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**Research Papers**

# EXPERIMENTAL AND COMPUTATIONAL STUDIES OF ALKALI HALIDE IONS: A VITAL RESEARCH FIELD

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## Abstract

*The article present a brief review of experimental and computational studies carried out for alkali halide ions under different conditions .The importance of studies in this subject area has led to significant amount of research work since last several decades. In the present review, few of such recent studies have been highlighted.*

**Keywords:** Computational techniques, Molecular dynamics, Monte Carlo method, equilibrium and non-equilibrium properties.

## 1. INTRODUCTION

Alkali halides have been in extensive use in large number of biological, chemical and technological processes [1-11]. This has been the prime reason for the significant amount of research works involving alkali halide ions since last many years [12-31]. Ions such as Na+, K+ play vital roles in various important processes crucial in biological and chemical systems. Moreover, in presence of water and other solvents/ media, these alkali metal ions exist as solvated ions and it is the solvation/ hydration of these ions which is a decisive factor in their activity/ application.

Various experimental methods such as Neutron spectroscopy[32-33], X-Rayscattering [34], Infrared and Raman spectroscopy [34-35] have been used to study kinetics and dynamics of ionic hydration/ solvation under varying conditions. On the other hand, methods like density functional theory and simulation techniques such as Molecular Dynamics and Monte Carlo Simulations are in use for theoretical studies.

## 2. EXPERIMENTAL STUDIES OF ALKALI HALIDE IONS

Several researchers have devoted their considerable time in the studies involving alkali halide and this research area still is active, attracting attention of many physical chemists and biological researchers.

In the early 70's, Tsuji and co-workers [36] studied thermodynamics of systems involving solid solutions of silver bromide and lithium bromide. They employed X- Ray diffraction method to determine the solubility limit in the AgBr-LiBr system. Their work also involved calculations of partial molar energy, partial molar entropy and the partial molar enthalpy using EMF measurements.

In the year 2001, Kameda and coworkers [] used Polarized Raman scattering and neutron diffraction measurements to study solvation structure of Li+ in concentrated LiBr non aqueous solution. Their studies revealed presence of a well-defined first solvation shell around Li+ ion in the solution.Yamaguchi and co-workers [47] also employed neutron diffraction technique along with isotopic dilution method to study various aspects such as bond distances, hydration numbers and

orientational correlation of water) of LiCl and CsCl in concentrated aqueous solutions. They observed that the first-order-difference structure factors and radial distribution functions are dominated by the ion–water interactions for Li+and Cl−ions over ambient to the supercritical temperature range.

The technique of isothermal titration calorimetry in combination with MD simulations have been used by Luksicet al. [48] to study ion-selectivity in mixtures of hydrophobic polyelectrolytes with sodium halides in water.

Schmitt and coworkers [] in the following year reported studies on structured alkali halides for medical applications. Their measurements on doped alkali halide image plates (having needle structure) showed good modulation transfer function (MTF) and high sensitivity, which made a significant progress in image plate technology.

## 3. COMPUTATIONAL STUDIES OF ALKALI HALIDE IONS

A detailed analysis of solvation structure around the $Ca^{2+}$ ( an alkaline earth metal ion) and Cl- ion in aqueous media with varying ionic concentration has been reported by Chiavlo and Simonson using MD simulations to determine the actual coordination number of these ions in aqueous medium. In their subsequent studies, they used MD simulations to study ion pairing and counter ion condensation in aqueous electrolytes. Their work involved comparison of experimental data obtained from the neutron diffraction techniques with the MD simulation results involving LiCl in aqueous solutions.

The technique of MD simulation has been used by Zhu [39] to study the clustering of Na+-Br- ion pairs . He reported rate of nucleation using classical nucleation theory. Later on, Zhu and Chen [] studied the nucleation rate dependence of KBr ion pair/s on cluster size at various temperature using MD simulations.

An interesting work using MD simulations on aqueous RbBr- solution over wide range of solubility at room temperature has been reported by Harsanyi et al. [41]. They studied structural aspect of the ions using radial distribution functions. They also studied dynamical properties of the ions and bulk solvent.Alkali halide ion/s play crucial role in biology. A comparative MD studies of these biologically vital ions have been carried out by Jungwirth and co-workers [] at the air/water interface.

Fennell and co-workers [43] have reported a comprehensive analysis of ion association/solvation of alkali halides ion pairs in aqueous medium. They have performed MD simulations for the entire series of alkali metal halides ion pairs using different water models. Their work explored the important association and solvation aspects of ion pair/s in aqueous medium wherein water was modelled using different potential parameters.

Pusztai and co-workers [44] employed MD along with reverse MC technique to performed a detailed structural analysis of RbBr solution in a dilute aqueous solutions. They also compared results obtained using combination of these techniques with the experimental observations made using neutron diffraction technique. Subsequently, Pusztai and co-workers [45] used the same technique and carried out a detail study of CsBr in aqueous medium.

## 4. FUTURE PROSPECTS

Inspite of several studies (experimental and theoretical) on the systems of alkali halide, there are many aspects of structural solvation and properties (equilibrium and non-equilibrium) which still remain elusive. There are many studies (experimental as well as theoretical) which have been carried out for systems involving alkali halide ion/s, the system involved in many of these studies is aqueous. There are many biologically and commercially important non aqueous solvents which act as media wherein various ions and ion pairs exhibit properties which depends on solvation structures of these ions. Solvents such as DMSO (Dimethyl sulphoxides), methanol, ethanol, acetonitrile and acetone play vital role in various reactions and as reaction media. The aqueous mixtures of these solvents have several applications in biology, chemistry and in technology. It would be very interesting if studies are carried out to investigate the various aspects of ion/s and ion pairs/s in these pure non-aqueous solvents and their binary mixtures with water.

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