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Developing Practical Models of Complex Salts for Molten Salt Reactors

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Abstract: Molten salt reactors (MSRs) utilize salts as coolant or as the fuel and coolant together with fissile isotopes dissolved in the salt. It is necessary to therefore understand the behavior of the salts to effectively design, operate, and regulate such reactors, and thus there is a need for thermodynamic models for the salt systems. Molten salts, however, are difficult to represent as they exhibit short-range order that is dependent on both composition and temperature. A widely useful approach is the modified quasichemical model in the quadruplet approximation that provides for consideration of first- and second-nearest-neighbor coordination and interactions. Its use in the CALPHAD approach to system modeling requires fitting parameters using standard thermodynamic data such as phase equilibria, heat capacity, and others. A shortcoming of the model is its inability to directly vary coordination numbers with composition or temperature. Another issue is the difficulty in fitting model parameters using regression methods without already having very good initial values. The proposed paper will discuss these issues and note some practical methods for the effective generation of useful models.

Keywords: thermodynamic modeling; CALPHAD; molten salt; molten salt reactor; thermodynamic database; modified quasichemical model; fluoride salt; chloride salt; salt system

1. Introduction

The turn of the 21st century saw the return of interest in molten salt reactor (MSR) systems after more than three decades, as noted in the roadmap efforts at the Generation-IV International Forum in 2002 [1]. There are now several nations with enterprises underway to develop and deploy molten-salt-fueled, or solid fueled and molten-salt-cooled, reactor systems, although at the time of this writing none have yet entered the prototype stage. The previous successful effort was the Molten Salt Reactor Experiment (MSRE), a demonstration program at Oak Ridge National Laboratory that operated between 1965 and 1969. The reactor was an 8 MWt critical system operating with LiF-BeF$_2$-ZrF$_4$-UF$_4$ flowing through a graphite moderator at ~650°C [2].

The worldwide interest in MSRs encompasses a broad range of concepts that manifest as differing salt compositions. These vary from thermal reactors fueled/cooled with 66LiF-34BeF$_2$ mol%, known as FLiBe, to those for fast reactors with 46.5LiF-11.5NaF-42KF mol%, known as FLiNaK. As in most concepts, the coolant also contains the fuel, and these systems or their compositional variants will host dissolved fissile and fertile actinide fluorides. Chloride-based systems, reserved for fast reactors as the heavier fuel/coolant elements make thermalizing neutrons difficult, typically include LiCl-NaCl-MgCl$_2$ compositions, which for fuel host fissile actinide chloride(s).

The exceptionally valuable MSRE experience emphasized how important the ability to understand and control the dynamic (temporal and spatial) evolution of salts in a reactor is. The sources of such variation are:

- Burnup-generated fission product (FP) and transuranic (TRU) elements
- Addition of fresh fuel salt
• Evolving composition due to fission/isotopic decay/neutron absorption
• Graphite pickup (where salt directly contacts graphite moderator) and reaction
• Corrosion product dissolution/deposition
• In-leakage of contaminants (atmospheric oxygen and nitrogen)
• Adjustment of redox with halide addition
• Removal of dissolved/suspended fission and corrosion products, and TRU elements
• Off-gas removal
• Local and cycle temperature

The high-temperature environment of the fuel/cooling loop of a MSR and the nature of the phases (largely ionic liquids and solids together with gases/vapors, metals, and graphite) are expected to drive chemical and phase behavior toward equilibrium, and thus are governed by their thermodynamic properties, i.e., Gibbs energy. Even when the effects of radiation and kinetics, i.e., non-equilibrium phenomena, are controlling, knowledge of the equilibrium state provides limits of phase stability and ultimate chemical potential. Thus, the computed equilibrium state of the molten salt fuel/coolant can provide knowledge about

• Local composition/speciation
• Precipitating solid phases
• Liquid–liquid immiscibility
• State of dislodged graphite or alloy material
• Chemical potentials/redox related to corrosion behavior and transport
• Vapor pressures
• Thermal expansion/specific volume
• Input for phase field calculations: modeling reactions, nucleation, and grain growth
• Energetics for potentially computing viscosity

The path forward in developing thermal properties of MSR salt systems has emerged within a number of national programs, which for the U.S. can be seen in a current roadmap document [3]. As noted in the roadmap, a thermodynamic database focused on MSR modeling needs is a priority and has led to the development of the Molten Salt Thermal Properties Database-Thermochemical (MSTDB-TC) [4]. It joins other efforts such as the Joint Research Centre Molten Salt Database (JRCMSD) [5] and commercial databases such as the Scientific Group Thermodata Europe (SGTE) Molten Salt Database [6] as international resources. Common to these efforts is the effective use of the CALPHAD (CALculation of PHAse Diagrams) [7,8] approach to generate coherent sets of Gibbs functions/models that accurately predict phase equilibria and constituent chemical potentials, the process for which is described in Figure 1.
Means for addressing these issues have been developed as they are common to systems such as EXAFS, and the results from molecular dynamics calculations [9–12]. The effect can be seen in in situ studies of such as ab initio molecular dynamics (AIMD), as demonstrated by Nguyen et al. [14]. In silicate ions, as well as in salt systems.

Pelton and Blander [13] noted that SRO is observed in alloy liquids that are beyond salts. The difficulty in using standard thermochemical models for molten salts is their tendency to exhibit short-range order (SRO). Capturing the influence of this tendency as a function of temperature and composition requires representing the energetics beyond the nearest-neighbor atoms and their coordination. The effect can be seen in situ studies of molten salts, such as EXAFS, and the results from molecular dynamics calculations [9–12]. Means for addressing these issues have been developed as they are common to systems beyond salts. Pelton and Blander [13] noted that SRO is observed in alloy liquids that are combinations of relatively electropositive and electronegative metals (e.g., Cu-Au, Mg-Bi, and Li-Pb), and to a great extent in silicate-containing systems via the formation of orthosilicate ions, as well as in salt systems.

Ideally, it is possible to compute molten salt behavior using atomic scale methods such as ab initio molecular dynamics (AIMD), as demonstrated by Nguyen et al. [14]. In principle, one could eventually compute the behavior of many-element systems, however,
even simple pseudo-binaries such as LiCl-KCl are computationally costly to fully describe making the widespread use of AIMD impractical. An early, mesoscale approach used for the SGTE Molten Salt Database [15] effort is the two-sublattice ionic liquid model [6], which while allowing interaction among species on a fictive cation and anion sublattice, thus considering charge balance, does not address the influence of SRO. Another concept is that of associate species [16,17]. Essentially, SRO is represented by a mixture of complex liquid species in addition to the endmember components. These typically mimic the stoichiometry of stable crystalline phases in the system, as the concept makes the reasonable assumption that any SRO will be due to molecular clusters similar in stoichiometry to the solid phases. The energetics are found through appropriate choice of these associate species and adjusting their Gibbs formation energy to provide a fit to the system phase equilibria. Pelton [18] notes that the approach is problematic as it cannot be applied to systems exhibiting positive deviations from ideality and the results of extending models to higher-order systems are often poor.

A marked improvement in modeling systems with SRO is based on the quasichemical theory of Guggenheim [19], which more directly addresses species coordination within melts. The approach can appropriately address the steep minimum in mixing enthalpy as a function of composition (forming a deep eutectic) and similarly the bimodal mixing entropy due to SRO. It thus avoids the use of computationally prohibitive AIMD and the limitations of models such as the associate species. Pelton and Blander [13] adapted the quasichemical scheme such that minima in mixing enthalpy and entropy are not fixed at 50% composition as required by the Guggenheim theory, making for a more realistic approach. While this discussion is focused on molten salts, the methodology has been very effectively used for oxide systems (primarily silicates) as well, of which the analysis of CaO-MgO-SiO$_2$ by Jung et al. [20] is a good example. Pelton and coworkers have substantially expanded on the technique over the years which can now address complex reciprocal salts with a modified quasichemical model in the quadruplet approximation (MQMQA) [18,21–24].

2.1. Modified Quasichemical Model

A description of the governing relations for the MQMQA would be redundant with other excellent reviews, yet it is worthwhile to describe its working concepts. A reciprocal salt has two cations (A and B) and two anions (X and Y) and these can exhibit SRO as first nearest neighbors (FNN) and second nearest neighbors (SNN), which are cation–anion and cation–cation/anion–anion, respectively. These can be represented by quadruplets, allowing reciprocal reactions for FNNs

$$(A_2X_2) + (B_2X_2) = (A_2Y_2) + (B_2Y_2)$$

and for SNNs

$$(A_2X_2) + (ABXY) = (A_2XY) + (ABX_2)$$
$$(A_2Y_2) + (ABXY) = (A_2XY) + (ABY_2)$$
$$(B_2X_2) + (ABXY) = (B_2XY) + (ABX_2)$$
$$(B_2Y_2) + (ABXY) = (B_2XY) + (ABY_2)$$

One can assign a Gibbs energy of formation to each of the quadruplets which then allows for the managing of their interactions.

While the MQMQA addresses reciprocal salts, MSR applications generally utilize a single anion, fluorine, or chlorine (the exception would be in dealing with the iodine fission product, whose behavior is important to understand in performing accident analyses). For the same anion systems, the MQM simplifies to the pair exchange reaction for FNNs

$$(A_2X_2) + (B_2X_2) = 2(ABX_2)$$

where the exchange Gibbs energy, $\Delta G_{AB/X}$, is related to the pair formation, and in this approach is expanded in a polynomial representing interactions among the components,
which are related to parameters dependent on the cation–cation pair fractions. These are generally empirically determined via fitting the model to data.

For salt melts the relationship between maximum SRO, and thus the most negative heat of mixing, is represented by the cation–cation coordination numbers \( Z_{A/XX}^A/AB \) and \( Z_{A/XX}^B/AB \). These are used to impose the condition of charge neutrality, such that

\[
\frac{q_A}{Z_{A/XX}^A} + \frac{q_B}{Z_{A/XX}^B/AB} = \frac{q_X}{Z_{A/XX}^A} + \frac{q_X}{Z_{A/XX}^B/AB}
\]

where \( q_i \) are the absolute values of the cation and anion charge on \( i \). The relation also allows the cation–cation coordination numbers to define the values for the anion–anion coordination numbers.

### 2.2. Determining Coordination Numbers

As can be appreciated from the MQM relations, the choice of coordination numbers, which are fixed for each component, can be important for obtaining accurate models of salt melts. The values are typically selected from observation of the composition at the greatest SRO and minimum in heat of mixing, or mixing enthalpy. For salts and similar systems, these can be related to eutectic and crystalline phase composition, as these correspond to Gibbs energy minima.

The use of fixed coordination numbers across the entire composition of a salt typically obtained from phase stoichiometries and charge has been common. Unfortunately, in more complex systems where one or more cations have a charge of >1 and the pseudo-binary phase diagram has more than one eutectic, it is apparent that the coordination in the melt is varying. Ultimately, the choice of the single set of coordination numbers will, in those cases, prevent the resulting MQM relations from accurately representing the melt across all compositions.

### 2.3. Coordination Numbers and MQM Generation

The issue of variable coordination numbers is illustrated in a comparison of analyses performed with and without that assumption. An analysis of fluoride fuel salt for MSR applications by Benes and Konings [25] reasonably well reproduces the experimental phase diagram for the pseudo-binary NaF–BeF₂ using measurements confined to less than 60 mol% BeF₂. Their MQM representation utilized single endmembers for the fluorides and thus the fixed coordination numbers

\[
Z_{Na/FF}^{NaNa/FF} = 3; Z_{Na/FF}^{BeNa/FF} = 3
\]

with that for F-F equal to 3.

A later effort on the NaF–BeF₂ pseudo-binary by Robelin and Chartrand [26] endeavored to extend the application of the MQM with variable coordination numbers by adopting two endmembers for BeF₂, which they identified as Be\(_{IV}\)F\(_2\), the four-coordinated beryllium with fluorine, and the dimer Be\(_2\)F\(_4\). These yielded still better agreement with the observed higher BeF₂-content phase equilibria by allowing compositions to be computed with coordination numbers intermediate between the monomer and dimer determined by the ratio of these endmembers. The values adopted for each of the endmembers were

\[
Z_{Na/FF}^{NaNa/FF} = 6; Z_{Na/FF}^{BeIV/BeIV} = 6
\]

\[
Z_{BeIV/FF}^{BeIVBeIV/FF} = 4.8; Z_{BeIV/FF}^{BeIVBeIV/FF} = 2.4
\]

\[
Z_{Be/FF}^{Be2Be/FF} = 6; Z_{Be/FF}^{Be2Be/FF} = 1.5
\]

\[
Z_{Na/FF}^{NaBeIV/FF} = 3; Z_{Na/FF}^{NaBeIV/FF} = 6
\]
can be used with a global energy minimization routine to determine the equilibrium state of phases at a fixed temperature, pressure, and composition. The self-consistent set of thermodynamic functions that have been measured, estimated, or computed from first principles are used to fit parameters of Gibbs functions. These include those that represent interactions among components in solid and liquid solutions, which in-clude variable stoichiometry solid phases. The term used to describe the comprehensive analysis of a system to obtain a fully representative set of Gibbs functions and models is an assessment. Sets of the thermodynamic functions that have been measured, estimated, or computed from first principles are used to fit parameters of Gibbs functions. These include those that represent interactions among components in solid and liquid solutions, which in-clude variable stoichiometry solid phases. The process for integrating the information and the fitting methodology (regression analysis) is termed optimization. When the results of the optimization allow the determined Gibbs functions to be used in global energy minimization calculations (the computing of equilibria) that reproduce the known phase

\[
Z_{NaBeIV/FF}^{Na} = 3; \quad Z_{NaBeIV/FF}^{BeIV} = 6 \\
Z_{NaBr2/FF}^{Na} = 2; \quad Z_{NaBr2/FF}^{Br2} = 6
\]

These yielded an improved fit to the system and thus an improved reproduction of the entire phase diagram (Figure 2). The variation in concentration of BeIVF2 and Be2F4 is shown in the inset in the phase diagram of Figure 2. In the current work, it is likely that additional endmembers will be needed for uranium-containing systems and systems with ZrF4 as well. While other MSR salt constituents will have valences >1 and yield more complex pseudo-binary phase diagrams, they will be present at low concentrations and therefore the use of variable coordination numbers will likely not be warranted.

![Phase diagram](image)

Figure 2. Overlaid phase diagrams based on melt models for NaF-BeF2 using [26] and not using [25] multiple endmembers for BeF2. The selected experimental data points are those of Roy et al. [27] and Novoselova [28]. The inset indicates the relative concentration of the monomer and dimer of BeF2 at 850 °C based on the Robelin and Chartrand [26] MQM representation.

3. Performing System Assessments for Salts

The term used to describe the comprehensive analysis of a system to obtain a fully representative set of Gibbs functions and models is an assessment. Sets of the thermo-chemical relations for phases and vapor species in a system constitute its full description and can be used with a global energy minimization routine to determine the equilibrium state of phases at a fixed temperature, pressure, and composition. The self-consistent set of Gibbs functions accurately describe the phase equilibria and characteristics of the phases in the systems. Following the CALPHAD approach (Figure 1), multiple sources and types of information are used in optimizations of model parameters for Gibbs function relations. Put simply, all relevant, reliable, consistent, and acceptably accurate values for determining thermodynamic functions that have been measured, estimated, or computed from first principles are used to fit parameters of Gibbs functions. These include those that represent interactions among components in solid and liquid solutions, which include variable stoichiometry solid phases. The process for integrating the information and the fitting methodology (regression analysis) is termed optimization. When the results of the optimization allow the determined Gibbs functions to be used in global energy minimization calculations (the computing of equilibria) that reproduce the known phase
equilibria (diagrams) and other characteristics (e.g., elemental chemical potentials), then
the process has been successful.

There are two overriding issues, however, that can cause system optimizations to be
difficult or impossible. The first is the lack of sufficient, consistent, and accurate data
that will allow successful fitting to Gibbs functions and solution models. The second is
the difficulty in performing a regression analysis to fit often disparate types, or even
the same type of data to a model, whether for a variable stoichiometry solid phase (e.g.,
sublattice model) or liquid (e.g., MQM). The solution to the first problem is the obvious
generation of the required data by appropriate means. The solution to the second problem,
however, has yet to be fully resolved. It is possible to have an adequately complete and
accurate set of information to allow, for example, the fitting of MQM parameters for a salt
melt, including Gibbs functions for crystalline phases, yet have great difficulty successfully
performing a regression analysis to successfully determine the parameters. Even for
the simpler systems where variability in coordination numbers is not an issue, it can be
difficult to obtain a successful fit to solution models.

Currently, there is no widely available solution to the problem of easily performing
regression analysis for more complex solution models, and particularly for MQM. It has
always been something of an art to fit data to successfully optimize a system for more than
very simple systems and models. It has depended on a close understanding of the likely
behavior of a system, with the goal of successfully reproducing behavior with a minimum
number of parameters. Tools such as the optimization modules in the FactSage\textsuperscript{TM} [29] and
Thermo-Calc [30] software suites offer the promise of fitting the parameters, however, for
the optimizations to be successful they generally require initial estimates for the regression
analyses that are close to final values. Obviously, this severely decreases the value of
these routines.

4. Higher-Order Systems and Example Applications

There are a significant number of assessed pseudo-binary salt systems of interest for
MSRs, however, models for melts with multiple components will be needed that reflect that
complexity of salt compositions. The base systems for fuel salts such as FLiBe, FLiNaK,
and LiCl-NaCl-MgCl\textsubscript{2} will also contain some concentrations of the same halide actinide.
Thus, a MQM addressing systems with at least four component halides will be required to
well represent MSR salts. In addition, the nuclear processes of a reactor generate \sim60 different
elements as fission products or transuranics, albeit ranging from low concentrations to
trace amounts. There are also corrosion products or contaminant elements that dissolve in
the salt. Given this potentially large number of constituents, the task of obtaining solution
descriptions that include all possible interactions among all the components, in principle,
would be impossibly large. The effort becomes tractable, however, as it is statistically
apparent that the low-concentration elements will be proximate almost solely with, and
thus solely energetically interact with, the major fuel salt constituents, obviating the need
for addressing very large numbers of interactions. There thus remains a substantially more
restricted set of systems to be addressed. The MQM can accommodate multiple compo-
nents, with the expressions well described by Pelton [18]. These require interpolation from
lower-order systems, and examples of which are becoming more common as attempts to
represent more complex systems expand.

An example of a set of interpolated systems is seen in the five endmember LiF-BeF\textsubscript{2}-
UF\textsubscript{5.4}-PuF\textsubscript{3} system developed for the MSTDB-TC. The types of information that can be
generated from such models can be seen in Figure 3a, which illustrates computed liquidus
projections for the LiF-BeF\textsubscript{2}-UF\textsubscript{4} where all composition additionally contains 10 mol\% UF\textsubscript{4}
and 1 mol\% PuF\textsubscript{3}. For example, it is clear that the actinide content markedly increases
the salt melting point from that of FLiBe of 456 °C, with an actinide salt solid solution
the first precipitating phase. A closer look at the effect of actinide fluorides is seen in
Figure 3b, which reflects the significant increase in liquidus temperature particularly due
to the presence of PuF\textsubscript{3}.
Adjustment of the UF\textsubscript{3}-UF\textsubscript{4} ratio in MSR systems is expected to be used to control fluorine potential, and therefore the propensity for a corrosive attack of structural alloys and the vapor pressure of some species. That type of critical information is also available from these kinds of thermochemical models, as seen in Figure 4 which provides 750 °C computed RT ln(p\textsubscript{F\textsubscript{2}}) values for FLiBe containing 10 mol% UF\textsubscript{3} as a function of the UF\textsubscript{3}/UF\textsubscript{4} ratio. On the plot are also indicated the RT ln(p\textsubscript{F\textsubscript{2}}) values for equilibria between the major Hastelloy-N elements (71Ni-16Mo-7Cr-4Fe mass) and their fluorides (except for molybdenum, which has values that are significantly more positive). Accurate calculations also require consideration of the activities of the metals in the alloy, i.e., alloy solid solution or secondary phase models. These were obtained from the SGTE 2020 Alloy Database [24] and the phases equilibrated with the salt in calculating the indicated equilibrium reactions of Figure 4. The equilibria thus provide thresholds such that more positive system RT ln(p\textsubscript{F\textsubscript{2}}) values will cause the fluoride of the metal to be more stable than the element as an alloy constituent and thus indicate the potential for corrosion. The understanding that the mechanism of corrosive attack in nickel alloys is the fluoriding and dissolution of chromium is again made apparent in the results in Figure 4 where the reaction (Cr)\textsubscript{H-N} + F\textsubscript{2}(g) = CrF\textsubscript{2}(l) occurs at the most negative values of RT ln(p\textsubscript{F\textsubscript{2}}) among the alloy constituents.

Figure 3. The models for the LiF-BeF\textsubscript{2}-UF\textsubscript{4} -UF\textsubscript{3}-PuF\textsubscript{3} system of MSTDB-TC [4] were used to (a) compute the liquidus projections for the pseudo-ternary LiF-BeF\textsubscript{2}-UF\textsubscript{4} phase diagram with fixed content of 10 mol% UF\textsubscript{3} and 1 mol% PuF\textsubscript{3} (labeled phase regions indicate the first precipitating phase) and (b) demonstrate the influence on the liquidus temperature of FLiBe of added components such as UF\textsubscript{4} and PuF\textsubscript{3}. 

An example of a set of interpolated systems is seen in the five endmember LiF-BeF\textsubscript{2}-UF\textsubscript{4} -UF\textsubscript{3}-PuF\textsubscript{3} system of MSTDB-TC [4] were used to (a) compute the liquidus projections for the pseudo-ternary LiF-BeF\textsubscript{2}-UF\textsubscript{4} phase diagram with fixed content of 10 mol% UF\textsubscript{3} and 1 mol% PuF\textsubscript{3} (labeled phase regions indicate the first precipitating phase) and (b) demonstrate the influence on the liquidus temperature of FLiBe of added components such as UF\textsubscript{4} and PuF\textsubscript{3}. 

Figure 4. The equilibria thus provide thresholds such that more positive system RT ln(p\textsubscript{F\textsubscript{2}}) values for equilibria between the major Hastelloy-N elements (71Ni-16Mo-7Cr-4Fe mass) and their fluorides (except for molybdenum, which has values that are significantly more positive). Accurate calculations also require consideration of the activities of the metals in the alloy, i.e., alloy solid solution or secondary phase models. These were obtained from the SGTE 2020 Alloy Database [24] and the phases equilibrated with the salt in calculating the indicated equilibrium reactions of Figure 4. The equilibria thus provide thresholds such that more positive system RT ln(p\textsubscript{F\textsubscript{2}}) values will cause the fluoride of the metal to be more stable than the element as an alloy constituent and thus indicate the potential for corrosion. The understanding that the mechanism of corrosive attack in nickel alloys is the fluoriding and dissolution of chromium is again made apparent in the results in Figure 4 where the reaction (Cr)\textsubscript{H-N} + F\textsubscript{2}(g) = CrF\textsubscript{2}(l) occurs at the most negative values of RT ln(p\textsubscript{F\textsubscript{2}}) among the alloy constituents.
Thermochemical representations of MSR salt systems are key components for the modeling and simulation of reactor systems. Yet, having a practical model for the salt melt is a significant challenge given the issues of accommodating SRO that includes variation in species coordination over large ranges of temperature and composition, as well as facilitating interpolation to higher-order systems. Simple solution models do not capture the effect of SRO, and approaches such as AIMD are not practical given unknowns, high computational costs, and inadequate levels of accuracy. The MQM has offered an extremely useful compromise in that although it does not incorporate all the complexity of salt melt structures, it provides a sufficient framework to include variation in the energetics of the salt and uses a simplified, but adequate view of structure in the melt. This capability together with its treatment of structure with endmember building blocks has allowed the reproduction of many-element system behavior. Generating MQM relations, however, involves understanding potential SRO variations in a system and knowing when it is necessary to add the complexity of multiple same-element endmembers. Salt melt MQMs coupled with those for intermediate compounds and solid solutions have successfully reproduced phase equilibria and thermochemistry, and has made possible the generation of complex melt databases, including the current MSTDB-TC [4].

In the current work, potential applications of salt system models were briefly explored, including compositional dependence of liquidus temperature and the potential for salt attack on a nickel-based alloy for use in proposed MSRs. The latter, in particular, demonstrates how salt thermochemical models used together with the understanding of other material systems, in this case Hastelloy-N, can offer guidance with regard to reactor design and operation. It is envisioned that this thermochemical capability, coupled with modeling and simulation codes for salt corrosion, will provide for an ultimate ability to predict the stability of reactor materials.

Finally, while much phase equilibria and thermodynamic information is available for salt systems of interest for MSRs, much more is yet needed and hopefully will be generated by the substantial number of researchers addressing these issues worldwide. Beyond that, however, there remain substantial materials science questions for molten salts whose resolution will aid modeling and database efforts. Among these is understanding and modeling atomic coordination in molten salts as a function of temperature and composition. This will require the continuing effort of both those engaged in first principles and
molecular dynamics calculations, and those making difficult, critical measurements of melt structural properties.

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