Nanoparticle Ionic Materials for Energy and Sustainability

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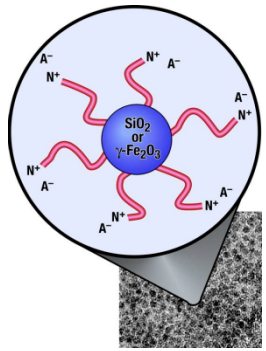
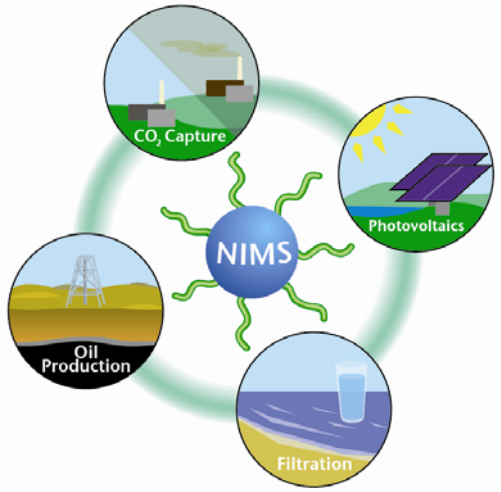
Chemical and Biomolecular Engineering & Materials Science and Engineering

Cornell University

Vision

We envision a Center for Research and Education that provides a dynamic venue for fundamental scientific studies, graduate education, and technological innovations addressing emerging problems critical to the Kingdom, the region, and the world





Mission

- **Establish a pre-eminent research center focused on hybrid nanomaterials**
- **Educate a cadre of interdisciplinary, team-based researchers prepared to assume leadership roles in the Kingdom, the United States, and the world**
- **Support a culture of innovation and entrepreneurship**
- **Collaborate to build capacity at KAUST through several innovative programs**
- **Promote industrial partnerships to ensure 1) technological relevance of research in the Center and 2) rapid commercialization of new technologies**

Benefits to KAUST

Research and education programs at the Center will help

- build intellectual capacity at KAUST during its formative years

- propel KAUST to the forefront of
  - nanoscience/nanotechnology
  - polymers
  - complex fluids

Interactions with KAUST

- Incubate research programs of new KAUST faculty
- Establish a dynamic student and visiting scholar exchange program that links the two campuses
- Support KAUST with research infrastructure development and laboratory build-outs
  - KAUST Nanofabrication Facility (KNF)
- Develop joint curricula and education programs to help promote a culture of excellence
- Share best practices for graduate student recruitment and for enhancing the pipeline of students in science and engineering
- Assist KAUST in developing a culture of innovation and entrepreneurship through formal courses and experiential learning

Synergies

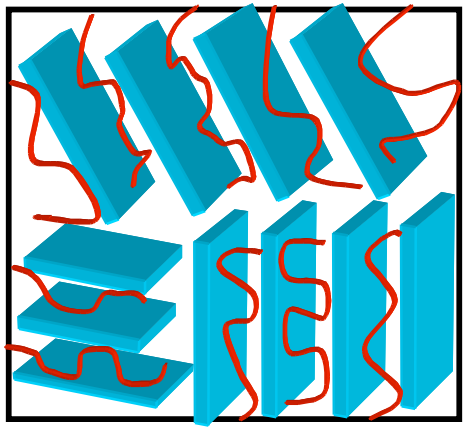
- Extensive experience administering large, multi-institution research centers in a cost-effective manner
  - High Energy Synchrotron Source (CHESS)
  - Center for Advanced Computing (CAC)
  - Cornell Center for Materials Research (CCMR)
  - Cornell Nanofabrication Facility (CNF)
- Graduate studies are based on field system
  - fosters collaborative research that transcends traditional disciplinary boundaries
- Land-grant mission
  - commitment to creating and disseminating scientific discoveries to the benefit of the state, nation, and the world

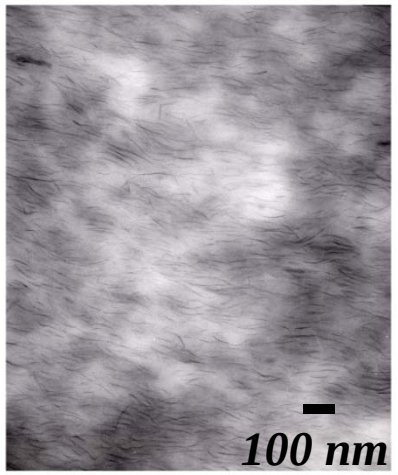
Scientific Focus: NIMS

- Organic-inorganic hybrids (composites) are attractive because they integrate the light-weight features, low-cost, and processability of polymers with functionality of inorganics

- Widespread interest in *nanocomposites* (composites with nanoscale components) has been motivated by the promise of unmatched performance, design flexibility, and lower unit and life-cycle costs
  - Market forecasts estimate the use of nanocomposites to reach $800M by 2011 (annual growth rate of 24%)

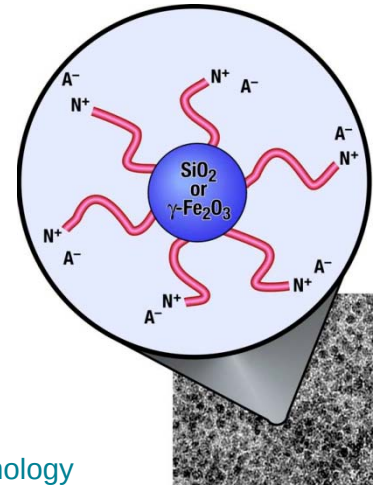
- Persistent challenges with poor miscibility, dispersion and interfacial strength prevent nanocomposites from realizing their full potential

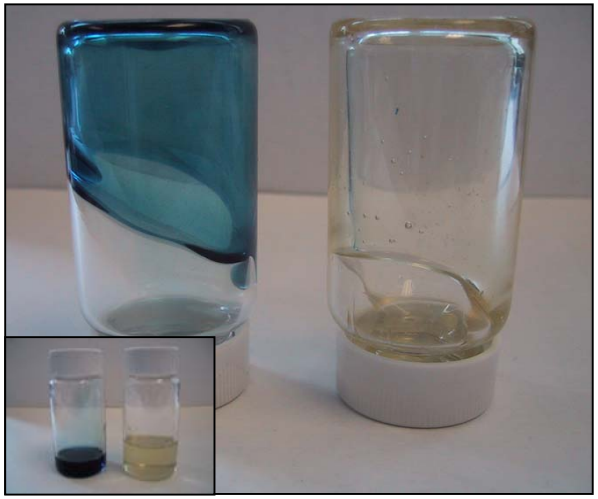




Scientific Focus: NIMS

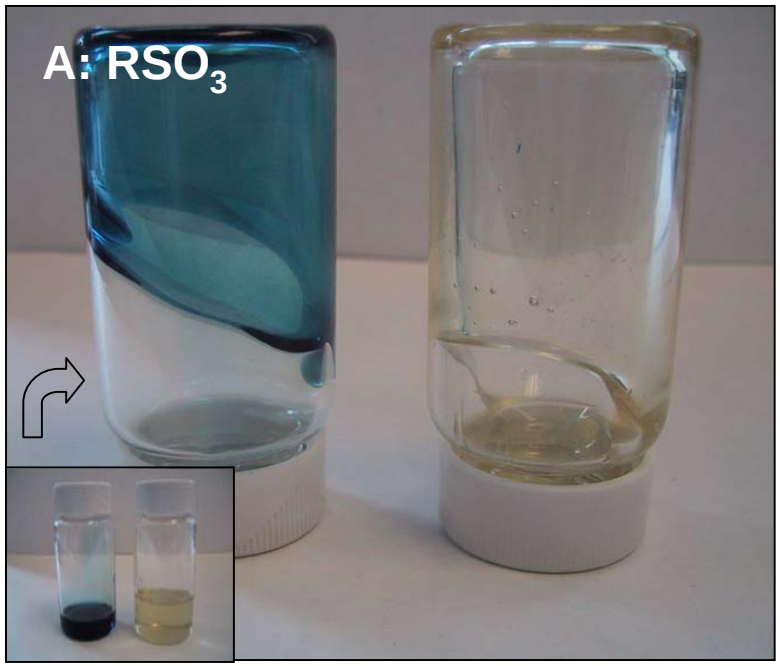
- **Nanoparticle ionic materials (NIMS) provide a highly tunable/functional materials platform that solves many of these technical challenges**
- **NIMS are a disruptive technology, enabling applications in multiple fields**
- **NIMS are ideal for research and education at the interface of nanotechnology, polymers and complex fluids**





NIMS: Solvent-Free Particle Fluids

SOLIDS ***LIQUIDS & GELS***



SiO_2 SiO_2 γ-Fe_2O_3

Cores: ***SiO_2***, ***TiO_2***, **γ–*Fe_2O_3***, ***ZnO***, ***SnO_2***, ***Au***, ***Pt***, ***Pd***, **CNTs**, ***C_{60}***

Science & Technology

- **“Solvent” is tethered to the cores**
  - zero vapor-pressure materials
- **Tunable materials properties**
  - liquid, gel, LC, solid (φ, T)
  - conductivity, magnetic susceptibility, refractive index
- **Controlled assembly**
  - despite nanometer size they reach **equilibrium** state
- **External fields can be used for assembly**

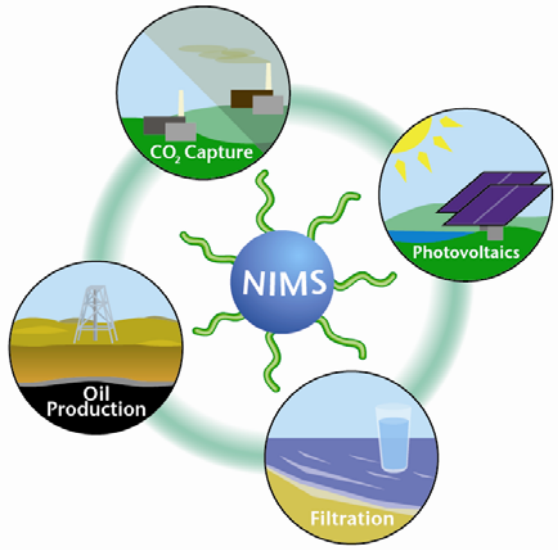
Research Program

NIMS: A new materials platform with many applications

Table 1. Applications of Nanoparticle Ionic Materials	
Property	**Applications**
Amphiphilicity	Membranes for water desalination; Surfactants and nanomaterial probes for oil and gas production
Birefringence	Reconfigurable optics
Chemical reactivity	Catalysts for CO_2 sequestration and polymerization
Electrical conductivity and semiconductivity	Photovoltaics and liquid processable semiconductors
High dielectric constant and zero vapor pressure	Media for CO_2 capture; Zero VOC solvents and inks
High index of refraction	Immersion photolithography, reconfigurable optics
Ionic conductivity	Solvent-free electrolytes for solar cells, batteries, and fuel cells.
Optical/absorption	Solar sensitizers, paints, UV filters
Thermal conductivity	Conducting lubricants & coolants
Tunable rheology	Displacement fluids and ferro fluids

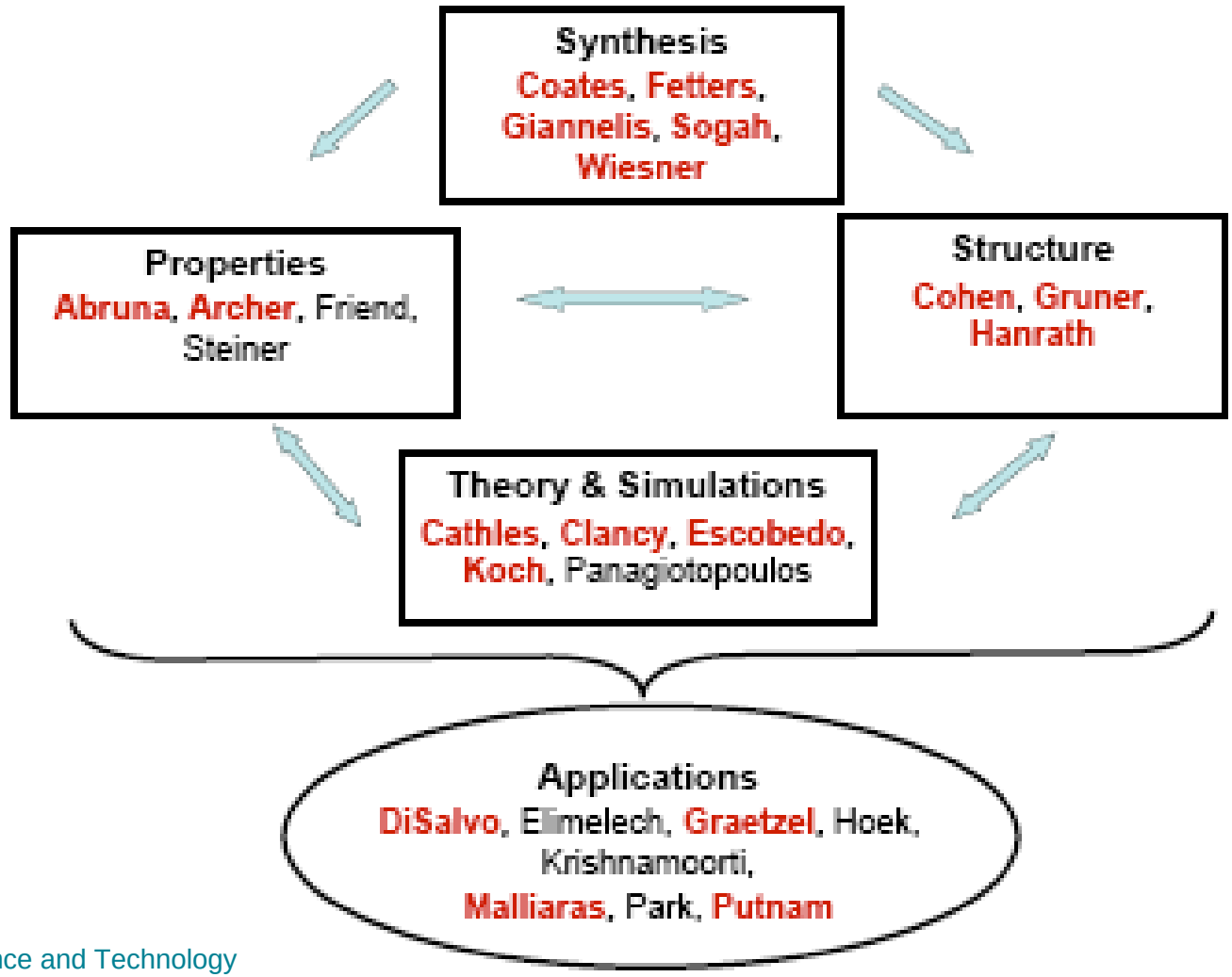
KAUST-CU Research Focus

- CO_2 capture and sequestration ★
- PVs and solid-state lighting
- Water treatment and desalination
- Nanomaterials for oil production



Global Interdisciplinary Team

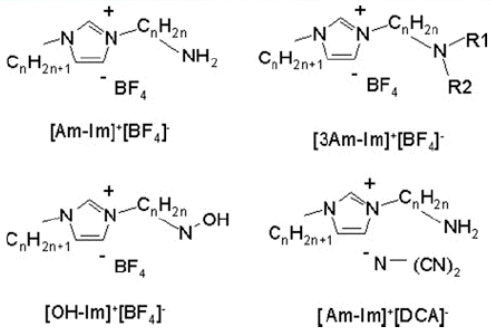
Cornell
Cambridge
Columbia
ETH Lausanne
Houston
Princeton
UCLA
Yale



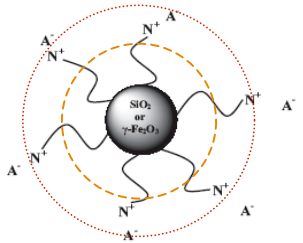
CO_2 Capture and Sequestration

- CO_2 is a greenhouse gas
- CO_2 sequestration involves three steps:

  capture, transportation, and disposal
  - Carbon dioxide capture is the most expensive

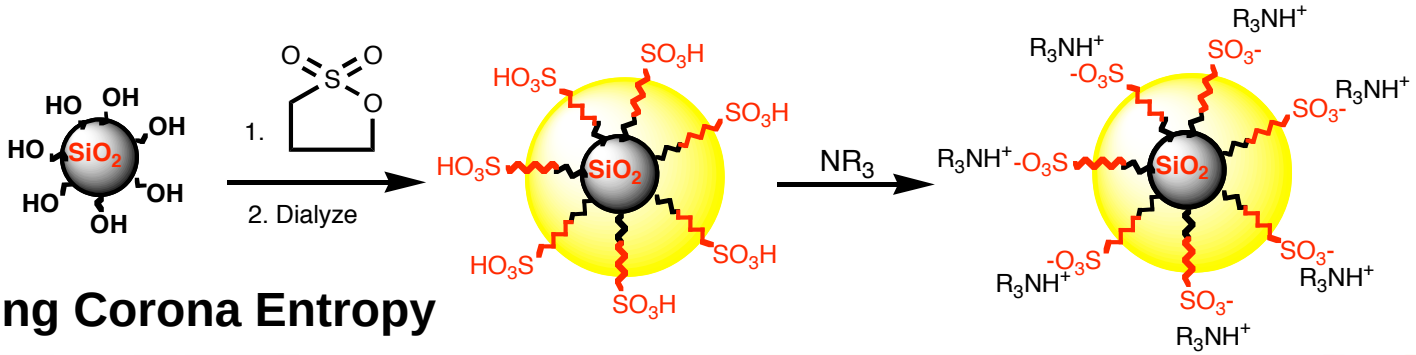


- A novel carbon capture technology under development utilizes an amine-functionalized Task-Specific Ionic Liquid (IL)

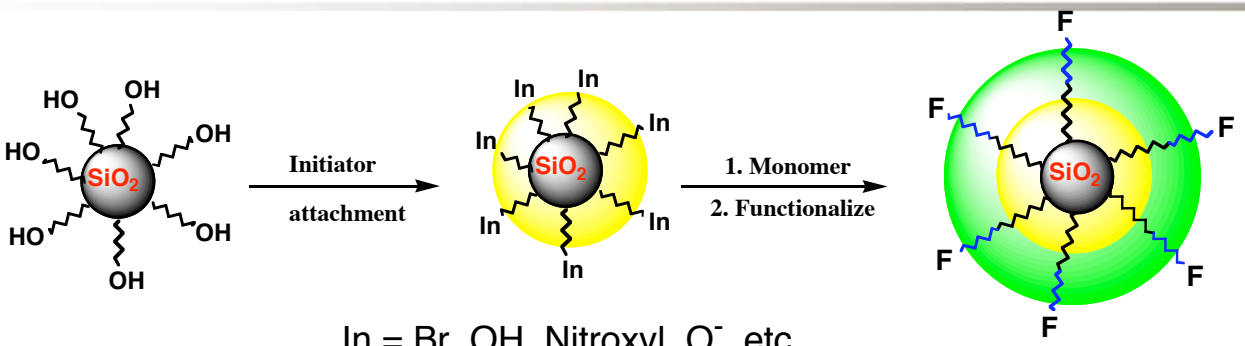


- NIMS are nanoscale analogs of ILs and offer numerous advantages for capture and sequestration
  - Solvation in NIMS is driven by enthalpic as well as by entropic interactions
  - NIMS with high-affinity nanoporous cores to enhance solubility can be designed
  - Recovery of the capture fluid facilitated by magnetic cores
  - Catalytically active cores can be introduced for sequestration (olivines)

Synthesizing Optimal NIMS for Carbon Capture



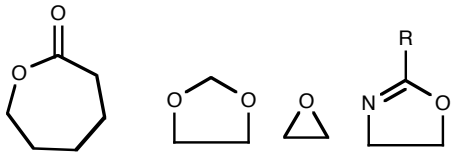
Controlling Corona Entropy



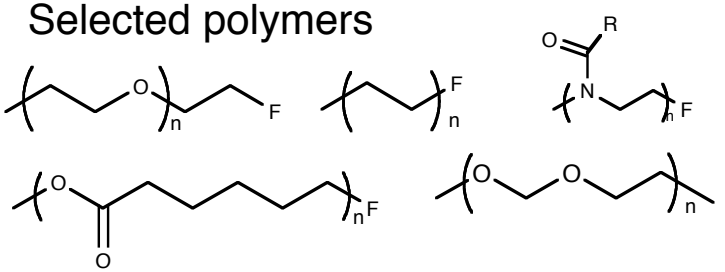
In = Br, OH, Nitroxyl, O^-, etc.

F = N^+, CO_2^-, SO_3^-, etc.

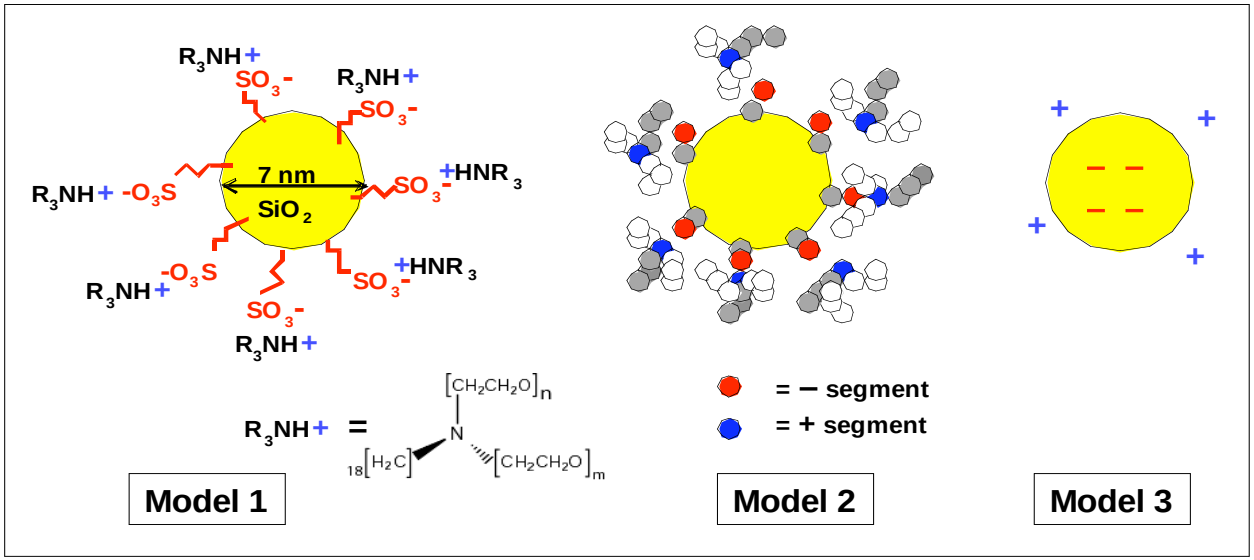
Selected Monomers



Selected polymers



Computer Simulation and Theory: Multiscale Approach



Length & Time Scales

Model 1
All-atom (MD)

- Generate effective interparticle potentials
- Structural packing of corona-canopy
- Effect of chemical composition

Theory and experiment to develop models for Interactions & Transport Properties

Model 2
Bead-spring model (MD, MC)

Bridge length-time scales

- Solid-liquid transitions

Structure (packing)

SAXS, TEM, SEM

Model 3
Mesoscopic model (BD)

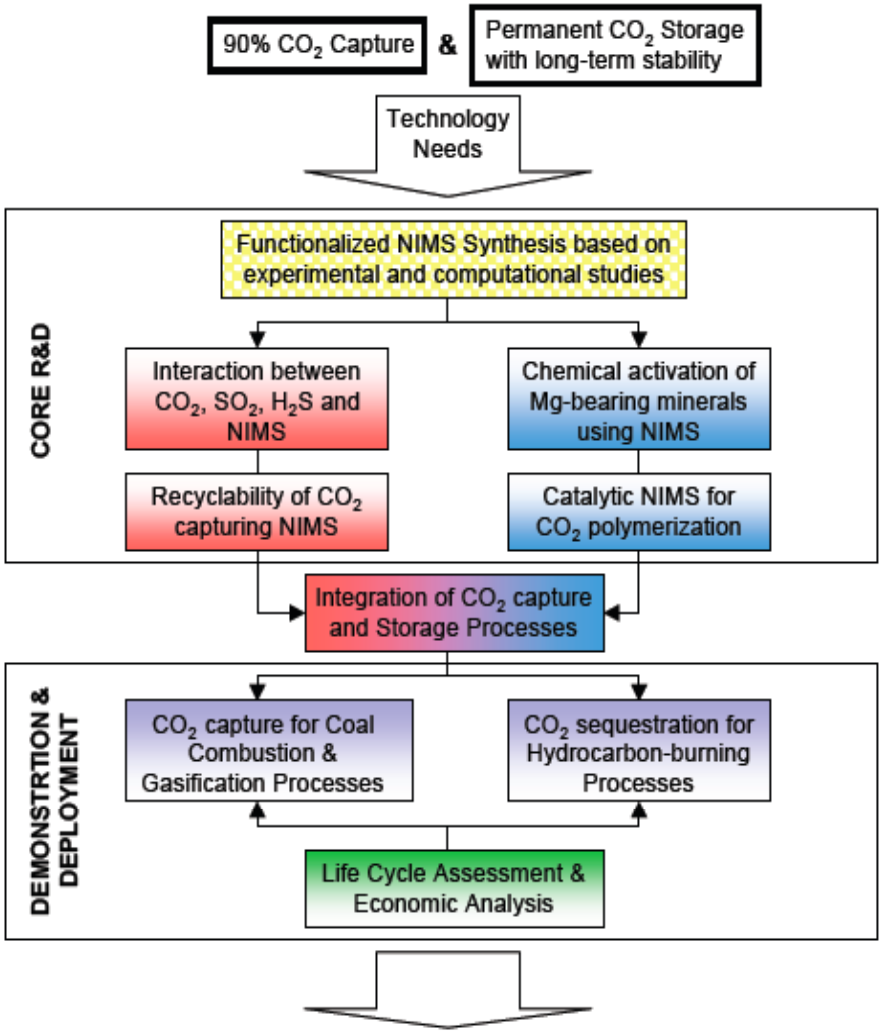
Simulate slow dynamic modes

- Shear flow properties
- Prediction & physical insights

Rheology (flow)

Std.& X-ray shear cells

Technology: Roadmap for CO_2 Thrust



Integrated Carbon Capture and Sequestration Technologies

Industrial Programs

- **BJ Services, Carbo Ceramics, Chevron, Corning, Kodak, Milliken, NanoH2O, NaturalNano, Orica, Summit Lubricants, and Union Carbide intend to participate as industrial partners to drive forward the applications**

- **KensaGroup - tech transfer partner to ensure that technologies emerging from the Center are transitioned rapidly into the marketplace**

CO_2 Capture & Sequestration	Photovoltaics & Energy Systems	Water Treatment & Desalination	Oil & Gas Production	Graduate Education
			BJ Services	BJ Services
			Carbo Ceramics	Carbo Ceramics
			Chevron	Chevron
	Corning	Corning		Corning
	Kodak			Kodak
	Milliken	Milliken		Milliken
		$NanoH_2O$		$NanoH_2O$
NaturalNano	NaturalNano			NaturalNano
Orica				Orica
			Summit Lubricants	Summit Lubricants
Union Carbide				Union Carbide

Thank You