



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
SHORT ABSTRACT OF THESIS

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Thesis Title: Quantum Chemical and Molecular Dynamics Insights into the Solvent Extraction and Stripping Mechanism of Metal Ions in Aqueous Biphasic Systems

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**SHORT ABSTRACT**

The doctoral work reports the modeling of transfer of metal ions from the aqueous phase to the organic solvents (i.e. octanol, nitrobenzene, o-NPHE and chloroform) and ionic liquids. The first chapter gives a brief introduction on crown ether, organic solvents and ILs for extraction of metal ions. The second chapter presents the extraction of metal ions by a crown ether using organic solvents. The extraction of metal ions (i.e. Cs<sup>+</sup>, K<sup>+</sup>, Na<sup>+</sup> and Rb<sup>+</sup>) in presence of ionophore such as dibenzo-18-crown-6 (DB18C6) from nitrobenzene-water biphasic system is reported using MD simulations along with COSMO-RS (Conductor like Screening Model for Real Solvents) predictions and experimental validation. The high selectivity of Na<sup>+</sup>-DB18C6 complex over other complexes in nitrobenzene was also confirmed and validated by the experimental distribution coefficients and interaction energy. On the other hand, the selectivity for the Cs<sup>+</sup>-CBCBGA extraction was found to be higher than other metal ions, i.e. K<sup>+</sup>, Na<sup>+</sup> and Rb<sup>+</sup>. The high selectivity of the Cs<sup>+</sup>-CBCBGA complex over other complexes (i.e. K<sup>+</sup>, Rb<sup>+</sup> and Na<sup>+</sup>) in nitrobenzene was also confirmed and validated by the HOMO-LUMO energy gap and interaction energy. The third chapter presents the interfacial insights on the crown-ether-assisted metal ion extraction in IL–water binary system. In addition, MD studies on the extraction of Cs<sup>+</sup> from the aqueous phase to the BMIMTF2N phase in presence of crown ether (i.e. DB18C6, DB21C7, DCH18C6 and BPC6) is also reported. It was observed that the [BMIM]<sup>+</sup> was partitioned to the aqueous phase and it exchanged with Cs<sup>+</sup> in the presence or in absence of CE. The selectivities of Cs<sup>+</sup> and Na<sup>+</sup> with dibenzo-18-crown-6 (DB18C6) with methanol as the diluent have been compared and validated by performing solvent extraction experiments and MD simulations. At the end of the chapter was stripping of metal ions (i.e. Cs<sup>+</sup> and Na<sup>+</sup>) in presence of ionophore (i.e. DB18C6) from the IL phase to the aqueous nitric acid phase by MD simulations. The results of simulation were validated by experiments. Chapter 4 summarizes the important findings of this doctoral work and suggests future directions of work. This chapter describes a future direction involving MD studies on the extraction of cesium ions by functionalized carbon nanotubes in the IL-water biphasic system.