Water plays a vital role in many physical and chemical processes. However, its structure and dynamics at a molecular level yet not fully understood. Computer simulations at the atomic scale play an important role in understanding the microscopic structure of water. However, the quality of the simulated results significantly depends on the accuracy of the interaction potential used in the simulation. The difficulty in producing a correct description of the interaction potential for water lies in the delicate balance between covalent bonds, hydrogen bonds and the weak van der Waals interactions. Unfortunately, the widely used classical point charge model fails to produce that balance in specific cases, especially when bulk water symmetry is broken. A solution to this problem is to use a fully ab initio model that can describe these balances of strong and weak forces more perfectly.

In this talk, I will present an ab initio model of water using a revised version of the PBE DFT functional along with dispersion correction that can produce a near quantitative agreement for the structure of bulk ambient water. Interestingly, this successful modeling of water allows us to use simulation in conjunction with experiment to study more complex chemical phenomenon in water. As an example, I will show how DFT MD along with simulated XANES spectra provide unprecedented information of solvation structure around ions and elucidate the CaCO3 nucleation mechanisms in water.