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Multiscale modelling of solvation of ions in droplets with applications in atmospheric and electrosprayed aerosols

Charged droplets with multiple ions are ubiquitous in atmospheric and man-made aerosols. The chemistry within the droplets is very intriguing and different from that of their bulk analogues. Overall the knowledge of the reaction mechanisms and solvation properties of the dissolved species in the droplet environment is still limited. In this project the ion spatial distribution in droplets will be studied by molecular dynamics methods. An example of the systems under investigation is shown in the first illustration, where the blue sphere represents sodium ions and the remaining molecules are water molecules. The second illustration shows the electric field on the surface of a fluctuating droplet. The molecular modelling will take place using classical molecular dynamics and the results are compared with the solution of the non-linear Poisson Boltzmann (PB) equation. The software for the solution of the non-linear PB has been created in the group. Molecular dynamics is performed using the software NAMD. The electric field on the droplet surface is computed with methods and software developed in the group.