Towards the understanding of the structure of Choline Chloride based DES using classical molecular dynamics and fragmentation simulations

Forcefield parametrization and benchmarking the density functional approximation methods.

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Contents

Table 1: Various methods studied in this work.

Method	Implementation height

1 Introduction

The invention of DES lead to the studies of wide-range of applications as their nature and tailoring help in significant processes. The modeling of DES as helps as they explain the experimental observations and help in the design of DES. In this thesis, the DES systems considered are:

1. Urea - Choline Chloride (1:2 molar ratio) colloquially called Reline.
2. Evernic Acid - Usinic Acid NADES found in the lichen *EverniaPrunastri*

And the following modeling strategies/tools were utilised for this purpose:

1. Molecular Dynamics
2. Fragmentation Simulations

2 Summary of third year work

Since the last CSI, the following projects were undertaken and certain protocols and work flows were developed based on the benchmarking of certain semi-empirical and density functional approximation methods. The following projects were undertaken:

1. **Developing the algorithm for fragmentation simulations of non-covalent clusters**
2. Studying the stability and water retention properties of the proposed NADES systems in lichen EverniaPrunastri.

3 Benchmarking density functional approximations

4 Local Energy Decomposition

Systems Studied:

1. $[1Ch + 1U + 2Cl]^{-1}$ $(m/z = 235)$
2. $[1Ch + 2U + 2Cl]^{-1}$ $(m/z = 295)$
3. $[1Ch + 3U + 2Cl]^{-1}$ $(m/z = 355)$
4. $[2Ch + 0U + 3Cl]^{-1}$ $(m/z = 313)$