U.S. DEPARTMENT OF ENERGY | Office of Nuclear Energy

FY2018 NUCLEAR ENERGY UNIVERSITY PROGRAMS
CINR WEBINAR – OCTOBER 25, 2017

RC-2: Salt Behavior in Molten Salt Reactors

RC-2.1: Predicting the Chemical Speciation, Structure, and Dynamics of Salt Solutions for Molten Salt Reactors

RC-2.2: Development of Molten Salt Reactor Fuel Salt Irradiation Capabilities

RC-2.3: Understand the Structure and Speciation of Molten Salt at the Atomic and Molecular Scale

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MSR National Technical Director – Dr. Lou Qualls (ORNL)

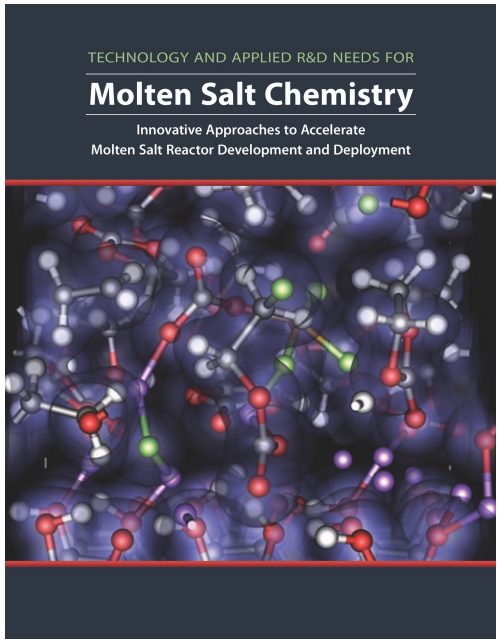
ELIGIBLE TO LEAD: UNIVERSITIES ONLY
Up to 3 years; $800K

NTRD
Nuclear Technology Research & Development

NEUP RC-2: Salt Behavior in Molten Salt Reactors

- Our NEUP solicitation seeks to support innovative research at universities that may offer enhanced safety, functionality and affordability of molten salt technologies.
- Our planned path forward:
  - ✓ To re-establish robust core competencies and R&D capabilities in Molten Salt Chemistry at DOE national laboratories and U.S. universities
  - ✓ To support MSR research community to train broad-based next generation expertise
  - ✓ To provide a technical basis, in coordination with MSR developers, for supporting the U.S. industries' goal for commercialization of MSR technologies

In April 2017, the Office of Nuclear Technology Research and Development sponsored a Molten Salt Chemistry Workshop at Oak Ridge National Laboratory. A report entitled "*Technology and Applied R&D Needs for Molten Salt Chemistry*" is available at: https://www.ornl.gov/content/molten-salt-chemistry-workshop



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The report identified six priority research directions:

- ✓ Understanding, Predicting and Optimizing the Physical Properties of Molten Salts
- ✓ Understanding the Structure, Dynamics, and Chemical Properties of Molten Salts
- ✓ Understanding Fission and Activation Product Chemistry and Radiation Chemistry
- ✓ Understanding Materials Compatibility and Interfacial Phenomena
- ✓ Guiding Next Generation Materials for Molten Salt Reactors
- ✓ Creating a Virtual Reactor Simulation

Expected Outcomes from NEUP Projects

- **Engage top talents from broad university communities to advance molten salt science and technology**
- **Should focus on innovative approaches:**
  - ✓ To transform the performance and efficiency of molten salt technology to further reduce technology cost, technical risks, and uncertainties;
  - ✓ To lead to new breakthroughs – addressing potential show-stoppers and longer-term challenges; and
  - ✓ To inspire and provide training for future MSR researchers/developers.
- **Capitalize on recent breakthroughs in nanoscience and technology, advanced characterization tools and instrumentation methods, and computation and predictive modeling capabilities**

RC-2.1:
Predicting the Chemical Speciation, Structure, and Dynamics of Salt Solutions for Molten Salt Reactors

Develop and use first-principles molecular dynamics simulations and computational electronic structure methods to extend the limited experimental data sets in covering a broad range of chemical evolution and environments.

Proposals are requested to better understand, predict, and optimize the physical properties/thermochemical behavior of molten salts.

- ❑ Build multi-component models for prediction of phase diagrams;
- ❑ Apply molecular dynamics simulations to predict thermophysical and transport properties; and
- ❑ Develop innovative method to validate thermochemical database.

RC-2.2:
Development of Molten Salt Reactor Fuel Salt Irradiation Capabilities

MSR presents a number of extreme environmental demands on reactor structural and functional materials. Complex processes and impacts due to radiation effects at the interfaces must be understood and controlled to ensure long-term material reliability.

Proposals are requested to better understand materials compatibility and interfacial phenomena to accelerate the rate and decrease the cost of fuel salt irradiation. Topics may include:

- ❑ Understand materials compatibility in molten salts reactor conditions;
- ❑ Understand and control degradation processes at the interface;
- ❑ Understand the combined effects of chemistry and radiation at the interface;
- ❑ Predict liquid-solid and liquid-gas interfacial interactions.

RC-2.3:
Understand the Structure and Speciation of Molten Salt at the Atomic and Molecular Scale

To understand how the structure and dynamics of molten salts impact their physical and chemical properties—such as viscosity, solubility, volatility, and thermal conductivity—it is necessary to determine the speciation of salt components as well as the local and intermediate structure at operationally relevant temperatures. Real-time spectroscopic and electrochemical methods can also help monitoring key chemical species in solution allowing for optimization of reactor performance and lifetime.

Proposals are requested to take advantage of recent breakthroughs in advanced characterization tools and instrumentation methods in conjunction with computation and predictive modeling capabilities.

- ❑ Determine salt molecular structure using scattering and spectroscopic methods;
- ❑ Develop novel electrochemistry and spectroscopy methods for online monitoring and predictive modeling; and
- ❑ Develop molten salts optical basicity scale to determine corrosivity and solubility of actinides.

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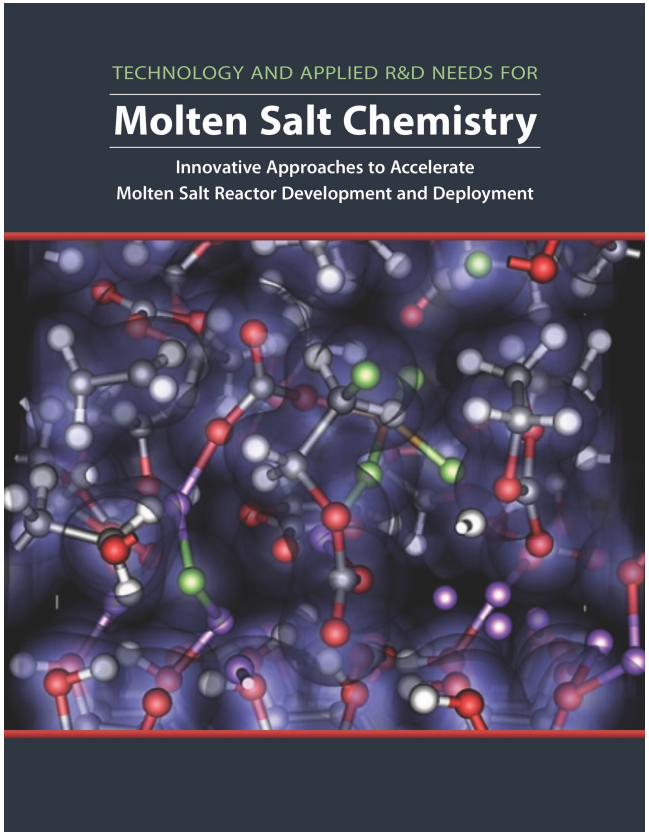

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