Physics 2013-2014 **PROJECT ##### (NOTE THIS WILL BE ADDED LATER)**

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Analytical and computational modelling of charged induced instabilities in droplets effected by charged macromolecules

Stability of charged droplets containing charge carriers such as protons, sodium or chloride ions and macromolecules that may be charged is a problem that appears in diverse fields such as electrospray ionization and deposition. It is also a fundamental problem in polymer physics. In this project we want to develop analytical theory for the instability of a droplet that contains a charged macromolecule and other charge carriers in the solvent, which are not attached to the macromolecule. The results of the analytical theory will be verified by molecular simulations. Poly (ethylene glycol) will be used as a model macromolecule. The proposed project is along the theoretical analysis we have done in the article by S. Consta and A. Malevanets, *Phys. Rev. Lett.* **109**: 148301 (2012).

During the project the students will become familiar with analytical theories that use electrostatics, molecular dynamics, Monte Carlo methods and theories of polymers. Knowledge of computer programming is helpful but not necessary. However, the student involved in the project should be willing to learn computer programming. In the first month of the project, the student is to learn how to program and prepare a molecular dynamics code on a simple system. Then the student should be able to transfer his/her knowledge to more complex systems. Our research group has expertise in the study of chemical and physical processes in droplets and hydration of complex molecules such as macromolecules in droplet and bulk environments [see S. Consta and A. Malevanets, *Phys. Rev. Lett.* **109**: 148301 (2012); *J. Chem. Phys.* **138**: 184312 (2013); S. Consta and J. K. Chung *J. Phys. Chem. B* **116**: 5777-5785 (2012); *J. Phys. Chem. B* **115**: 10447-10455 (2011)]. Please do not hesitate to contact me to discuss details of the project.