

## Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)

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**Mission Statement:** *To master molecular to mesoscale chemical and physical phenomena at interfaces in complex environments characterized by extremes in alkalinity and low-water activity, and driven far from equilibrium by ionizing ( $\gamma, \beta$ ) radiation.*

IDREAM is an Energy Frontier Research Center (EFRC) conducting fundamental science to support innovations in processing high-level radioactive wastes (HLW). IDREAM facilitates the transformation of HLW processing by elucidating the basic chemistry and physics required to control and manipulate interfacial phenomena in extreme HLW environments (e.g., heterogeneous and chemically complex). This foundational knowledge is required to achieve ***IDREAM's mission to master molecular-to-mesoscale chemical and physical phenomena at interfaces in complex environments characterized by extremes in alkalinity and low-water activity, and driven far from equilibrium by ionizing ( $\gamma, \beta$ ) radiation.*** Further, understanding these processes will enable prediction of waste aging over the many decades required to complete this difficult cleanup task. IDREAM activities focus on aluminum hydroxides and (oxy)hydroxides, as they are principal components of bulk waste materials to which a variety of other metal ions and radionuclides partition.

Through novel and highly integrated experimental, computational, and theoretical approaches, we propose to develop the ability to predict and control the critical physicochemical phenomena currently preventing the application of more efficient and cost-effective tank waste removal and processing strategies. Our work will span from the molecular scale (e.g., speciation and dynamics of key solution species), to interfacial dynamics (e.g., dissolution and precipitation rates and mechanisms), to particle scale (e.g., particle interactions), and will involve realistic conditions of extreme alkalinity, low water activity, and ionizing radiation. IDREAM will provide a scientific foundation for emergent phenomena in high-level radioactive waste (HLW) processing, such as dissolution rates, aging phenomena, and slurry behavior including adhesion, friction, gelation, and rheology.

As shown in the figure below, IDREAM is structured around three research thrusts and three cross-cutting thrusts:

**Research Thrust 1 (RT1): Molecular and Solution Processes.** Understand the roles of solvent dynamics, chemical reactivity, solute organization, and pre-nucleation species on overall molecular speciation in highly alkaline systems of concentrated electrolytes.

**Research Thrust 2 (RT2): Interfacial Structure and Reactivity.** Link fluid phase dynamics to nucleation, particle growth, and interfacial reactivity in highly alkaline systems of concentrated electrolytes.

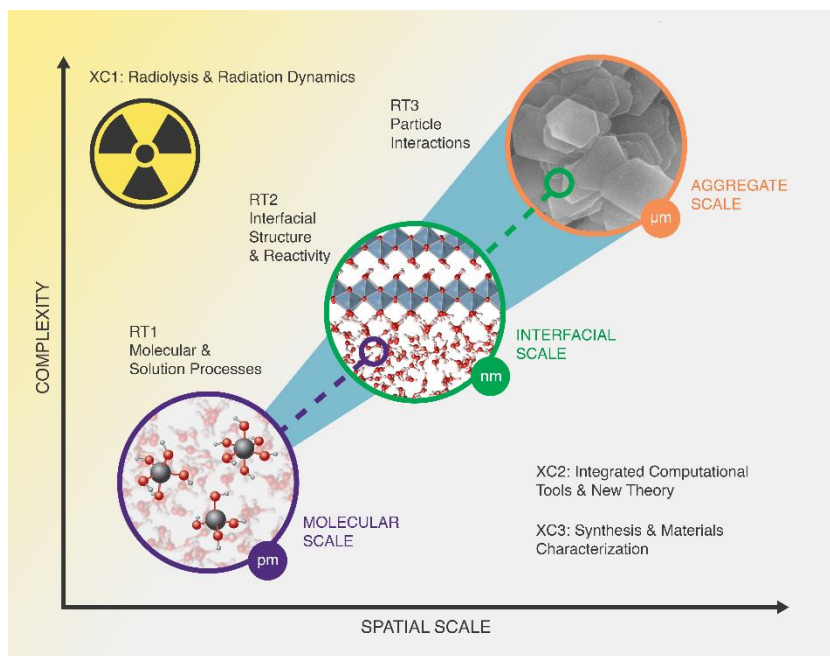
**Research Thrust 3 (RT3): Particle Interactions.** Quantify the chemical and physical phenomena leading to hierarchical microstructures of aggregates, and other response dynamics that couple across scales.

**Cross-Cutting Thrust 1 (XC1): Radiolysis and Radiation Dynamics.** Quantify the role of  $\beta$  and  $\gamma$  radiation in driving molecular speciation and interfacial reactivity far from equilibrium.

**Cross-Cutting Thrust 2 (XC2): Integrated Computational Tools and New Theory Development.** Develop and apply integrated computational approaches within and across research thrusts to enable foundational, new theories in interfacial chemistry to emerge.

**Cross-cutting Thrust 3 (XC3): Synthesis and Materials Characterization.** Understand and control the synthesis of aluminum oxides and oxyhydroxides to design and produce materials with well-defined characteristics.

IDREAM has a central theme of aluminum chemistry because it's commanding role in the processing of high level radioactive wastes. It is a primary component of the bulk solids to which other metal ions and radionuclides are partitioned, and must be dissolved and separated from radioactive contaminants. This focus provides an integrating theme across the four Research Goals. The integrated disciplinary perspective of IDREAM will accelerate the transformative understanding of complex interfacial phenomena that are driven far from equilibrium. We will exploit a broad range of characterization tools and computational resources within our collaborating institutions and at DOE user facilities.



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By better understanding chemical interactions across scales of time and space, we can explain poorly understood macroscale phenomena, such as waste stream rheology, slurry agglomeration, and control of precipitation. This will provide the foundation for accelerating the dissolution of the waste materials, its processing, and improving process systems. The knowledge gained in IDREAM will be broadly applicable to other complex heterogeneous processing problems related to materials and energy production.

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