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Modeling of proton transfer reactions in clusters using path integral methods

We intend to study a proton transfer reactions in a molecular cluster using path integral methods along the lines presented in [Ref. 1]. The modelling of these systems is significant for understanding the reactivity in atmospheric aerosols and for understanding the charge states of analytes detected by mass spectrometry [Ref. 2]. The cluster will be composed of solvent, certain reactive sites and protons modeled by path integrals methods. The software LAMPPS will be used in the study.

During the course of the project the student(s) will learn molecular modelling software packages and molecular dynamics and Monte Carlo methods. Knowledge of a programming language such as Python, C++, C is a desirable. Some knowledge of statistical mechanics, probabilities and statistics will be helpful for the project.

References

1. Consta, S., and Raymond Kapral. "Proton transfer in mesoscopic, molecular clusters." The Journal of Chemical Physics 101.12 (1994): 10908-10914.
2. Consta, S., et al. "Strengths and Weaknesses of Molecular Simulations of Electrosprayed Droplets." *Journal of The American Society for Mass Spectrometry* 29.12 (2018): 2287-2296.