Solid State and f-block Chemistry
Structures and Thermodynamics of nano, bulk-size lanthanide and actinide (transuranium actinides) materials

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Research Programs

Nuclear Waste Forms and Fuels
- Structural stability of lanthanide/actinide phosphate and silicates, MXO₉-(n/2)O (M = La, An; X = P, Si)
- Structural and thermodynamic stability
- Role and position of water in the structure
- Influence of mixing La/An in the matrix

- Various sized An₂O₃, the size-dependent structural and thermodynamic features
- Unknown size-dependent thermodynamic features relevant to environmental concerns

Critical Material Ceramics and Minerals
- Lanthanide silicate ceramic in aerospace thermal coating application
- Structural and thermal stability
- Thermal oxidation behavior
- Bulk moduli of U-X compounds
- Phase diagrams of U-X

- Material science of accident tolerant fuel, U-X and molten salt fuel

Thermodynamics of Transuranium solids
- Thermodynamics of Pu oxides/salts
- Pu calorimetry capability at NSC
- Protocols that ensure safely conducted calorimetric experiments
- Spectrocalorimetry development

Structures under Various P-T

Phase equilibria under various P-T conditions
- Long-range structures as functions of T, P, or combined
- Various sized An₂O₃, the size-dependent structural and thermodynamic features

Local structures by X-ray scattering
- Determine the atomic arrangement
- Local structures as a function of T, in the melts vs. solids

Chemistry probed by X-ray absorption
- Determine the oxidation state, bonding information, and coordination of Ln, An solutions and solids
- Lab-based XAS and XES commissioned in 2021 summer

Thermodynamic Capabilities

High Temperature Oxide Melts Solution Calorimetry
- Isoperibol Type, 500–1000 °C
- Heats of reactions
- Heats of formation
- Heats of mixing
- Refractory, volatile-bearing, air-sensitive, molten-salt, or variable valence materials can be studied

Differential Scanning Calorimetry
Thermogravimetric Analysis
- Study thermal stability and reaction energetics at high temperature up to 2400 °C
- Determine the transition/melting/crystallization related thermal processes
- Determine heat capacity and melting points
- Study kinetics of crystallization and transition

Resonant Ultrasonic Spectroscopy
- Bulk, Shear, Young’s Moduli and Poisson’s ratio
- Mechanical performance at high temperature

About the Group

Summary of Research
- Current research focuses include:
  - Thermodynamics of lanthanides, actinides-containing phases, nuclear fuels and wastes
  - Complex and nanosized materials
  - Critical material mineralization
  - Minerals and materials under high-temperature, high-pressure, and other extreme conditions

- Students in the group will be trained in:
  - Handling rad materials and inorganic synthesis
  - X-ray and neutron-based characterizations
  - Static compression (high pressure)
  - Thermal analysis techniques (DSC, TG, high T calorimetry)
  - Elastic techniques (RUS)

Interested Systems
- U-, Tb-, (Np-, Pu-) containing minerals/solids
- Oxides, silicates, phosphates, etc.
- U-X intermetallics and HEA
- Chloride- and fluoride-based molten salts

Instrumentation
- Thermodynamic instruments
  - High T Isoperibol Calorimeter
  - Ultra High T DSC/TGA
  - High T resonant ultrascan spectroscopy

- High-pressure Apparatus
  - Diamond Anvil Cells (DAC)
  - Hydrothermal DAC

- Synthesis and Characterization Capabilities
  - High T Furnaces and Tube Furnace
  - Schlenk Line
  - Inert-gas Glovebox and Rad Glovebox
  - Micro-balances
  - X-ray Fluorescence Spectrometer
  - Lab-based X-ray spectrometer (XAS and XES)

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