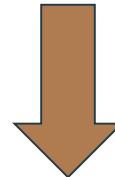


Thank you to:



Breaking the Crystal Lattice

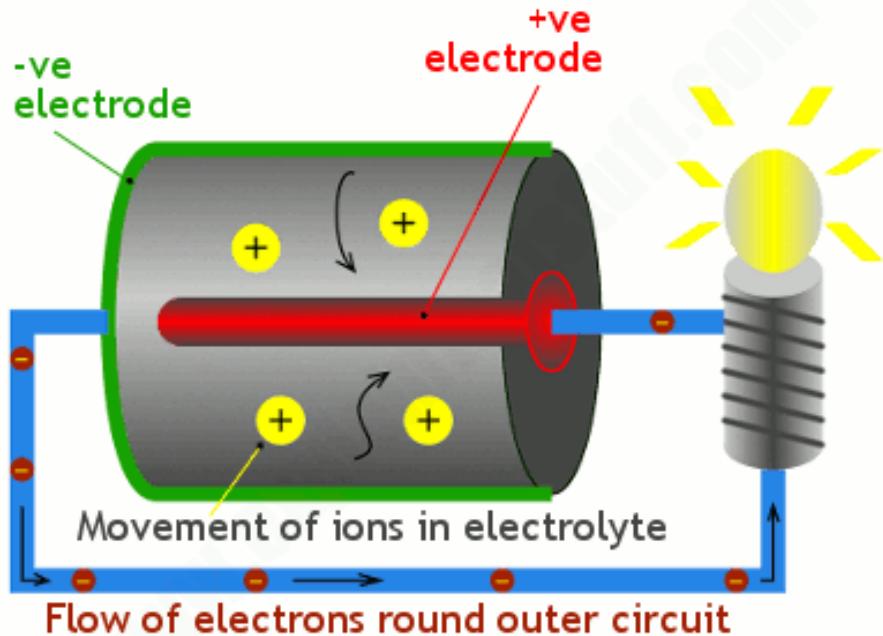


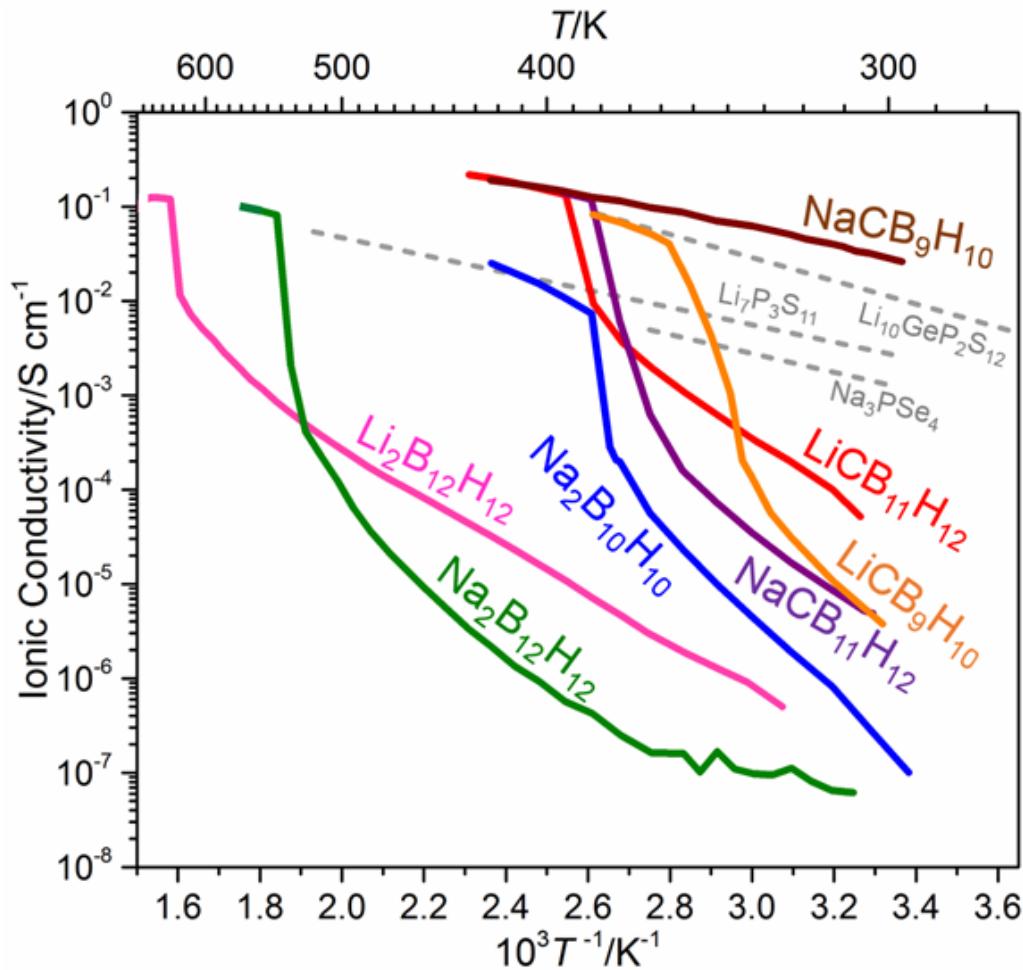
Improving Salt Conductivity

Małgorzata (Maggie) Psurek

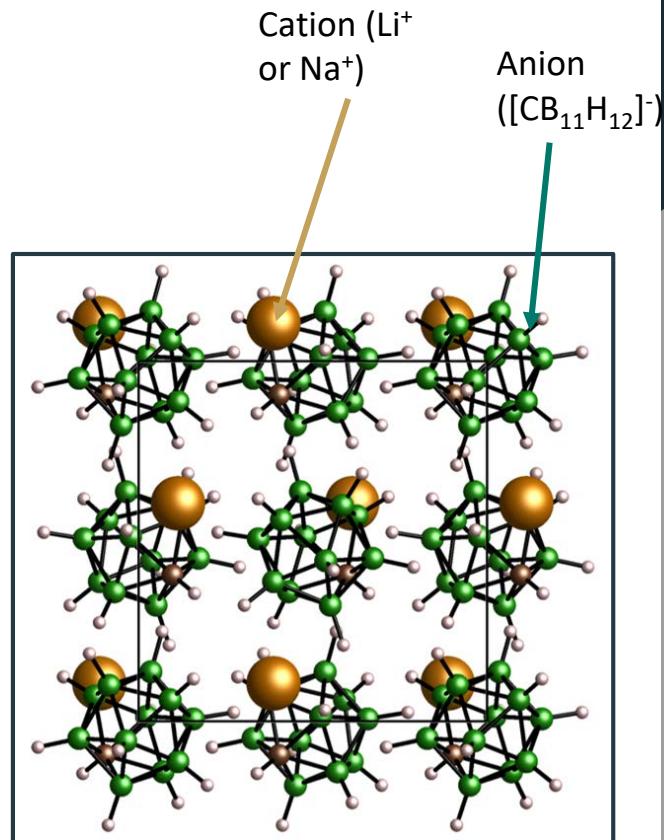
Goal: Solid State batteries

- ❖ Safer
- ❖ Non-hazardous, non-flammable
- ❖ Possibly cheaper
- ❖ Sodium: more eco-friendly

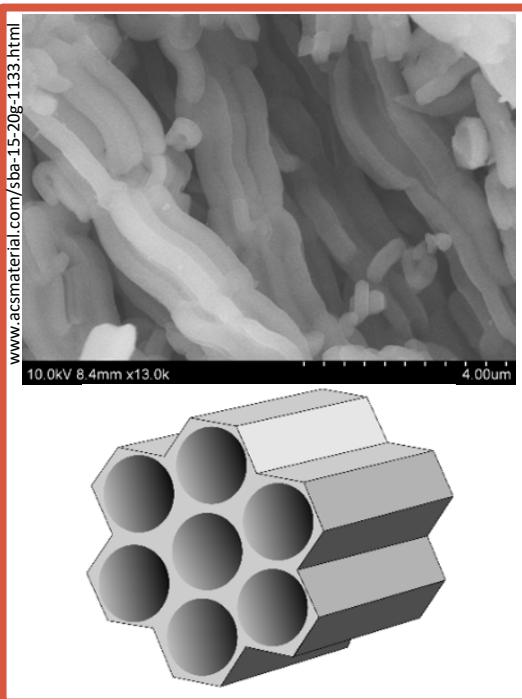




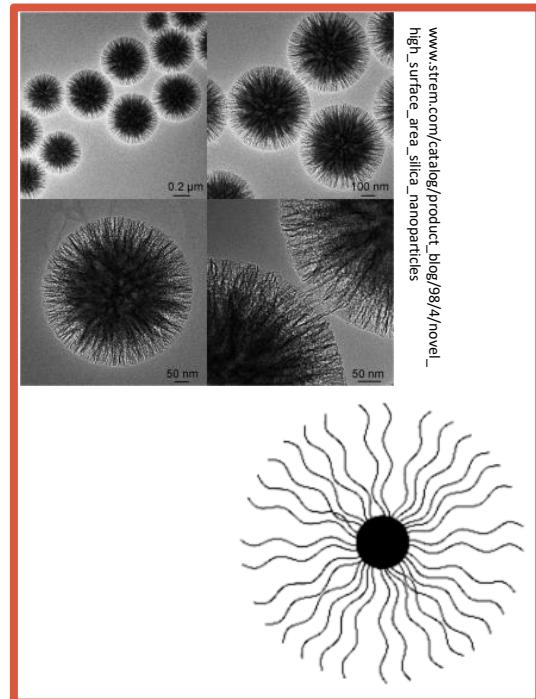
Images courtesy of Dr. Terrence Udovic



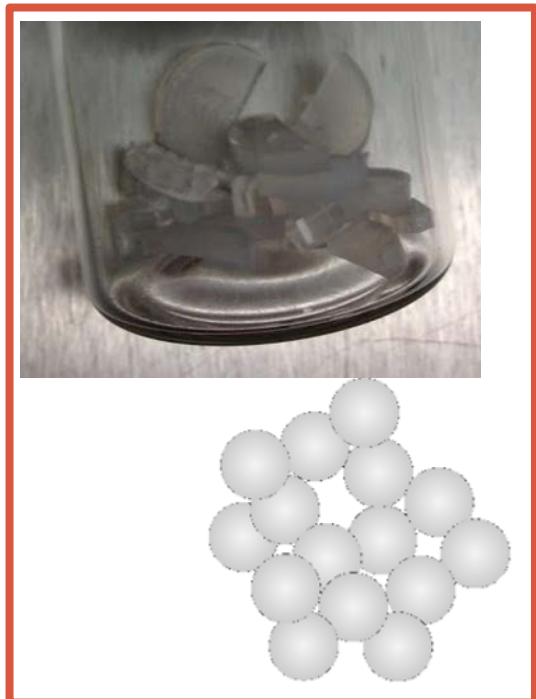
Materials: Silica (SiO_2)



SBA-15 (8nm and 12 nm pores)



High Surface Area (HSA) Silica
(900-1100 nm particles)

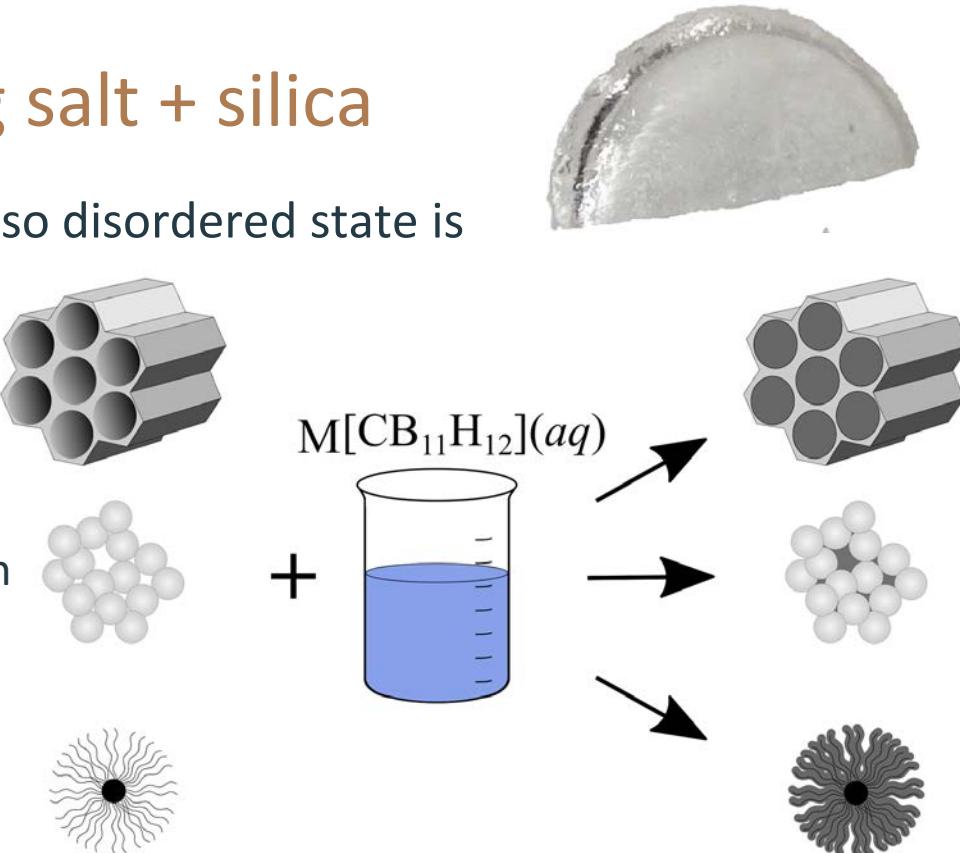


Porous SiO_2 disks (made of
7nm and 13 nm spheres)

Digital drawings courtesy of Mikael Andersson

Methods: combining salt + silica

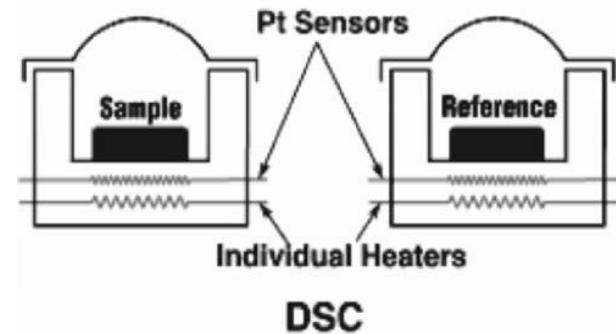
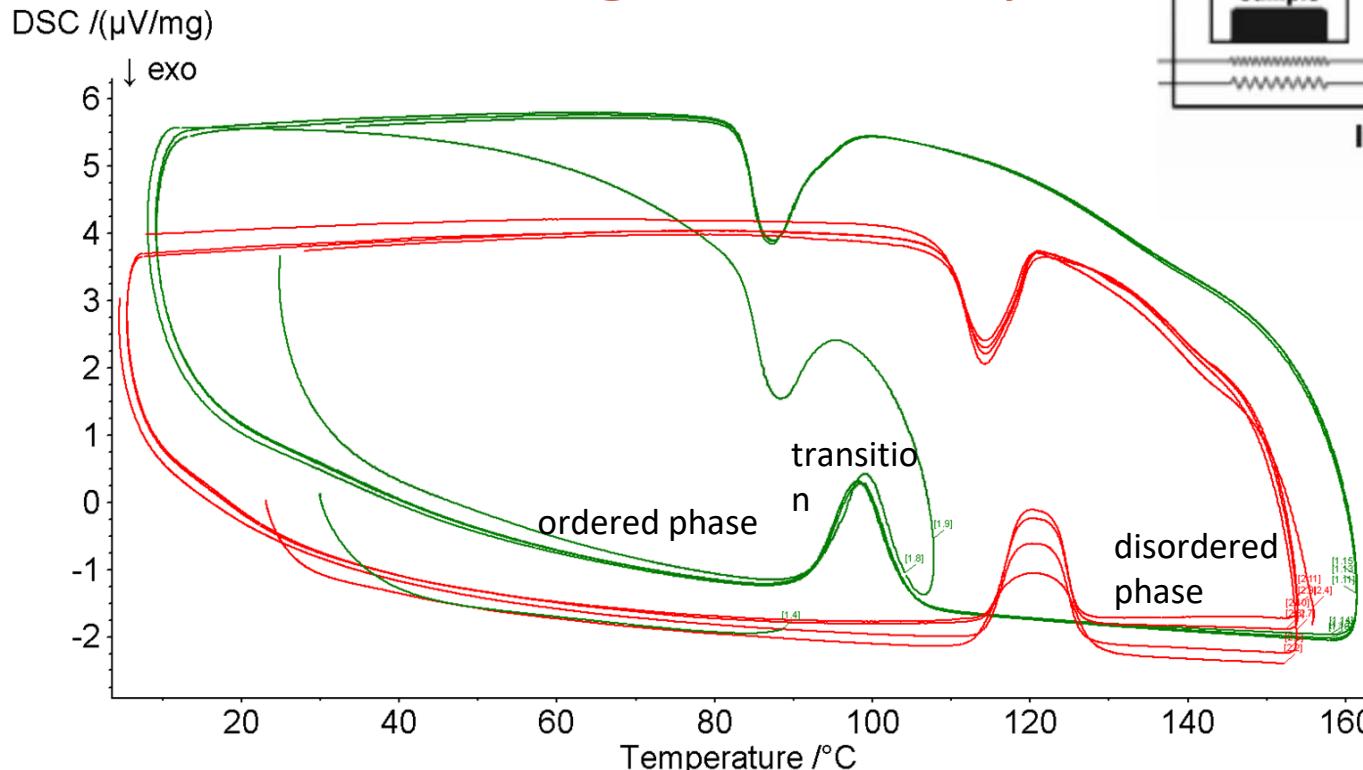
- ❖ Purpose: nano-confine the salt so disordered state is favoured
- ❖ Method
 - Make saturated solution
 - mix into silica
 - Or add by capillary action
 - Dry under vacuum



Original schematic provided by Mikael Andersson

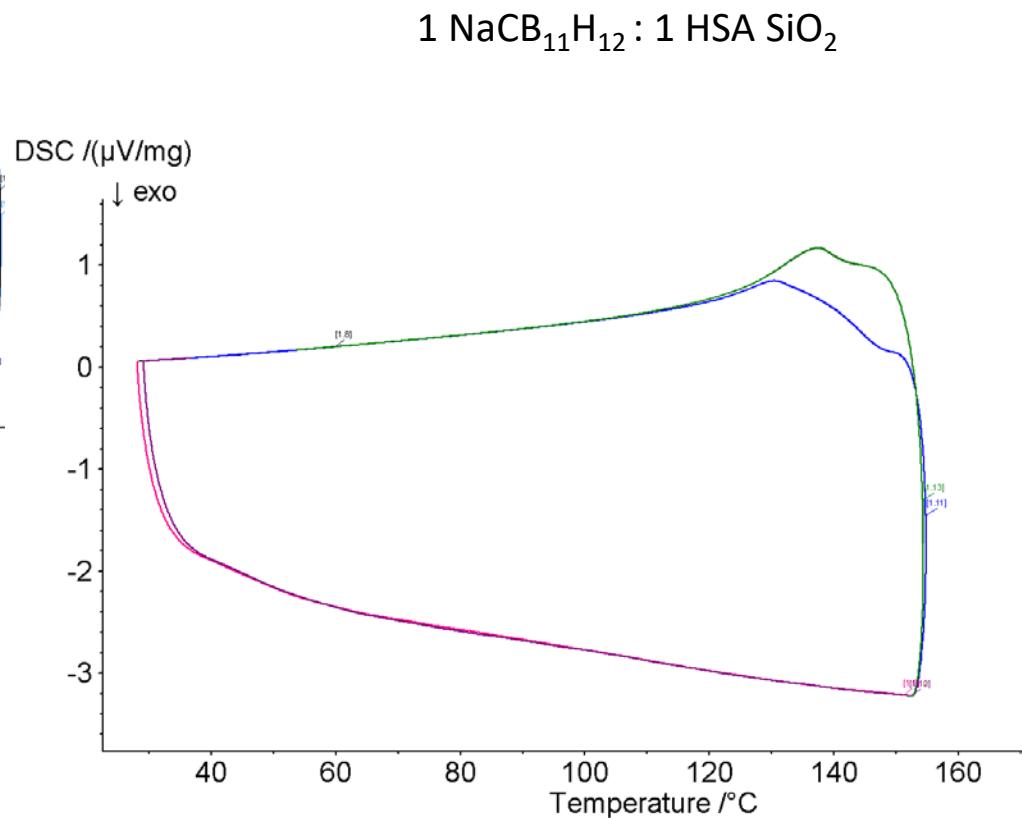
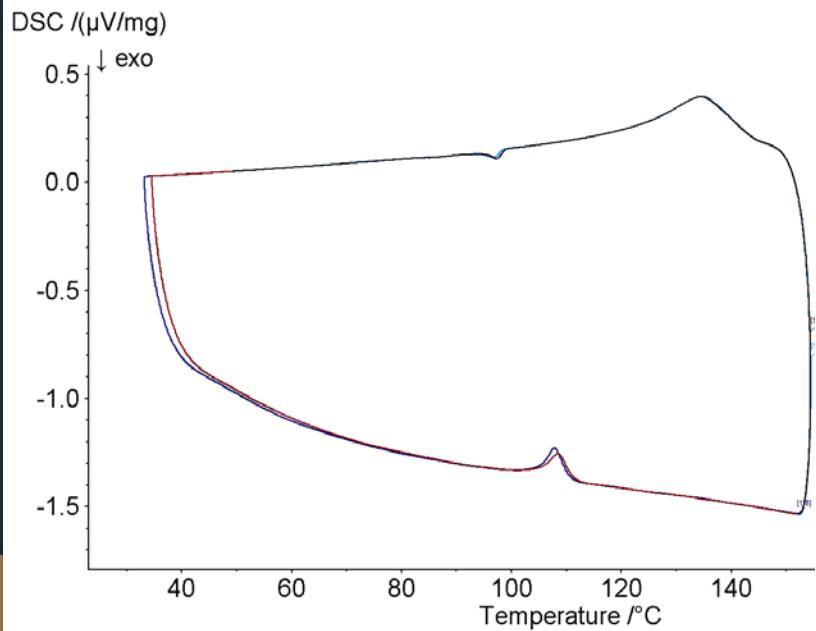
How do we know it works?

Differential Scanning Calorimetry

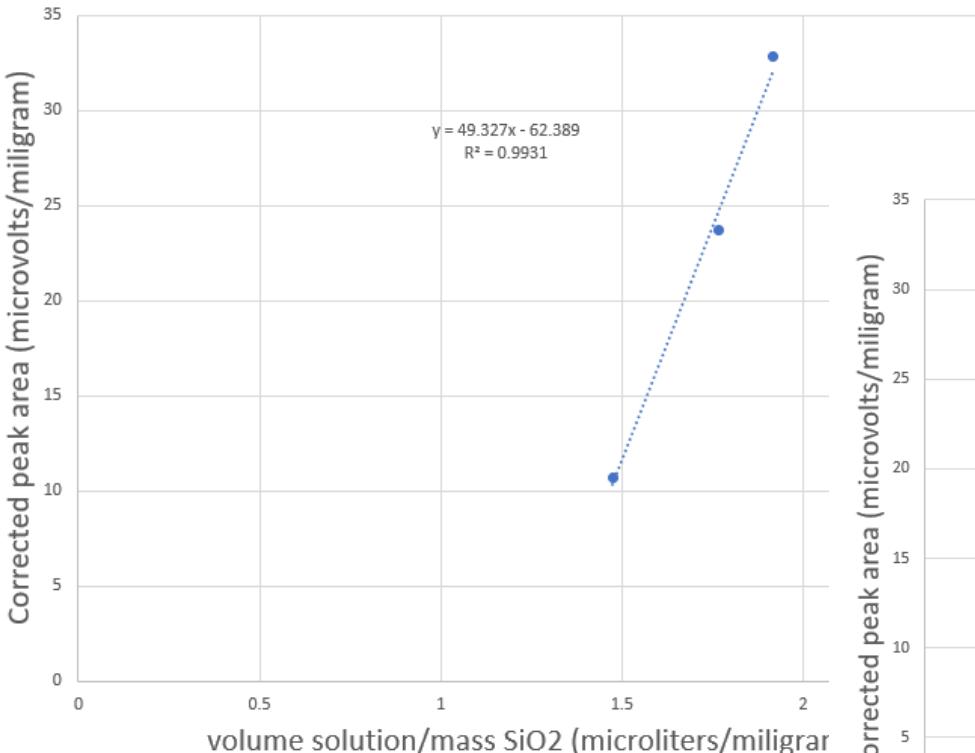


Green (left peaks) = bulk
 $\text{NaCB}_{11}\text{H}_{12}$

Red (right peaks) = bulk
 $\text{LiCB}_{11}\text{H}_{12}$

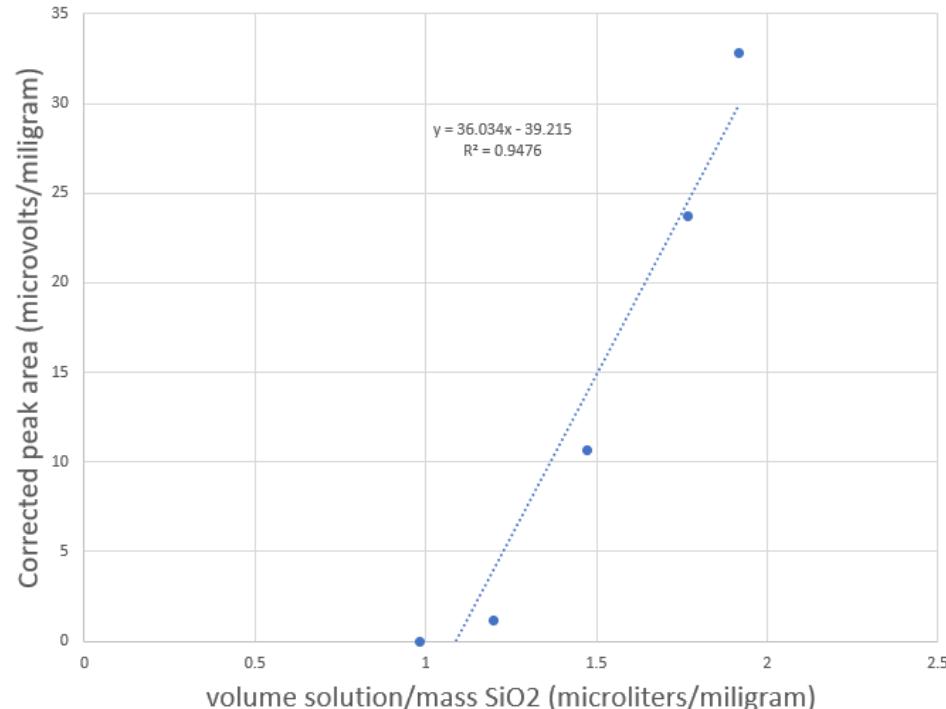


DSC peaks of NaCB11H12:HSA mixtures



Graph including all final DSC results for Na--:HSA ratios

All DSC peaks of NaCB11H12:HSA mixtures



Graph used to estimate correct volume/mass ratio.
X-int = 1.265 μL solution/mg SiO₂

1.2 NaCB₁₁H₁₂ : 1 HSA SiO₂

DSC /(μ V/mg)

↓ exo

8
6
4
2
0
-2
-4
-6

20 40 60 80 100 120 140

Temperature /°C

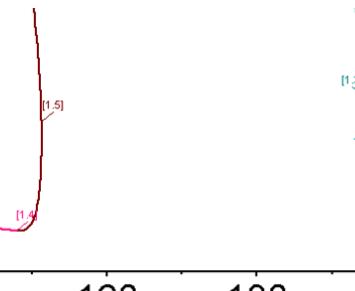
DSC /(μ V/mg)

↓ exo

-4.0
-4.5
-5.0
-5.5
-6.0
-6.5
-7.0

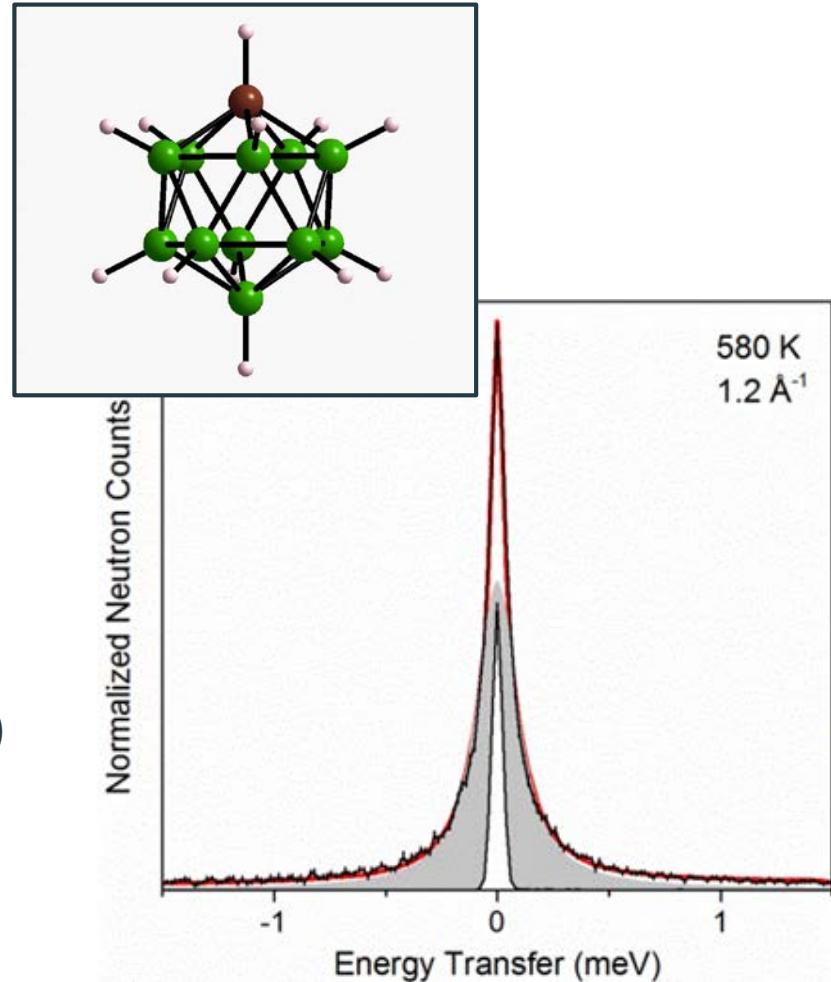
80 90 100 110
Temperature /°C

Area: 2.069 μ Vs/mg

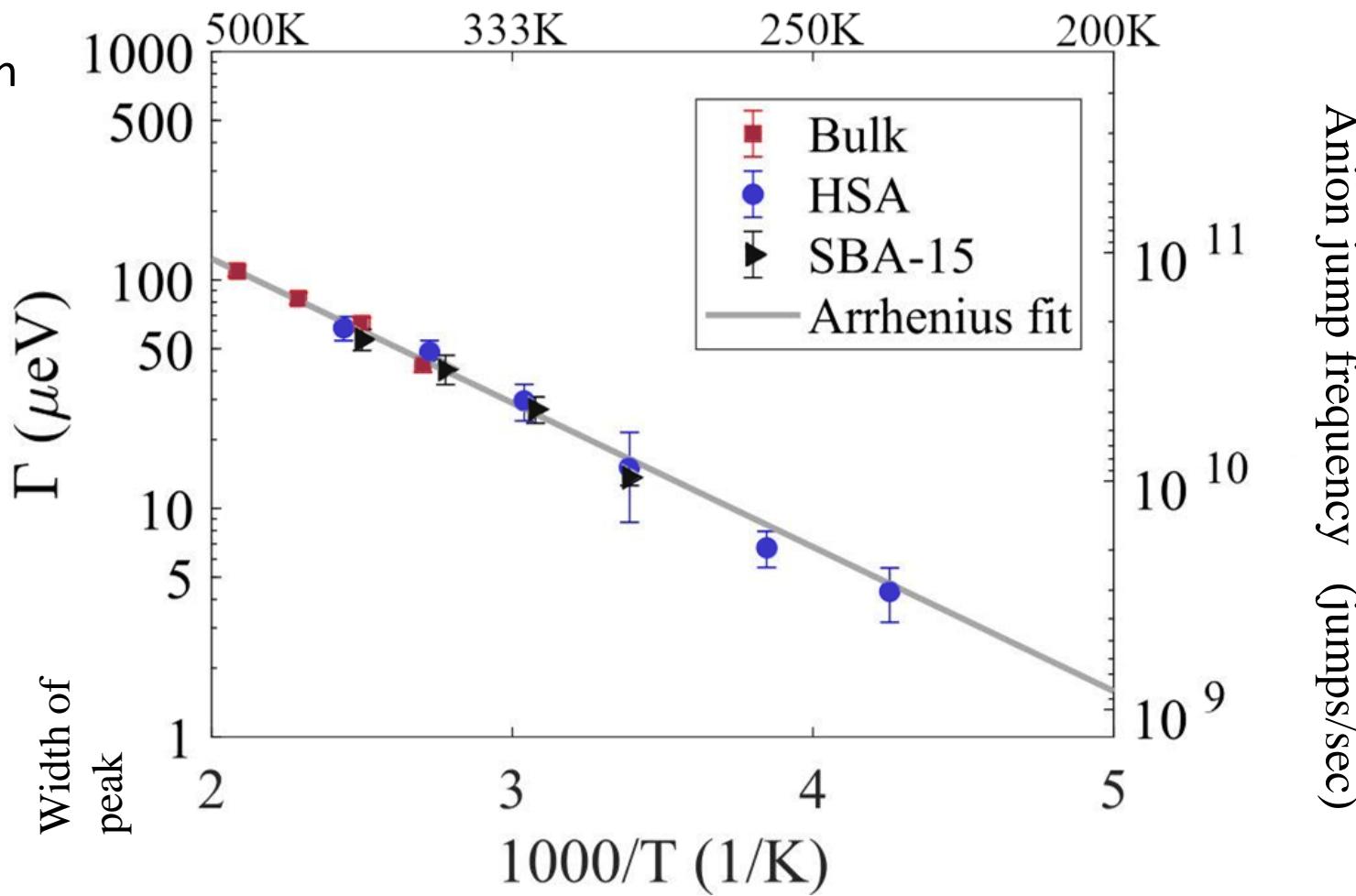


Quasielastic Neutron Scattering

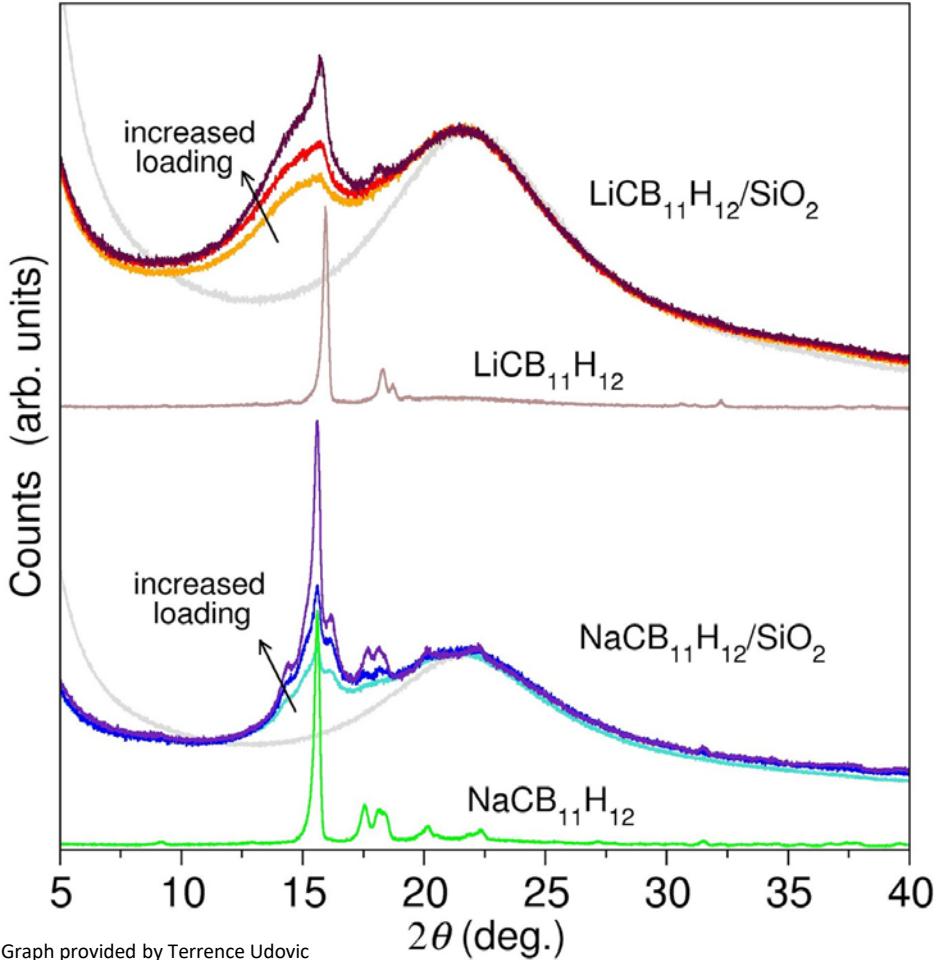
- ❖ High Flux Backscattering Spectrometer (HEBS)
- ❖ Disk-chopper Spectrometer (DCS)
- ❖ Measures hydrogen dynamics
 - No movement → elastic (no E change)
 - Movement → inelastic (E lost or gained)
 - More movement → broader peak



Speed of anion rotation over temperature range



X-ray Crystallography



1.5 Li-- : 1 HSA

1.2 Li-- : 1 HSA

1 Li-- : 1 HSA

$\text{LiCB}_{11}\text{H}_{12}$

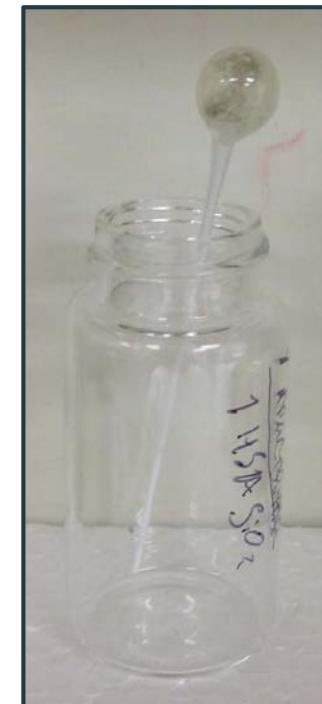
hydrate

1.8 Na-- : 1 HSA

1.2 Na-- : 1 HSA

1 Na-- : 1 HSA

$\text{NaCB}_{11}\text{H}_{12}$ hydrate



True test: Conductivity

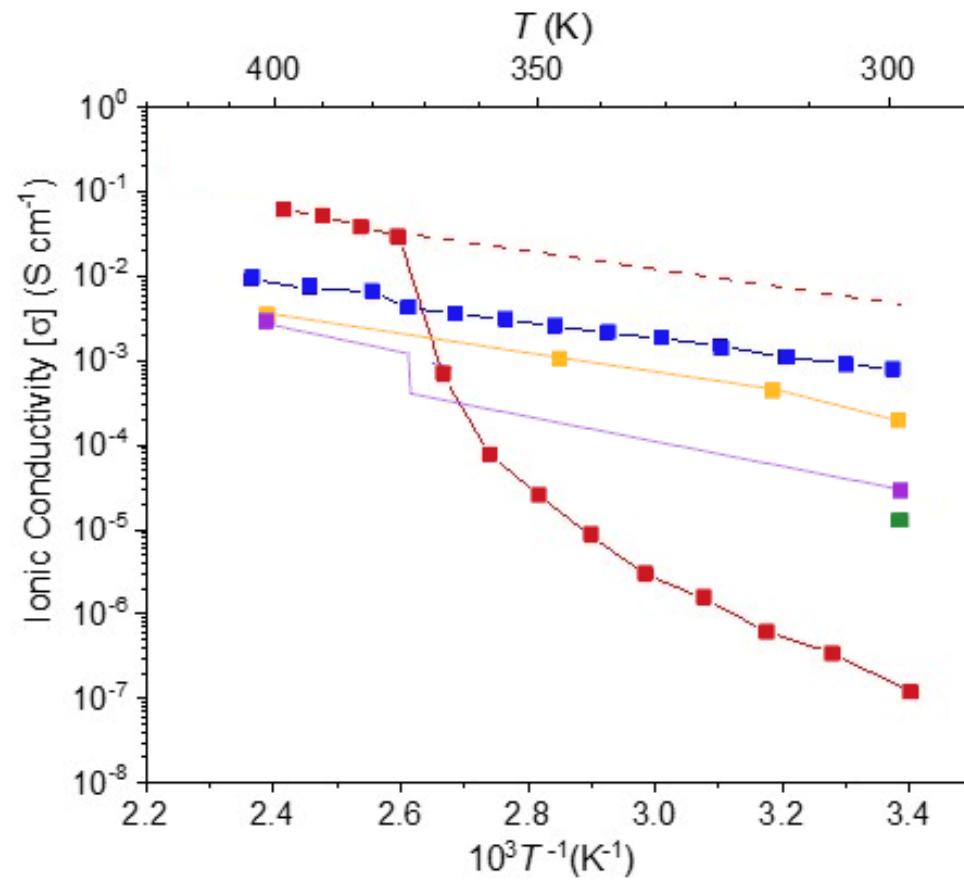
Blue = $\text{NaCB}_{11}\text{H}_{12}$ in SBA-15 with 8nm pores

Red = $\text{NaCB}_{11}\text{H}_{12}$

Green = Once-filled porous SiO_2 disk

Orange = 1.5 μL solution
 $\text{NaCB}_{11}\text{H}_{12} / 1 \text{ mg HSA SiO}_2$

Purple = 1.8 μL solution
 $\text{NaCB}_{11}\text{H}_{12} / 1 \text{ mg HSA SiO}_2$





Possible Next Steps

- ❖ Measure conductivity of more samples
 - Loading samples more than once
 - 12nm SBA-15
 - More durable SiO_2 disks
- ❖ More compressive force on HSA SiO_2
- ❖ Different system for measuring conductivity -
larger temperature range
- ❖ Looking at filled silica under microscope



References & Thank You

Terrence Udovic

Mikael Anderson

Juscelino Leão



- ❖ Dimitrievska M, Shea P, Kweon K, Bercx M, Varley J, Tang W, Skripov A, Stavila V, Udovic T, Wood B. 2018. Carbon Incorporation and Anion Dynamics as Synergistic Drivers for Ultrafast Diffusion in Superionic $\text{LiCB}_{11}\text{H}_{12}$ and $\text{NaCB}_{11}\text{H}_{12}$. *Advanced Energy Materials*. 8(15):1703246.
- ❖ Tang W, Unemoto A, Zhou W, Stavila V, Matsuo M, Wu H, Orimo S, Udovic T. 2015. Unparalleled lithium and sodium superionic conduction in solid electrolytes with large monovalent cage-like anions. *Energy & Environmental Science*. 8(12):3637-3645