INL/MIS-24-79525-Revision-0

Interrogating the physical properties of molten salts at the atomic scale with NMR and all-atom molecular dynamics

August 2024

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Changing the World's Energy Future

Idaho National Laboratory

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Interrogating the physical properties of molten salts at the atomic scale with NMR and all-atom molecular dynamics

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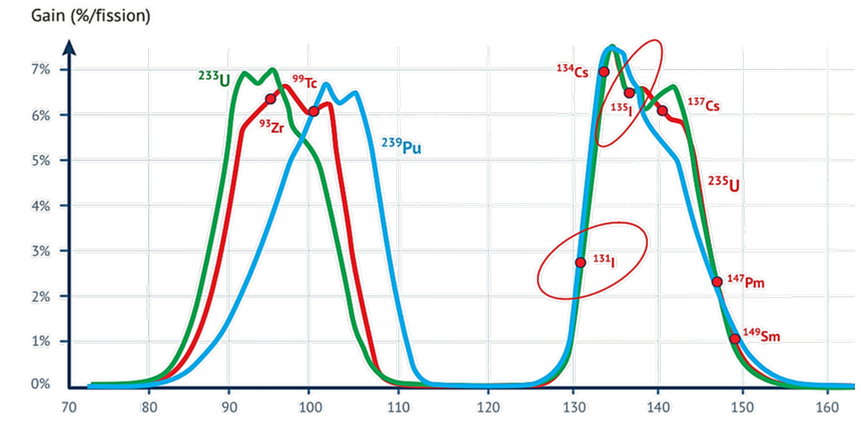
Background and Motivation

- In the Molten Salt Reactor Experiment (MSRE) up to 70% of the fission product Iodine was unaccounted for.*, demonstrating a gap in our understanding of fundamental molten salt reactor chemistry
- In this work we seek to combine experiment and simulation to interrogate the physical properties of molten salt (MS) media in the presence of Iodide at the atomic scale

*Compere *et al.*, Fission Product Behavior in the Molten Salt Reactor Experiment. ORNL-4865, **1975**.

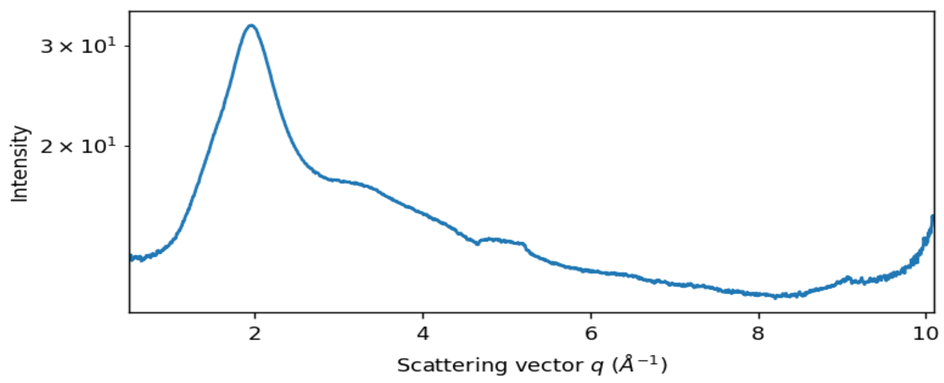


^{235}U, ^{239}Pu, and ^{233}U thermal neutron fission products

Image Courtesy: www.energyencyclopedia.com/en/nuclear-energy/the-nuclear-power-industry/fission-products

Synchrotron X-Ray Diffraction (XRD)

LiCl-KCl Eutectic (126 °C)

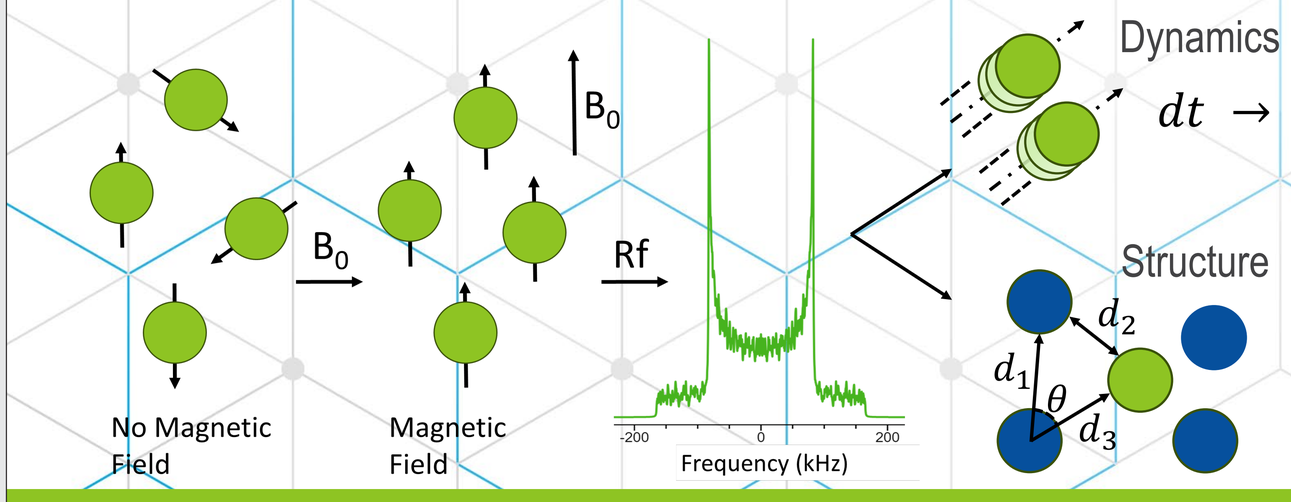


Plot showing the total x-ray diffraction of LiCl-KCl eutectic at 126 °C. XRD is primarily used to determine the bulk structure of molten salts.

- Techniques like XRD do not provide site-resolved information about the structure and dynamics of MS.
- By combining information from XRD and techniques that possess atomic resolution we can obtain a more thorough understanding of MS behavior

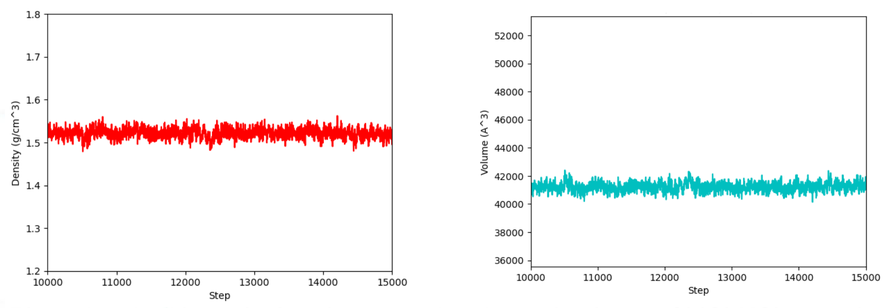
Nuclear Magnetic Resonance (NMR)

- NMR takes advantage of the inherent nuclear spin of certain nuclei to probe their site-specific structure and dynamics.

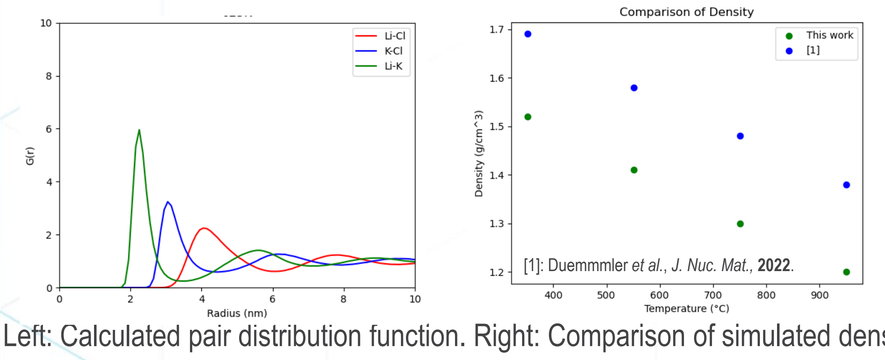


All-atom Molecular Dynamics

- Molecular dynamic (MD) simulations solve the equations of motion in a stepwise manner to evolve the defined system forward in time.
- At each of these 'timesteps' the energies and forces of each atom are also calculated giving insight into the simulated system.



Plots showing the calculated system density and volume of LiCl-KCl eutectic at 351 °C.



Left: Calculated pair distribution function. Right: Comparison of simulated density with measured density [1].

Conclusions

- NMR and MD can be used to interrogate MS at the relevant length/timescales
- Future Work
  - Combine high temperature NMR and MD simulations to study the LiCl-KCl eutectic in the presence of CsI

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