

## Abstract

The water dimer consists of two water molecules loosely bound by a hydrogen bond. The hydrogen bond in water dimer has received the most theoretical attention. The water dimer is small in size and obtaining experimental results for this species is difficult. So, it is an ideal candidate to be a model system for studying hydrogen bonding in water. In first part of this project, the water dimer,  $(\text{H}_2\text{O})_2$ , has been used as a model for optimization of the structure of dimers using electrostatics. A hydrogen bond network is also found in ammonia clusters and it plays a key role in understanding the properties of species which are embedded in ammonia. The structures of neutral ammonia clusters dictate this network. In the second part, we concentrated on hydrogen bonded neutral clusters of ammonia,  $(\text{NH}_3)_n$  ( $n = 2-6$ ) and these clusters have been theoretically investigated employing the basis set aug-cc-pvdz at the Hartree-Fock (HF) level as well as with M06L level of theory.