

2ND ANNUAL **ENERGY & INNOVATION** CONFERENCE

Soft Materials: Capabilities and Successes

David Luebke

Carbon Capture Technical Coordinator, NETL



Carnegie Mellon



University of Pittsburgh

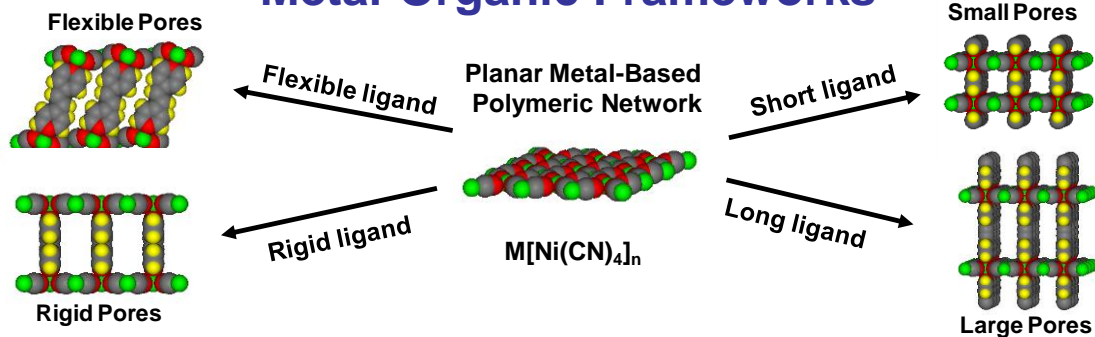
VirginiaTech

West Virginia University

URS

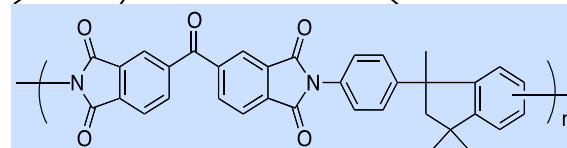
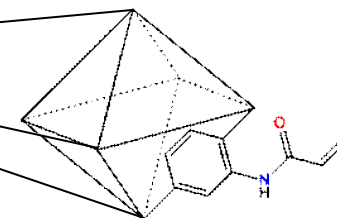
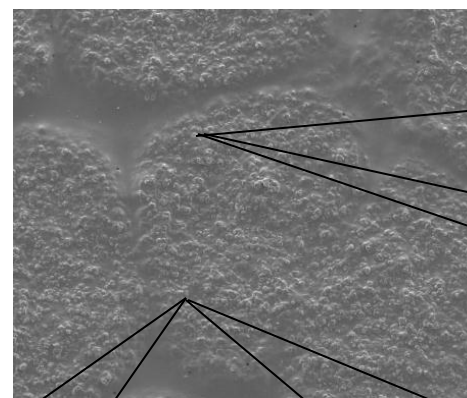
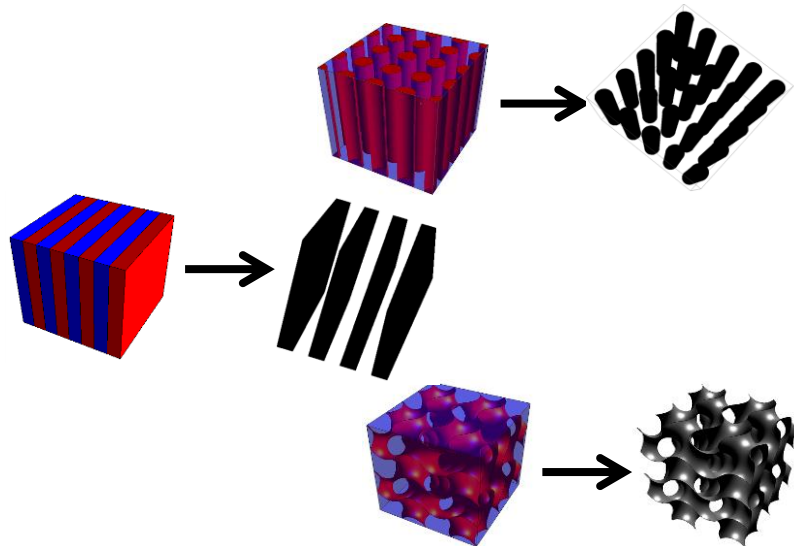
What are soft materials?

Metal-Organic Frameworks



Ionic Liquids

Polymers and Derivatives



Composites

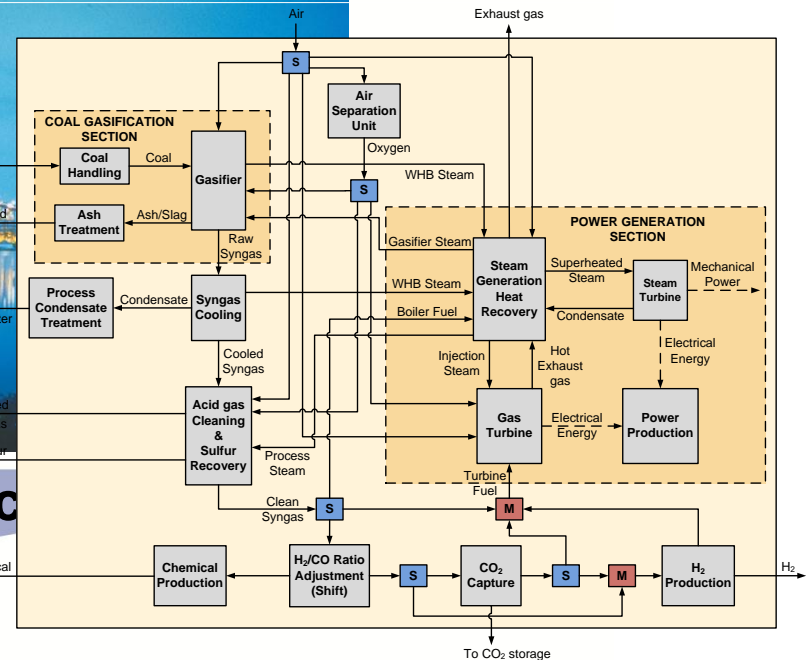
**What does the
NETL-RUA bring to
the table?**



Unrivaled Understanding of Energy Applications



Energy Tec

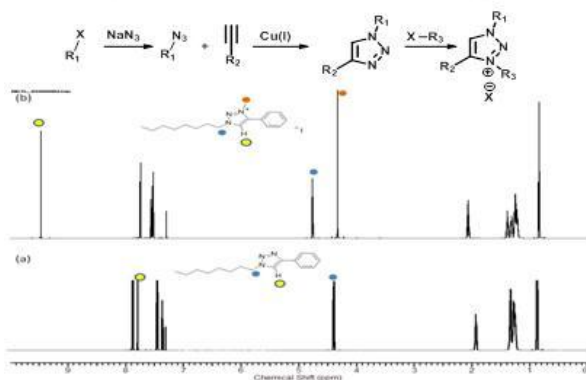


Expertise

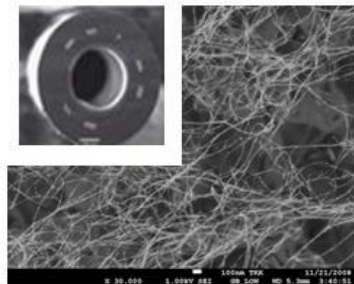
Tools

Results Based Technology Development

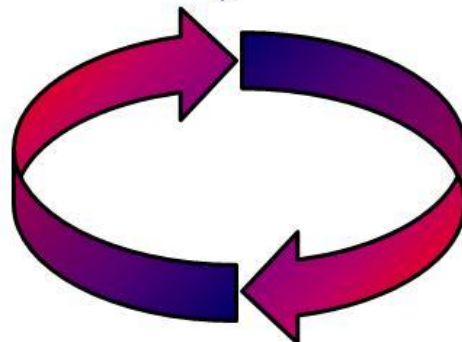
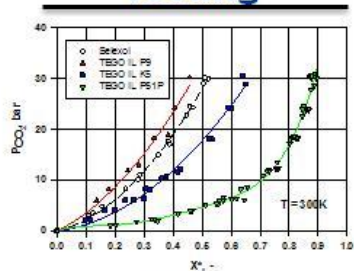
Characterization



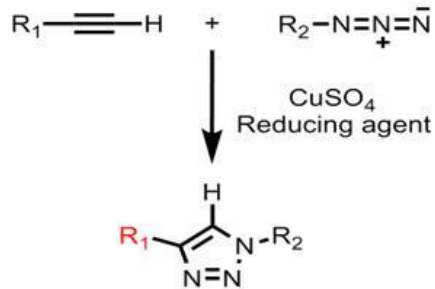
Fabrication



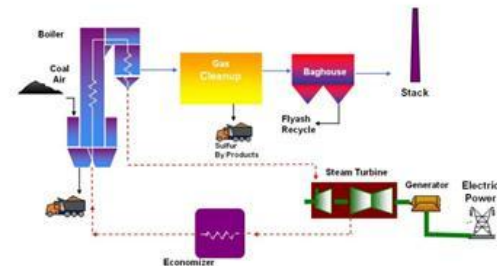
Performance Testing



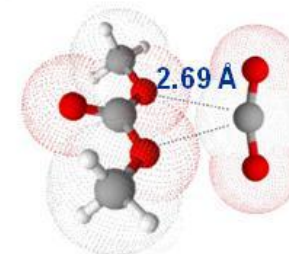
Synthesis



Systems Analysis



Modeling

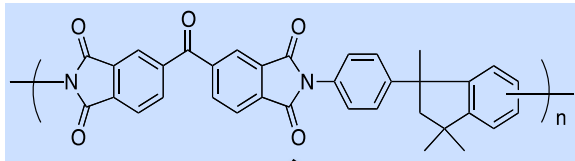


Strength in Collaboration



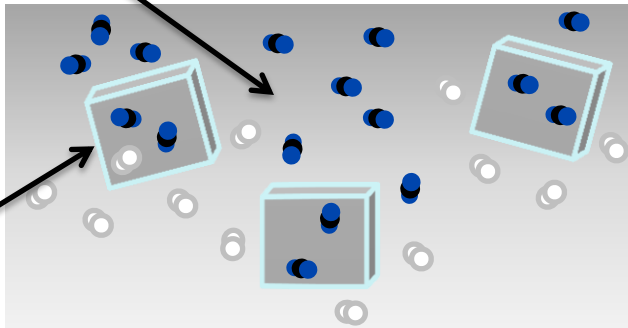
Internal Collaborative Research

Mixed Matrix Membranes



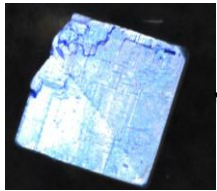
Polymer Membrane

Brian Adzima, ORISE
Hunaid Nulwala, CMU



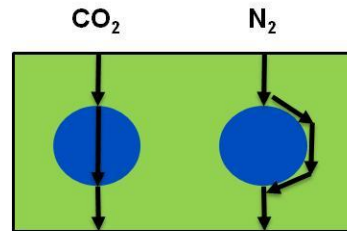
MMM

David Hopkinson, DOE
Shan Wickramanayake, URS

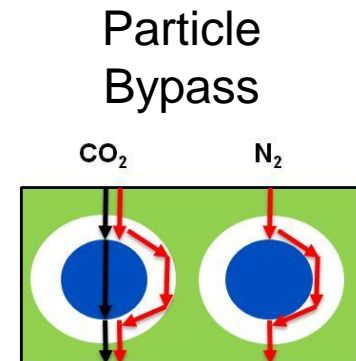


MOF

Brian Kail, URS
Nathaniel Rosi, Pitt



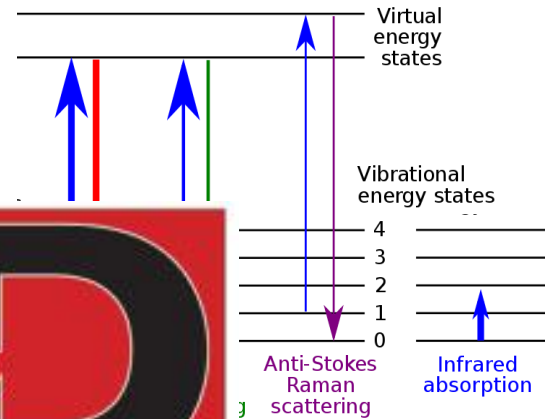
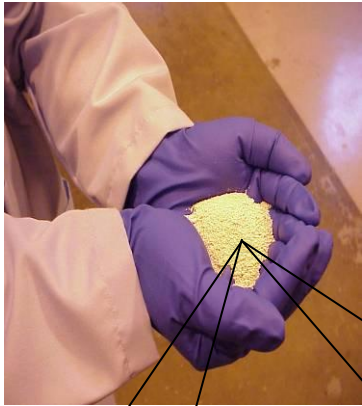
“True” MMM Transport



Particle Bypass

Internal Collaborative Research

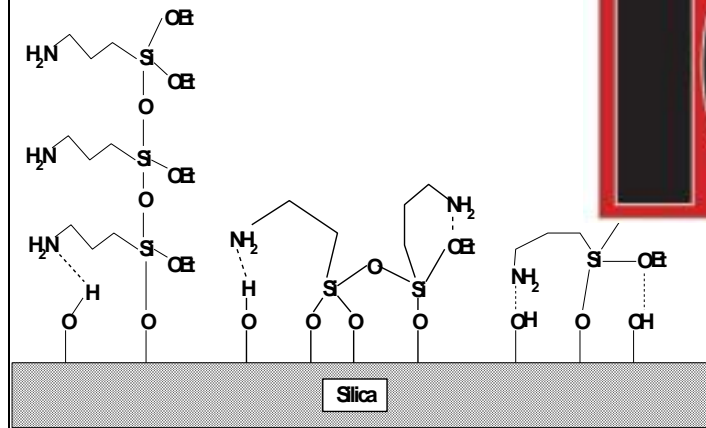
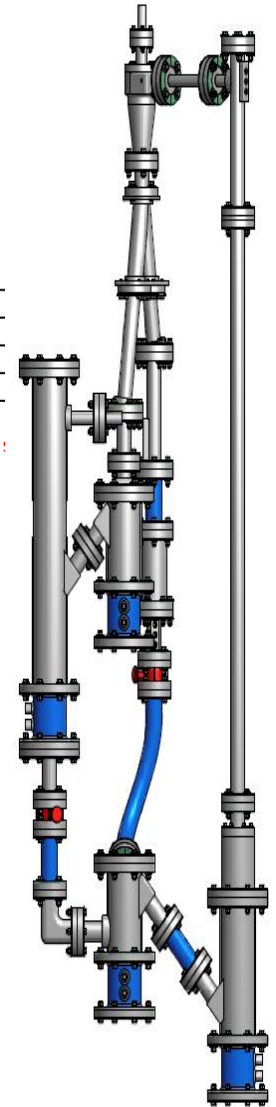
Supported Amine Sorbents



Lin, CMU
 Iman, DOE
 Krishnan, Pitt

Scale-up

Larry Shadle, DOE
 Scott Chen, CCS



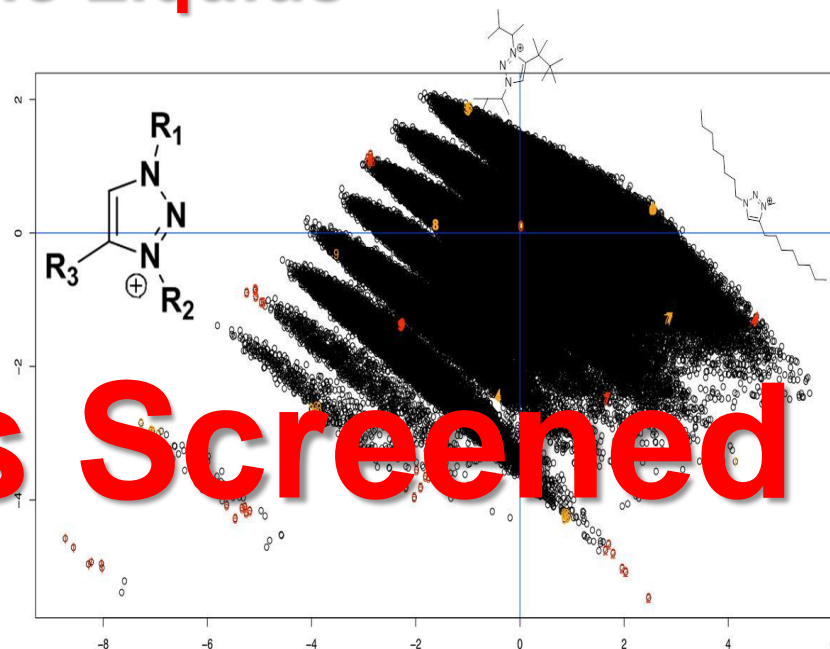
McMahan Gray, DOE
 Bingyun Li, WVU



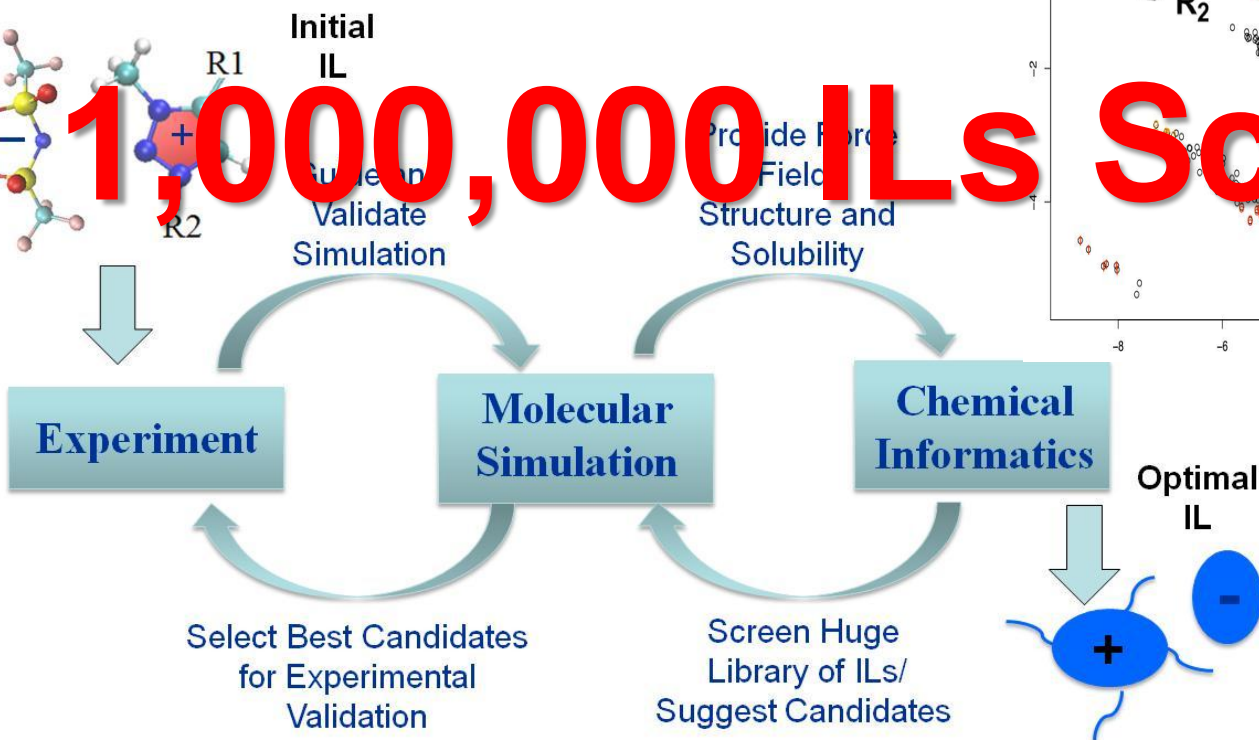
External Collaborative Research

Triazolium Ionic Liquids

Hunaid Nulwala, CMU
Robert Thompson, URS
Michael Larthey, ORISE



1,000,000 ILs Screened



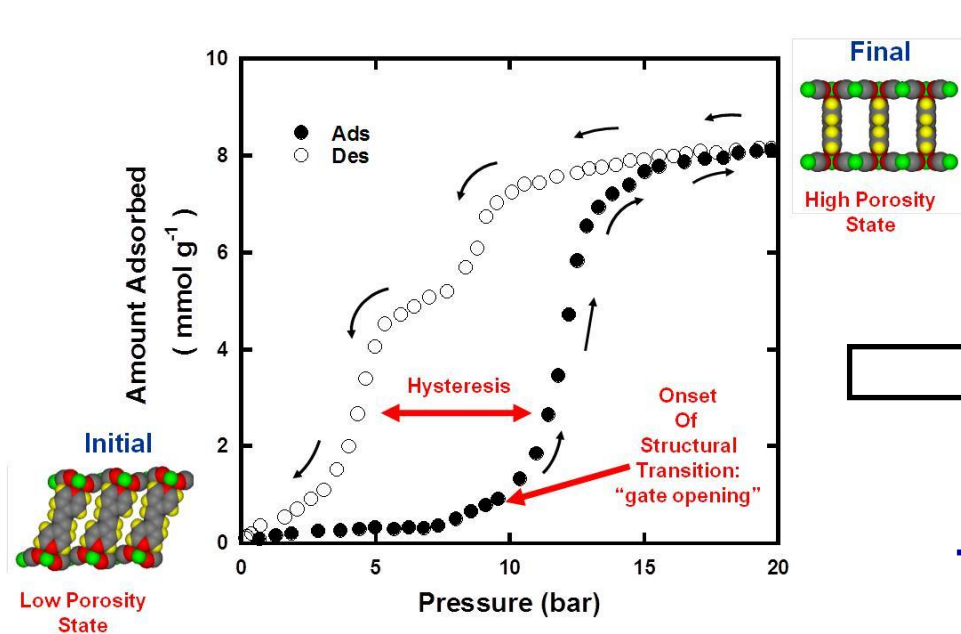
Berend Smit, Berkeley

Maciej Haranczyk, Berkeley

Jeff Kortright, LBNL

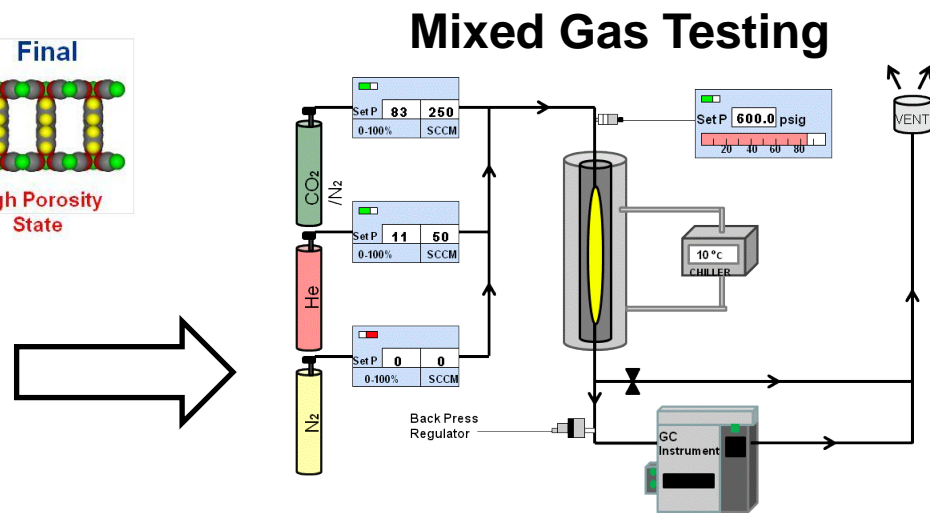
External Collaborative Research

Structurally Dynamic MOFs

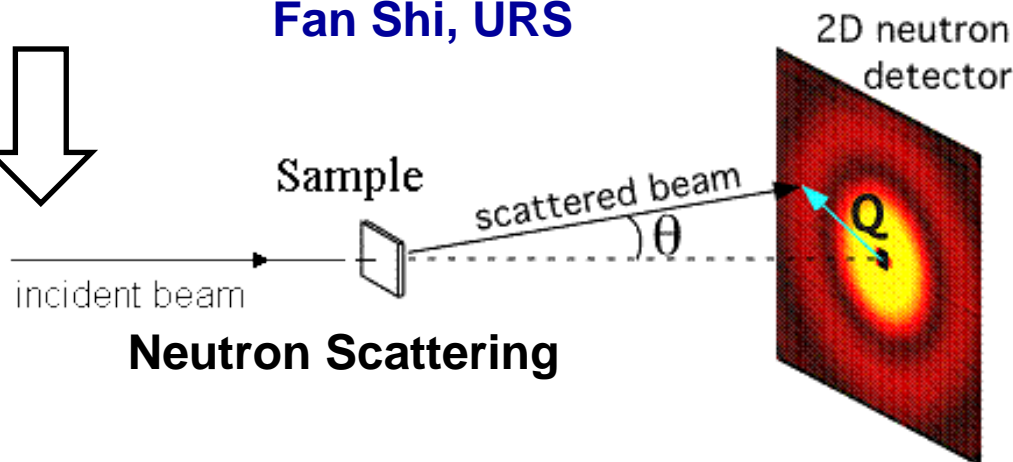
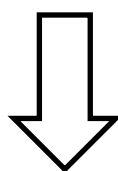


Christopher Matranga, DOE
Jeff Culp, URS

Andrew Allen, NIST

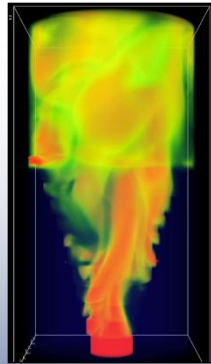
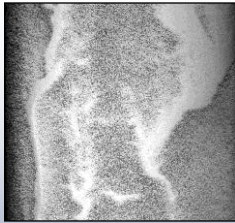
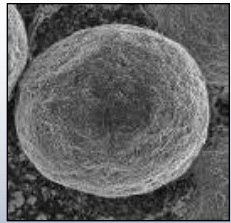


Tom Brown, DOE
Fan Shi, URS



Neutron Scattering

External Collaborative Research Carbon Capture Simulation Initiative



Identify promising concepts



Reduce the time for design & troubleshooting



Quantify the technical risk, to enable reaching larger scales, earlier



Stabilize the cost during commercial deployment

National Labs



Academia

Carnegie Mellon



West Virginia University

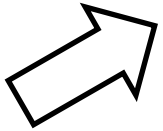
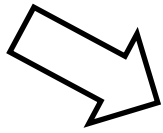


Industry

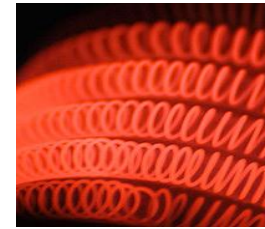
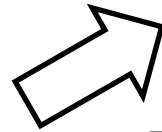


External Collaborative Research

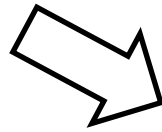
Adhesives/Coatings Based on CO₂



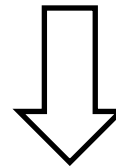
Simple Mixing



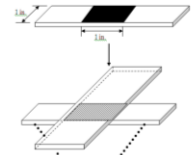
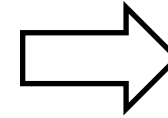
Thermal Curing



UV Curing



Electronics
Composites



Glass Adhesive
Metal Adhesive
Fiber Binder

CO₂-based
Precursor

Shawn Duffy, PPG

Larry Fitzgerald, PPG

Robert Schmeltzer, PPG

Max Dizard, IW

Hunaid Nulwala, CMU

Dave Luebke, DOE

NETL-RUA Capabilities

Computational

- **Monte Carlo (MC)**
 - In-house software: MPI parallel *MCMDMS*
 - NVT, NTP, Continuous Fraction Component, Gibbs, grand canonical, Osmotic, Hybrid MD/MC
 - NP_{xy}T, NP_{zz}T, Isostress Osmotic, Isostress Grand Canonical
- **Molecular Dynamics (MD)**
 - Free software: LAMMPS, NAMD, VMD
 - Classical Atomistic and Coarse-grained Force Field Development
 - Reactive Force Field Development
- **Ab Initio**
 - Wave Function Methods: HF, MP2, CC, SAPT, MCSCF, MRPT
 - DFT Methods: LDA, GGA, Exact-exchange Hybrids, Meta-GGA, Dispersion Corrected, Long-range Corrected
 - Energy, Geom. Opt., Transition State Opt., Vib. Freq., Atomic Charges, MD, QM/MM
 - Cluster or Periodic Models
 - Software: VASP, G09, MOLPRO, Q-CHEM, PSI4, CPMD, CP2K
- **Chemical Informatics**

Synthesis

- **Scale**
 - 1 mg – 1 kg
- **Reaction Classes**
 - Click
 - Controlled Radical Polymerization
 - Free Radical Polymerization
 - Organometallic Synthesis
 - Friedel-Crafts Acylation

Fabrication

- **Thin Films**
 - Reverse Phase Inversion
 - Knife Casting
 - Spin Coating
- **Fibers**
 - Hollow
 - Solid
- **Composites**
 - Supported Ionic Liquid Membranes
 - Mixed Matrix Membranes

Imaging

- **Optical Microscopy**
- **SEM**
- **TEM**
- **CT Scanning**
- **AFM**
- **Neutron**
 - SANS
 - USANS

Chromatography

- **GC**
 - TCD
 - FID
 - MS
- **LC**
 - HPLC
 - LC-MS
- **GPC**

NETL-RUA Capabilities

Spectroscopy

- **FTIR**
 - ATR
 - High Pressure
 - DRIFTS
- **UV-Vis**
- **Raman**
 - High Pressure
- **NMR**
 - Solution (700 MHz)
 - Solid State (500 MHz)
 - Pulse Field Gradient
 - Nuclear Spin Relaxation Kinetics
- **X-rays**
 - Soft X-rays
 - Single Crystal
 - Powder

Gas Solubility

- **Solids/Liquids**
 - Microbalance
 - Sievert's Method
 - Single Pass Flow
 - Recirculating Flow
 - Breakthrough
- **Liquids Only**
 - CSTR

Membrane Performance

- **Isochoric**
- **Flow**
 - High Accuracy
 - High Throughput
- **Gas-liquid Porosimetry**
 - Bubble Point
 - Pore Size Distribution
 - Membrane Burst Pressure

Other Analytical

- **DSC**
 - Modulated
- **MS**
 - ESI
 - MS-MS
 - TOF-ESI
- **TGA**
- **ICP**
 - MS
 - OES
- **BET**
- **Viscometry**
- **Densimetry**
- **Karl Fischer**
- **Goniometry**
 - Contact Angle
 - Surface Tension
- **DMA**
 - Dynamic Modulus
 - Tensile Strength

NETL-RUA: **Creating Technology Solutions**

- **Unrivaled Understanding of Energy Applications**
- **Results-based Technology Development Approach**
- **Vast Array of Expertise and Facilities within NETL-RUA**
- **Collaborations with World Class Research Organizations**
- **Proven Record of Achieving Technology Solutions**



Contact Information

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