The famous Miller experiment to model the primordial soup demonstrated that amino acids can form spontaneously as the essential building blocks of life in solutions. It is, however, still an open question how self-recognition processes influence the transformation of these spontaneously formed amino acids in solvents into higher ordered structures in the solid state, thereby creating chiral materials and catalytically competent structures. The understanding of the first steps of molecular self-assembly processes in such environments will thus give important clues towards the understanding of biological evolution. Most of intermolecular interactions are not very strong and their formation is related to and affected by small changes in the molecular structure and the crystallisation conditions. Continuing our investigations on aggregation of substituted aromatic molecules in the solid state, we studied the influence and boundaries of weak directing substituents like deuterium on the aggregation of small molecules. Hydrogen/deuterium (H/D)-exchange, the smallest possible modification of a molecule, is generally seen as a non-dominating parameter in the formation of crystal structures of chemical compounds. On the other hand, it could already be shown that the aggregation of molecules in the solid state of polymorphic N-heterocycle systems like pyridine-N-oxide or acridine can be very sensitive to small changes of the isotopic substitution pattern of the selected molecules. Within our project, the molecular aggregation of amino acids in solution with the formation of molecular aggregates and pre-nucleation clusters in deuterated and non-deuterated systems, and in particular the role of the solvent in these processes, will be studied in both experiment and theory.


Keywords: molecular aggregation, amino acids, deuteration effect