C)	30.3 (20°C)	102.2 (20°C)	2M KOH @ 25°C, 9days, No degradation 2M KOH @ 60°C, 9days, Loss of IEC=50%	

Will also scope automated machine reading of the literature - see Olivetti, et al.

...165 and counting

Need Robust Naming Conventions for Database

Backbone – poly(2,6-dimethyl-1,4-phenylene oxide)



Tether - Methylene (benzyl)

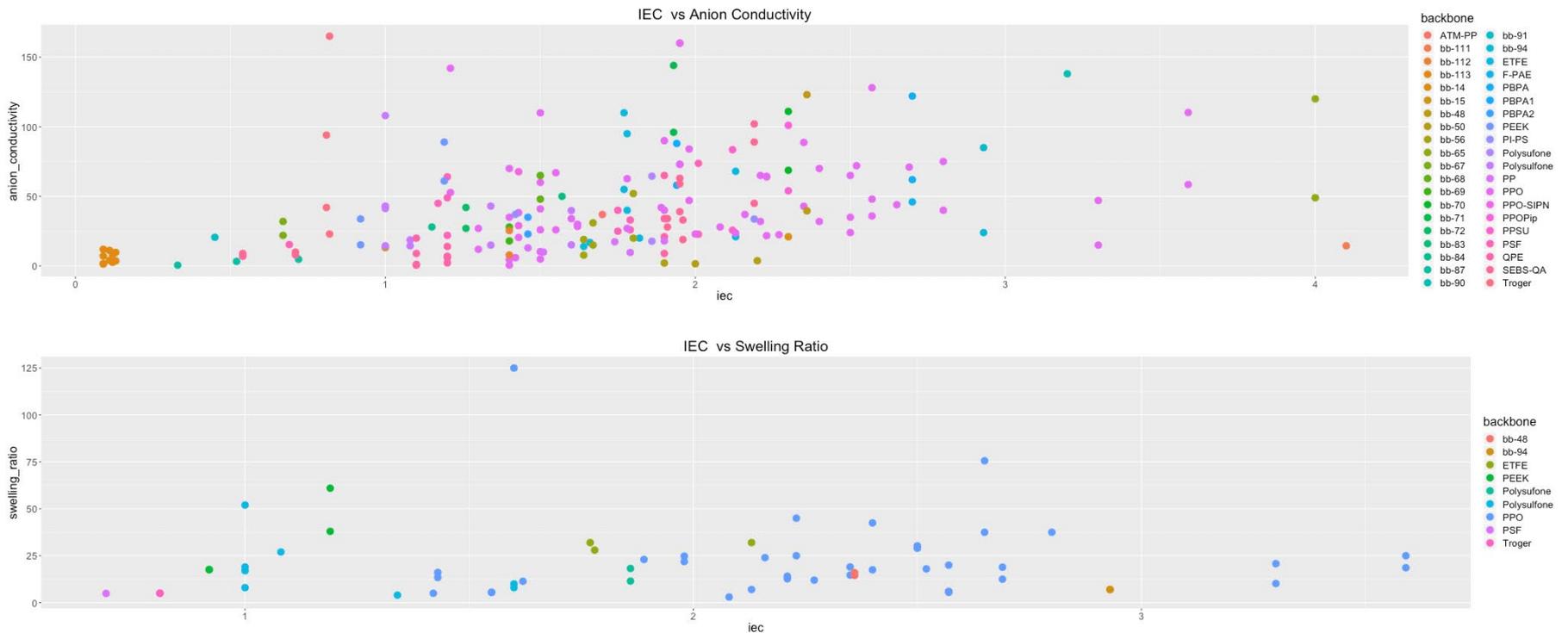
One structure:

- 1 backbone
- 1 tether
- 1 or multiple cations
- 0,1 or multiple comonomers

- Cation – Hexyl, dimethyl, alkyl
- Anion – depends on how it is characterized
- We should leave this as a variable since results are reported with different anions.

Database Allows for Large-Scale, Customized Analysis – Potential for Machine Learning

Need database curation and structure coding for automated analysis of structure-function relationships of these materials.



Where We're Headed

OPV Database

Search

Email Updates

OPV Data Management

To search by selecting building blocks based on pictures of their structure, use Advanced Search, by clicking the "Search" tab at the top of this page. Results for T-core-T small molecules are found in the "Oligomer" tab. To limit searches to these small molecules, search by "T." for tag name.

Energy Diagram: select up to 6 structures / oligomers by clicking the "plus buttons" to populate an energy level diagram for display and printing

structure graph

Tag Name (Example: BDT_)

b3lyp/6-31g(d)



Polymer Oligomer

603 records

Display 20

1 2 3 4 5 6 7 8 9 10 31

	Max O#	Thumb	Tag	HOMO	LUMO	Opt LUMO	Gap	Sum f Osc (n=2)	Spectral Overlap (n=2)	Basis
	4		BDT_MeO-MeO-H-H_CTD_Me-Me	-5.115	-3.238	-3.433	1.682	2.094	4597.662	b3lyp/6-31g(d)
	4		BDT_Th-Th-H-H_Th_H-H_CTD_Me-Me_Th_H-H	-4.824	-2.935	-3.272	1.552	3.824	9957.934	b3lyp/6-31g(d)
	2		BDT_Th-Th-H-H_Th_H-H_TPD_Me_Th_H-H	-4.901	-2.924	-3.284	1.617	3.852	9137.942	b3lyp/6-31g(d)
	3		BDT_Th-Th-H-H_CTD_Me-Me	-5.086	-3.201	-3.407	1.679	2.018	4566.334	b3lyp/6-31g(d)
	4		BDT_Th-Th-H-H_TPD_Me	-5.103	-3.032	-3.278	1.825	2.214	4038.037	b3lyp/6-31g(d)
	2		FLR_Me-MeO-H-H-H-H-H_H_CTD.HH	-5.312	-3.005	-3.329	1.983	2.013	3102.140	b3lyp/6-31g(d)
	2		FLR_MeO-Me-H-H-H-H-H_H_CTD.HH	-5.330	-2.982	-3.313	2.017	1.958	3006.523	b3lyp/6-31g(d)

https://organicelectronics.nrel.gov/project/detail/project_id/19

HydroGEN Data Hub

The submission point for data collected from research conducted by the Advanced Water Splitting Materials National Laboratory Consortium



Register

Request a HydroGEN account.



Discover

Search the repository.



Submit Data

Upload and archive your data.
Share data with others.



Energy Materials Network
U.S. Department of Energy



Sandia National Laboratories



Things to do

- Naming and structure coding
- Finalize schema and build in flexibility for expansion
- Leverage data tools from NREL OPV database
- Expand database entries through the end of the supplement and consider curated user submissions
- Chart pathway forward for use in EMN with DOE